

VnmrJ Command and Parameter Reference

*Varian, Inc. NMR Systems
With VnmrJ 2.3A Software*

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Notational Conventions

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abort	Terminate action of calling macro and all higher macros (C)	37
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abortoff	Terminate normal functioning of abort in a macro (C)	38
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acct	Writes records for operator login and logoff (M)	39
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acosyold	Automatic analysis of COSY data, old algorithm (C)	40
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Acqmeter	Open Acqmeter window (U)	42
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activestudy	Active study name (P)	47
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addi	Start interactive add/subtract mode (C)	48
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alfa	Set alfa delay before acquisition (P)	53
alock	Automatic lock control (P)	53
ampmode	Independent control of amplifier mode (P)	54
amptype	Amplifier type (P)	54
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analyze	Generalized curve fitting (C)	55
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N

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newshm	Interactively create a shim method with options (M)	368
nextpl	Display the next 3D plane (M)	369
nfni	Number of increments in 1st indirectly detected dimension (P)	369
ni2	Number of increments in 2nd indirectly detected dimension (P) ...	369
ni3	Number of increments in 3rd indirectly detected dimension (P)....	370
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nimax	Maximum limit of ni (P)	370
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nli	Find integral values (C)	370
nlivast	Produces a text file of integral regions without a sum region (M) .	371
nlivast2	Produces a text file with normalized integral regions (M)	371
nlivast3	Produces a text file with normalized integral regions (M)	371
nll	Find line frequencies and intensities (C)	371
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nm2d	Select Automatic 2D normalization (M)	372
Noesy	Convert the parameter to a NOESY experiment (M)	373
Noesy1d	Convert the parameter set to a Noesy1d experiment (M).....	373
noise	Measure noise level of FID (C)	373
noisemult	Control noise multiplier for automatic 2D processing (M)	374

noislm	Limit noise in spectrum (M)	374
notebook	Notebook name (P)	374
np	Number of data points (P)	375
npoint	Number of points for fp peak search (P)	375
nrecords	Determine number of lines in a file (M)	375
nt	Number of transients (P)	375
ntrig	Number of trigger signals to wait before acquisition (P)	376
ntype3d	Specify whether f_1 or f_2 display expected to be N-type (P)	376
nuctable	Display VNMR style nucleus table for a given H1 frequency (M)	376
numrcvrs	Number of receivers in the system (P)	376
numreg	Return the number of regions in a spectrum (C)	377
numrfch	Number of rf channels (P)	377

O

off	Make a parameter inactive (C)	379
on	Make a parameter active or test its state (C)	379
operator	Operator name (P)	380
operatorlogin	Sets workspace and parameters for the operator (M)	380
opx	Open shape definition file for Pbox (M)	380
oscoef	Digital filter coefficients for over sampling (P)	381
osfb	Digital filter bandwidth for oversampling (P)	381
osfilt	Oversampling filter for real-time DSP (P)	382
oslsfrq	Bandpass filter offset for oversampling (P)	382
overrange	Frequency synthesizer overrange (P)	382
oversamp	Oversampling factor for acquisition (P)	383
owner	Operating system account owner (P)	384

P

p1	Enter pulse width for p1 in degrees (C)	389
p1	First pulse width (P)	389
p1pat	Shape of excitation pulse (P)	389
p2pul	Set up sequence for PFG testing (M)	390
p31	Automated phosphorus acquisition (M)	390
p31p	Process 1D phosphorus spectra (M)	390
pa	Set phase angle mode in directly detected dimension (C)	391
pa1	Set phase angle mode in 1st indirectly detected dimension (C)	391
pacosy	Plot automatic COSY analysis (C)	392
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padept	Perform adept analysis and plot resulting spectra (C)	393
page	Submit plot and change plotter page (C)	393
page	Name of page (P)	394
panellevel	Display level for VnmrJ interface pages (P)	394
pap	Plot out “all” parameters (C)	394
par2d	Create 2D acquisition, processing, and display parameters (M)	395
par3d	Create 3D acquisition, processing, and display parameters (M)	395
par3rf	Get display templates for 3rd rf channel parameters (M)	395
par4d	Create 4D acquisition parameters (M)	395
paramedit	Edit a parameter and its attributes with user-selected editor (C)	396
paramvi	Edit a parameter and its attributes with vi editor (M)	396
pards	Create additional parameters used by downsampling (M)	397
parfidss	Create parameters for time-domain solvent subtraction (M)	397
parfix	Update parameter sets (M)	398
parlc	Create parameters for LC-NMR experiments (M)	398
parl12d	Create parameters for 2D peak picking (M)	399
parlp	Create parameters for linear prediction (M)	399
parmax	Parameter maximum values (P)	399
parmin	Parameter minimum values (P)	400
paros	Create additional parameters used by oversampling (M)	400
parstep	Parameter step size values (P)	400
parversion	Version of parameter set (P)	401
path3d	Path to currently displayed 2D planes from a 3D data set (P)	401

paxis	Plot horizontal LC axis (M)	401
Pbox	Pulse shaping software (U)	402
pbox_bw	Define excitation band (M)	403
pbox_bws	Define excitation band for solvent suppression (notch) pulses (M)	403
pbox_dmf	Extract dmf value from pbox.cal or Pbox shape file (M)	403
pbox_dres	Extract dres value from pbox.cal or Pbox shape file (M)	404
pbox_name	Extract name of last shape generated by Pbox from pbox.cal (M)	404
pbox_pw	Extract pulse length from pbox.cal or Pbox shape file (M)	404
pbox_pwr	Extract power level from Pbox.cal or Pbox shape file (M)	404
pbox_pwrfl	Extract fine power level from pbox.cal or Pbox shape file (M)	405
pboxget	Extract Pbox calibration data (M)	405
pboxpar	Add parameter definition to the Pbox.inp file (M)	406
pboxrst	Reset temporary Pbox variables (M)	406
pboxunits	Converts to Pbox default units (M)	406
pcon	Plot contours on a plotter (C)	406
pcss	Calculate and show proton chemical shifts spectrum (M)	407
peak	Find tallest peak in specified region (C)	407
peak2d	Return information about maximum in 2D data (C)	408
pen	Select a pen or color for drawing (C)	408
pexpl	Plot exponential or polynomial curves (C)	409
pexpladd	Add another diffusion analysis to current plot (M)	409
pfgon	Pulsed field gradient amplifiers on/off control (P)	409
pffw	Plot FIDs in whitewash mode (C)	410
pge	Convert parameter set to PGE pulse sequence (M)	410
pge_calib	Calibrate gradient strengths for PGE pulse sequence (M)	410
pge_data	Extract data from single element of PGE pulse sequence (M)	411
pge_output	Output results from PGE pulse sequence (M)	411
pge_process	Automated processing of data from PGE pulse sequence (M)	411
pge_results	Calculate diffusion constant for integral region (M)	411
pge_setup	Set up gradient control parameters for PGE pulse sequence (M)	412
ph	Set phased mode in directly detected dimension (C)	412
ph1	Set phased mode in 1st indirectly detected dimension (C)	413
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phase	Change frequency-independent phase ρ (M)	414
phase	Phase selection (P)	414
phase1	Phase of first pulse (P)	414
phase2	Phase selection for 3D acquisition (P)	414
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phasing	Control update region during interactive phasing (P)	415
phfid	Zero-order phasing constant for the $n\rho$ FID (P)	415
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pin	Pneumatics Router Interlock ((P)	417
pintvast	Plots of integral regions (M)	417
pir	Plot integral amplitudes below spectrum (C)	418
pirn	Plot normalized integral amplitudes below spectrum (M)	418
piv	Plot integral values below spectrum (M)	418
pivn	Plot normalized integral values below spectrum (M)	418
pl	Plot spectra (C)	419
pl2d	Plot 2D spectra in whitewash mode (C)	420
plane	Currently displayed 3D plane type (P)	420
plapt	Plot APT-type spectra automatically (M)	421
plarray	Plotting macro for arrayed 1D spectra (M)	421
plate_glue	Define a glue order for plotting and display (U)	421
plc	Plot a carbon spectrum (M)	422
plcosy	Plot COSY- and NOESY-type spectra automatically (M)	422
pldept	Plot DEPT data, edited or unedited (M)	423
plfid	Plot FIDs (C)	423
plfit	Plot deconvolution analysis (M)	424

plgrid	Plot a grid on a 2D plot (M).....	424
plh	Plot proton spectrum (M).....	424
plhet2dj	Plot heteronuclear J-resolved 2D spectra automatically (M).....	424
plhom2dj	Plot homonuclear J-resolved 2D spectra automatically (M)	425
plhxcor	Plot X,H-correlation 2D spectrum (M).....	426
pll	Plot a line list (M)	427
pll2d	Plot results of 2D peak picking (C)	427
plockport	Port number to use to lock out multiple ProTune processes (P).....	427
plot	Automatically plot spectra (M).....	428
plot1d	Plotting macro for simple (non-arrayed) 1D spectra (M)	428
plot2D	Plot 2D spectra (M).....	429
plotfile	Plot to a file (M).....	429
plothiresprep	High resolution plot output preparation (M).....	430
plotmanual	Plot manually (M)	430
plotlogo	Plots a logo (M)	430
plotpreview	Creates temporary plots of the current plot output (M)	430
plotside	Plot spectrum on side (M).....	430
plotter	Plotter device (P)	430
plottop	Plot spectrum on top (M)	430
plottopside	Plot spectrum on top and side (M).....	431
plp	Plot phosphorus spectrum (M).....	431
plplanes	Plot a series of 3D planes (M)	431
plt2Darg	Plot 2D arguments (P).....	432
plttext	Plot text file (M)	432
pltmod	Plotter display mode (P)	432
plvast	Plot VAST data in a stacked 1D-NMR matrix format (M).....	433
plvast2d	Plot VAST data in a stacked pseudo-2D format (M)	433
plww	Plot spectra in whitewash mode (C)	434
pmode	Processing mode for 2D data (P)	434
poly0	Display mean of the data in regression.inp file (M)	435
pp	Decoupler pulse length (P)	435
ppa	Plot a parameter list in plain English (M).....	436
ppcal	Proton decoupler pulse calibration (M)	436
ppf	Plot peak frequencies over spectrum (C).....	436
pph	Print pulse header (M)	437
ppmm	Resolution on printers and plotters (P)	437
pprofile	Plot pulse excitation profile (M).....	437
pps	Plot pulse sequence (C).....	438
prealfa	Specify a delay for longer ring down (P).....	438
prep	Run prepare acquisition macro (M)	438
Presat	Set up parameters for presat ¹ H experiment (M).....	439
prevpl	Display the previous 3D plane (M).....	439
prescan	Study queue prescan (P).....	439
prescan_CoilTable	Read or update the CoilTable File (M)	439
prescan_tn	Return tn string for a given atomic number (M).....	439
printer	Printer device (P)	440
printfile	Path to the print-to-file image (P)	440
printformat	Format of saved-to-file image (P).....	440
printlayout	Layout of printed image (P).....	440
printoff	Stop sending text to printer and start print operation (C)	440
printon	Direct text output to printer (C).....	440
printregion	Screen region to be printed (P)	441
printsize	Size of printed image (P)	441
printsend	Defines where image will print (P).....	441
probe	Probe type (P)	441
probeConnect	Specify which nucleus can be acquired on each RF channel (P)....	441
Probe_edit	Edit probe for specific nucleus (U).....	442
probe_edit	Edit probe for specific nucleus (M)	442
probe_protection	Probe protection control (P).....	442
proc	Type of processing on np FID (P).....	442
procl	Type of processing on ni interferogram (P)	443
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proc2	Type of processing on ni2 interferogram (P)	444
proc2d	Process 2D spectra (M)	444
proccarray	Process arrayed 1D spectra (M)	445
process	Generic automatic processing (M)	445
procplot	Automatically process FIDs (M)	445
profile	Set up pulse sequence for gradient calibration (M)	446
proj	Project 2D data (C)	446
Proton	Set up parameters for ¹ H experiment (M)	447
protune	Macro to start ProTune (M)	447
protune	Shell script for start ProTune operation (U)	448
protunegui	Macro to start ProTune in graphical user interface (M)	448
prune	Prune extra parameters from current tree (C)	448
pscale	Plot scale below spectrum or FID (C)	449
pseudo	Set default parameters for pseudo-echo weighting (M)	449
psg	Display pulse sequence generation errors (M)	450
psggen	Compile a user PSG object library (M,U)	450
psgset	Set up parameters for various pulse sequences (M)	450
psgupdateon	Enable update of acquisition parameters (C)	450
psgupdateoff	Prevent update of acquisition parameters (C)	451
pshape	Plot pulse shape or modulation pattern (M)	451
pshapef	Plot the last created pulse shape (M)	451
pshr	PostScript High Resolution plotting control (P)	451
pslabel	Pulse sequence label (P)	451
pslw	PostScript Line Width control (P)	452
pssl	Plot Arrayed Numbers (C)	452
ptext	Print out a text file (M)	453
ptspec3d	Region-selective 3D processing (P)	453
ptsval	PTS frequency synthesizer value (P)	454
pulseinfo	Shaped pulse information for calibration (M)	454
pulsetool	RF pulse shape analysis (U)	454
purge	Remove macro from memory (C)	455
puttxt	Put text file into a data file (C)	455
putwave	Write a wave into Pbox.inp file (M)	455
pw	Enter pulse width pw in degrees (C)	456
pw	Pulse width (P)	456
pw90	90° pulse width (P)	456
pwd	Display current working directory (C)	456
pwpat	Shape of refocusing pulse (P)	457
pwr	Set power mode in directly detected dimension (C)	457
pwr1	Set power mode in 1st indirectly detected dimension (C)	457
pwr2	Set power mode in 2nd indirectly detected dimension (C)	458
pwsadj	Adjust pulse interval time (M)	458
pxcal	Decoupler pulse calibration (M)	459
pxbss	Bloch-Siegert shift correction during Pbox pulse generation (P) ...	459
pxrep	Flag to set the level of Pbox reports (P)	459
pxset	Assign Pbox calibration data to experimental parameters (M)	459
pxshape	Generates a single-band shape file (M)	460
Pxsim	Simulate Bloch profile for a shaped pulse (U)	460
Pxspy	Create shape definition using Fourier coefficients (U)	461

Q

qcomp	Longer dead time for longer ring down (P)	463
QKexp	Set up quick experiment (M)	463
qtune	Tune probe using swept-tune graphical tool (C)	463
?	Display the value of an individual parameter (C)	464

R

r	Recall display parameter set (M)	466
r(n)	Recall some display parameters (C)	467
r1-r7	Real-value storage for macros (P)	467
ra	Resume acquisition stopped with sa command (C)	467

rcvrwt	Weighting for different receivers (P)	468
react	Recover from error conditions during werr processing (M)	468
readallshims	Read all shims from hardware (M)	469
readbrutape	Read Bruker data files from 9-track tape (U)	469
readfile	Read the contents of a text file into two parameters (C)	469
readhw	Read current values of acquisition hardware (C)	470
readlk	Read current lock level (C)	472
readparam	Read one of more parameters from a file (C)	472
readultra	Read shim coil setting for Ultra•nmr shim system (M)	473
real	Create a real variable without a value (C)	473
recon_all	Reconstruct images from 2D MRI fid data (C)	473
record	Record keyboard entries as a macro (M)	476
redor1	Set up parameters for REDOR1 pulse sequence (M)	476
redosy	Restore 2D DOSY display from sub experiment (M)	476
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reff2	Reference f2 Indirect Dimension from Observe Dimension (M) ...	477
reffrq	Reference frequency of reference line (P)	478
reffrq1	Reference freq. of reference line in 1st indirect dimension (P)	478
reffrq2	Reference freq. of reference line in 2nd indirect dimension (P)	478
refpos	Position of reference frequency (P)	479
refpos1	Position of reference frequency in 1st indirect dimension (P)	479
refpos2	Position of reference frequency in 2nd indirect dimension (P)	479
refsource1	Center frequency in 1st indirect dimension (P)	479
refsource2	Center frequency in 2nd indirect dimension (P)	480
region	Divide spectrum into regions (C)	480
relayh	Set up parameters for RELAYH pulse sequence (M)	481
rename	Move and/or rename a file (C)	481
reqparcheck	Flag which enables/disables required parameters (P)	481
reqparclear	Clears the parameters in required parameter list (M)	481
reqparlist	List of required parameters (P)	482
reqpartest	Tests whether required parameters are set (M)	482
resetf3	Reset parameters after a partial 3D Fourier transform (M)	483
resetplotter	Reset plotter to system plotter (M)	484
resolv	Set resolution enhancement parameters (M)	484
restorenuctable	Calculate & store accurate nuctable for current system (M)	484
resume	Resume paused acquisition queue (C)	484
return	Terminate execution of a macro (C)	485
rev	System software revision level (P)	485
revdate	System software preparation date (P)	485
rfband	RF band in use (P)	485
rfblk	Reverse FID block (C)	485
rfchannel	Independent control of rf channel selection (P)	486
rfchtype	Type of rf channel (P)	487
rfdata	Reverse FID data (C)	488
rfl	Reference peak position in directly detected dimension (P)	489
rfl1	Reference peak position in 1st indirectly detected dimension (P) ..	489
rfl2	Reference peak position in 2nd indirectly detected dimension (P) ..	489
rfp	Reference peak frequency in directly detected dimension (P)	490
rfp1	Reference peak freq. in 1st indirectly detected dimension (P)	490
rfp2	Reference peak freq. in 2nd indirectly detected dimension (P)	490
rftrace	Reverse FID trace (C)	490
rftype	Type of rf generation (P)	491
rfgw	RF waveform generator (P)	492
right	Set display limits to right half of screen (C)	492
rights	Determine an operator's specified right (C)	492
rinput	Input data for a regression analysis (M)	493
rl	Set reference line in directly detected dimension (M)	493
rl1	Set reference line in 1st indirectly detected dimension (M)	493
rl2	Set reference line in 2nd indirectly detected dimension (M)	494
rm	Delete file (C)	494
rmdir	Remove directory (C)	494
rmsAddData	Add transformed data files with weighting (U)	495

Roesy	Convert the parameter to a ROESY experiment (M)	495
Roesy1d	Convert the parameter set to a Roesy1d experiment (M)	495
rof1	Receiver gating time preceding pulse (P)	495
rof2	Receiver gating time following pulse (P)	495
rof3	Receiver gating time following T/R switch (P)	496
rotate	Rotate 2D data (C)	496
rotorsync	Rotor synchronization (P)	496
rp	Zero-order phase in directly detected dimension (P)	496
rp1	Zero-order phase in 1st indirectly detected dimension (P)	497
rp2	Zero-order phase in 2nd indirectly detected dimension (P)	497
rt	Retrieve FIDs (M)	497
rtcmx	Return Spinsight data into current experiment (C)	498
rtp	Retrieve parameters (M)	498
rts	Retrieve shim coil settings (C)	498
rttmp	Retrieve experiment data from experiment subfile (M)	499
rtv	Retrieve individual parameters (C)	499
rtx	Retrieve parameters based on rtx rules (C)	500
 S		
s	Save display parameters as a set (M)	505
s(n)	Save display parameters (C)	505
s2pul	Set up parameters for standard two-pulse sequence (M)	506
sa	Stop acquisition (C)	506
sample	Submit change sample, Autoshim experiment to acquisition (M) ..	506
samplename	Sample name (P)	507
save	Save data (M)	507
savefile	Base file name for saving files (P)	507
saveglobal	Save selected parameters from global tree (P)	507
sb	Sinebell constant in directly detected dimension (P)	508
sb1	Sinebell constant in 1st indirectly detected dimension (P)	508
sb2	Sinebell constant in 2nd indirectly detected dimension (P)	508
sbs	Sinebell shift in directly detected dimension (P)	508
sbs1	Sinebell shift in 1st indirectly detected dimension (P)	509
sbs2	Sinebell shift in 2nd indirectly detected dimension (P)	509
sc	Start of chart (P)	509
sc2	Start of chart in second direction (P)	510
scalelimits	Set limits for scales in regression (M)	510
scalesw	Set scaling factor for multipulse experiments (M)	510
scalesw	Scale spectral width in directly detected dimension (P)	510
scalesw1	Set f_1 scaling factor for 2D multipulse experiments (M)	511
scalesw1	Scale spectral width in 1st indirectly detected dimension (P)	511
scalesw2	Scale spectral width in 2nd indirectly detected dimension (P)	511
sd	Set first decoupler frequency to cursor position (M)	511
sd2	Set second decoupler frequency to cursor position (M)	511
sd3	Set third decoupler frequency to cursor position (M)	512
sda	Set first decoupler frequency array (M)	512
sd2a	Set second decoupler frequency array (M)	512
sd3a	Set third decoupler frequency array (M)	512
sdp	Show diffusion projection (M)	513
sel1d	Apptype macro for Selective 1D experiments (M)	513
select	Select spectrum, FID, trace, or 2D plane without display (C)	513
selex	Defines excitation band (M)	514
selexcit	Set up PFG selective excitation pulse sequence (M)	514
selexHT	Set up a selective Hadamard experiment (M)	514
send2vnmr	Send a command to VnmrJ (U)	515
seqfil	Pulse sequence name (P)	515
seqgen	Initiate compilation of user's pulse sequence (M,U)	515
serverport	Returns the VnmrJ network listening port value (C)	516
set2D	General setup for 2D experiments (M)	516
set2d	General setup for 2D experiments (M)	516
set3dproc	Set 3D processing (C)	517

setallshims	Set all shims into hardware (M).....	517
setcolor	Set colors for graphics window and for plotters (C).....	518
setdecpars	Set decoupler parameter values from probe file (M).....	519
setdec2pars	Set decoupler 2 parameter values from probe file (M).....	519
setdgroup	Set the Dgroup of a parameter in a tree (C).....	519
setenumerals	Set values of a string parameter in a tree (C).....	519
setether	Connect or reconnect host computer to Ethernet (U)	520
setexport	Set parameter bits for use with protocols (M)	520
setfrq	Set frequency of rf channels (C)	520
setgauss	Set a Gaussian fraction for lineshape (M)	521
setgcal	Set the gradient calibration constant (M).....	521
setgcoil	Assign sysgcoil configuration parameter (M)	521
setgrid	Divide graphics window into rows and columns (C)	522
setgroup	Set group of a parameter in a tree (C).....	522
sethtfrq1	Set a Hadamard frequency list from a line list ((M).....	523
sethw	Set values for hardware in acquisition system (C)	523
setint	Set value of an integral (M)	525
setlimit	Set limits of a parameter in a tree (C)	525
setlk	Set up lock parameters (M).....	526
setlockfreq	Set lock frequency (M)	526
setLP	Set up linear prediction in the direct dimension (M)	527
setLP1	Set F1 linear prediction parameters (M).....	527
setlp0	Set parameters for zero linear phase (M).....	527
setnoether	Disconnect host computer from Ethernet (U).....	527
setoffset	Calculate offset frequency for given nucleus and ppm (M)	528
setparams	Write parameter to current probe file (M)	528
setpen	Set maximum number of HP plotter pens (M)	528
setplotdev	Return characteristics of a named plotter (C)	529
setpower	Set power and pulsewidth for a given γB_1 value (M)	529
setprotect	Set protection mode of a parameter (C).....	529
setrc	Set receiver constants (M)	531
setref	Set frequency referencing (M).....	531
setref1	Set freq. referencing for 1st indirectly detected dimension (M).....	532
setref2	Set freq. referencing for 2nd indirect detected dimension (M).....	533
setscout	Set up a scout run (M).....	533
setssfilter	Set sslsfrq to the frequencies of each suppressed solvents (M).....	534
setsw	Set spectral width (M).....	534
setsw1	Set spectral width in evolution dimension (M).....	534
setsw2	Set spectral width in 2nd evolution dimension (M).....	534
setselfrqc	Set selective frequency and width (M)	535
setselinv	Set up selective inversion (M)	535
settcldefault	Select default display templates for pulse sequence (M).....	535
settone	Opens the Auto Tune Setup dialog (M).....	535
settype	Change type of a parameter (C).....	535
setup	Set up parameters for basic experiments (M)	536
setup_dosy	Set up gradient levels for DOSY experiments (M).....	536
setvalue	Set value of any parameter in a tree (C)	537
setwave	Write a wave definition string into Pbox.inp file (M).....	537
setwin	Activate selected window (C).....	538
sf	Start of FID (P)	538
sf1	Start of interferogram in 1st indirectly detected dimension (P).....	538
sf2	Start of interferogram in 2nd indirectly detected dimension (P)	538
sfrq	Transmitter frequency of observe nucleus (P).....	539
sh2pul	Set up for a shaped observe excitation sequence (M).....	539
shdec	Set up for shaped observe excitation sequence (M)	539
shell	Start a UNIX shell (C)	539
shelli	Start an interactive UNIX shell (C)	540
shim	Submit an Autoshim experiment to acquisition (C)	540
shimset	Type of shim set (P)	540
showconfig	Show system configuration settings (M)	542
showconsole	Show system configuration settings (U).....	542
showfit	Display numerical results of deconvolution (M)	542

showloginbox	Shows operator login dialog (M)	542
shownumx	Show x position of number (P)	542
shownumy	Show y position of number (P)	543
showoriginal	Restore first 2D spectrum in 3D DOSY experiment (M)	543
showplotter	Show list of currently defined plotters and printers (M)	543
showplotq	Display plot jobs in plot queue (M)	543
showprintq	Display print jobs in print queue (M)	543
showprotunegui	show the graphical interface while tuning (P)	543
showrfmon	Show RF Monitor Button in Hardware Bar (P).....	544
showstat	Display information about status of acquisition (M,U)	544
sin	Find sine value of an angle (C)	544
sine	Find values for a sine window function (M).....	544
sinebell	Select default parameters for sinebell weighting (M).....	545
sinesq	Find values for a sine-squared window function (M).....	545
size	Returns the number of elements in an arrayed parameter (O)	546
slfreq	Measured line frequencies (P)	546
slw	Spin simulation linewidth (P)	546
smaxf	Maximum frequency of any transition (P).....	546
sminf	Minimum frequency of any transition (P)	547
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sp1	Start of plot in 1st indirectly detected dimension (P)	549
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spcfrq	Display frequencies of rf channels (M)	550
specdc3d	3D spectral drift correction (P)	550
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spin	Sample spin rate (P)	551
spincad	Run SpinCAD program (C)	551
spingen	Compile SpinCAD pulse sequence (M,U).....	551
spinll	Set up a slfreq array (M)	552
spinner	Open the Spinner Control window (C)	553
spins	Perform spin simulation calculation (C)	554
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spmin	Take minimum of two spectra in add/subtract experiment (C).....	556
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sqinebell	Set up unshifted sinebell-squared window function (M).....	560
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Notational Conventions

The *VnmrJ Command and Parameter Reference* describes in detail the commands, macros, and parameters in VnmrJ software. Information new to VnmrJ in this version is shown by a change bar (as shown to the left of this paragraph).

Title Line Codes

Each entry has a letter in parentheses in the title line that identifies the type of entry:

(C)	VnmrJ command
(M)	VnmrJ macro command (from the <code>macLib</code> directory)
(O)	MAGICAL programming operator
(P)	VnmrJ parameter
(U)	UNIX command (not executable within VnmrJ)
(C,U) (M,U)	Executable from UNIX or VnmrJ (note that syntax is different)

Applicability

An entry with applicability information applies only to the system or accessory listed. If the entry does not include applicability information, the entry applies to all systems.

Command and Macro Syntax

Each command and macro entry includes the syntax used when entering it into the system. The following examples illustrate this syntax:

<code>halt</code>	If no parentheses are shown, enter the command or macro exactly as shown, e.g., enter <code>halt</code> .
<code>delexp(exp_num)</code>	If parentheses are shown, enter the command or macro name as shown, but replace arguments with a value, e.g., if <code>exp_num</code> is 5, enter <code>delexp(5)</code> .
<code>rttmp(file)</code>	Arguments can be a string (e.g., name of file or solvent), number, variable, or parameter (e.g., <code>pw</code>),. If a string, enclose it with single quote marks, e.g., if file is <code>samp02</code> , enter <code>rttmp('samp02')</code> . If number, variable, or parameter, do <i>not</i> use marks.
<code>rl<(frequency)></code>	Angle brackets (< and >) indicate optional input, e.g., if <code>frequency</code> not needed or the default value of <code>frequency</code> is acceptable, enter <code>rl</code> , but if <code>frequency</code> has a value such as 10, enter <code>rl(10)</code> .

Notational Conventions

<code>md(<from_exp,>to_exp)</code>	Arguments can also be optional. Use a comma to separate arguments, e.g., <code>md(2,3)</code> . Unless stated otherwise, the order of arguments is often important.
<code>nll<('pos')></code>	A keyword is frequently used as an argument. In the syntax, keywords are shown in single quotes and are entered exactly as shown, e.g., to use the optional keyword 'pos' for <code>nll</code> , enter <code>nll('pos')</code> .
<code>dc2d('f1' 'f2')</code>	A vertical bar indicates an OR condition, e.g., either 'f1' or 'f2' can be an argument to <code>dc2d</code> .
<code>sin(angle)<:n></code>	Some commands return values to a calling macro. This is shown by a colon followed by one or more variables, e.g., if <code>angle</code> is variable <code>x</code> and <code>n</code> is variable <code>rt</code> , then <code>sin(x):rt</code> returns the value of <code>sin(x)</code> to the calling macro via the variable <code>rt</code> .
<code>z(reset1,reset2,...)</code>	Three dots indicate the sequence of arguments continues. Unless a limit is given, you can enter one argument, two, three, or as many as needed.

Parameter Syntax

Parameter syntax is always in the form `parameter_name=value`. If `value` is a string, enclose it in single quote marks; otherwise, no marks are used, e.g., `auto='y'`, `plotter='ThinkJet'`, `spin=5`. Note that some parameters are not user-enterable.

Notational Conventions

Throughout all Varian, Inc. NMR manuals, typewriter-like characters identify commands, parameters, directories, file names, and text displayed on the screen.

Because pressing the Return key is required at the end of almost every command or line of text you type on the keyboard, assume this use of the Return key unless stated otherwise.

Other Sources of Information

For further information about an entry, refer to the manual listed under “See also.” For general coverage on VnmrJ, refer to the following manuals (each manual is also online):

VnmrJ Walkup

NMR Spectroscopy User Guide

VnmrJ Installation and Administration

VnmrJ Imaging NMR

A

aa	Abort acquisition with error (C)
abort	Terminate action of calling macro and all higher macros (C)
abortallacqs	Reset acquisition computer in a drastic situation (C)
abortoff	Terminate normal functioning of abort in a macro (C)
aborton	Restore normal functioning of abort in a macro (C)
abs	Find absolute value of a number (C)
AC1S-AC11S	Autocalibration macros (M)
ACbackup	Make backup copy of current probe file (M)
acct	Writes records for operator login and logoff (M)
ACreport	Print copy of probe file after autocalibration (M)
acos	Find arc cosine of number (C)
acosy	Automatic analysis of COSY data (C)
acosyold	Automatic analysis of COSY data, old algorithm (C)
acqdisp	Display message on the acquisition status line (C)
acqi	Interactive acquisition display process (C)
acqmeter	Open Acqmeter window (M)
Acqmeter	Open Acqmeter window (U)
acqmode	Acquisition mode (P)
acqstat	Open Acquisition Status window (M)
Acqstat	Open Acquisition Status window (U)
acqstatus	Acquisition status (P)
acquire	Acquire data (M)
actionid	Current study queue node id (P)
activestudy	Active study name (P)
add	Add current FID to add/subtract experiment (C)
addi	Start interactive add/subtract mode (C)
addnucleus	Add new nucleus to existing probe file (M)
addpar	Add selected parameters to current experiment (M)
addparams	Add parameter to current probe file (M)
addprobe	Create new probe directory and probe file (M)
adept	Automatic DEPT analysis and spectrum editing (C)
aexppl	Automatic plot of spectral expansion (M)
ai	Select absolute-intensity mode (C)
aig	Absolute-intensity group (P)
alfa	Set alfa delay before acquisition (P)
alock	Automatic lock control (P)
ampmode	Independent control of amplifier mode (P)
amptype	Amplifier type (P)
analyz	Calculate standard peak height (M)
analyze	Generalized curve fitting (C)
ap	Print out “all” parameters (C)
ap	“All” parameters display control (P)
apa	Plot parameters automatically (M)

A

<code>aph</code>	Automatic phase adjustment of spectra (C)
<code>aph0</code>	Automatic phase of zero-order term (C)
<code>aphb</code>	Auto phasing for Bruker data (C)
<code>aphx</code>	Perform optimized automatic phasing (M)
<code>appdirs</code>	Starts Applications Directory Editor (M)
<code>appmode</code>	Application mode (P)
<code>apptype</code>	Application type (P)
<code>Apt</code>	Set up parameters for APT experiment (M)
<code>aptaph</code>	Automatic processing for APT spectra (M)
<code>array</code>	Easy entry of linearly spaced array values (M)
<code>array</code>	Parameter order and precedence (P)
<code>arraydim</code>	Dimension of experiment (P)
<code>asin</code>	Find arc sine of number (C)
<code>asize</code>	Make plot resolution along f_1 and f_2 the same (M)
<code>assign</code>	Assign transitions to experimental lines (M)
<code>at</code>	Acquisition time (P)
<code>atan</code>	Find arc tangent of a number (C)
<code>atan2</code>	Find arc tangent of two numbers (C)
<code>atcmd</code>	Call a macro at a specified time (M)
<code>atext</code>	Append string to current experiment text file (M)
<code>attval</code>	Calculate pulse width (M)
<code>atune</code>	ProTune Present (P)
<code>au</code>	Submit experiment to acquisition and process data (M)
<code>AuCALch3i</code>	Set up autocalibration with CH ₃ I sample (M)
<code>AuCALch3i1</code>	Get autocalibration with CH ₃ I sample (M)
<code>AuCALch3oh</code>	Set up autocalibration with Autotest sample (M)
<code>AuCALch3oh1</code>	Get autocalibration with Autotest sample (M)
<code>Aucalibz0</code>	Automatic Hz to DAC calibration for Z0 (M)
<code>AuCdec</code>	Carbon decoupler calibration macro (M)
<code>AuCgrad</code>	Carbon/proton gradient ratio calibration macro (M)
<code>AuCobs</code>	Carbon observe calibration macro (M)
<code>audiofilter</code>	Audio filter board type (P)
<code>Aufindz0</code>	Automatic adjustment of Z0 (M)
<code>Augcal</code>	Probe gcal calibration macro (M)
<code>Augmap</code>	Automated gradient map generation (M)
<code>Augmapz0</code>	Automatic lock gradient map generation and z0 calibration (M)
<code>AuHdec</code>	Proton decoupler calibration (M)
<code>AuHobs</code>	Proton observe calibration macro (M)
<code>Aumakegmap</code>	Auto lock gradient map generation (M)
<code>AuNuc</code>	Get parameters for a given nucleus (M)
<code>auto</code>	Prepare for an automation run (C)
<code>auto</code>	Automation mode active (P)
<code>auto_au</code>	Controlling macro for automation (M)
<code>Autobackup</code>	Back up current probe file (M)
<code>autodept</code>	Automated complete analysis of DEPT data (M)
<code>autodir</code>	Automation directory absolute path (P)
<code>autogo</code>	Start automation run (C)

<code>autolist</code>	Set up and start chained acquisition (M)
<code>autoname</code>	Create path for data storage (C)
<code>autoname</code>	Prefix for automation data file (P)
<code>autora</code>	Resume suspended automation run (C)
<code>autosuspend</code>	Suspend current automation run (C)
<code>autoscale</code>	Resume autoscaling after limits set by <code>scaleglimits</code> macro (M)
<code>autostack</code>	Automatic stacking for processing and plotting arrays (M)
<code>autotest</code>	Open Auto Test Window (C)
<code>autotime</code>	Displays approximate time for automation (M)
<code>av</code>	Set abs. value mode in directly detected dimension (C)
<code>av1</code>	Set abs. value mode in 1st indirectly detected dimension (C)
<code>av2</code>	Set abs. value mode in 2nd indirectly detected dimension (C)
<code>averag</code>	Calculate average and standard deviation of input (C)
<code>awc</code>	Additive weighting const. in directly detected dimension (P)
<code>awc1</code>	Additive weighting const. in 1st indirectly detected dimension (P)
<code>awc2</code>	Additive weighting const. in 2nd indirectly detected dimension (P)
<code>axis</code>	Provide axis labels and scaling factors (C)
<code>axis</code>	Axis label for displays and plots (P)
<code>axisf</code>	Axis label for FID displays and plots (P)

aa Abort acquisition with error (C)

Syntax: `aa`

Description: Aborts an experiment that has been submitted to acquisition. If the experiment is active, it is aborted immediately, all data is discarded, and the experiment is interpreted as an error. Any data collected from an earlier block size transfer is retained. If any `werr` processing is defined, that processing occurs, followed by any queued experiments. The `login` name, and the FID directory path in `file` are used as keys to find the proper experiment to abort.

In some circumstances, there is a delay between the time `go` is entered and the acquisition is started. During this time, instructions based on the selected pulse sequence are being generated. This is signified by the letters “PSG” appearing in the upper left corner of the status window. An `aa` command issued under these circumstances reports that no acquisition is active but it instead stops the instruction generation process and the message “PSG aborted” appears.

See also: *NMR Spectroscopy User Guide*

Related:	<code>file</code>	File name of a parameter set (P)
	<code>go</code>	Submit experiment to acquisition (C)
	<code>halt</code>	Abort acquisition with no error (C)
	<code>werr</code>	Specify action when error occurs (C)
	<code>werr</code>	When error (P)

abort Terminate action of calling macro and all higher macros (C)

Syntax: `abort`

Description: Terminates the action of the calling macro and all higher levels of nested macros. `abort` is used only in macros and not entered from the keyboard. It generates an error condition, which is the reason why the calling macro and any

parent (nested) macros above will also be aborted. To exit from the execution of a macro without generating an error, use `return`.

See also: *VnmrJ User Programming*

Related: `abortoff` Terminate normal functioning of `abort` in a macro (C)
`aborton` Restore normal functioning of `abort` in a macro (C)
`return` Terminate execution of a macro (C)

abortallacqs Reset acquisition computer in a drastic situation (C)

Syntax: `abortallacqs`

Description: Reboots the acquisition system from the host computer. Wait at least 30 seconds before attempting new acquisitions.

See also: *NMR Spectroscopy User Guide*

abortoff Terminate normal functioning of abort in a macro (C)

Syntax: `abortoff`

Description: Changes the action of an `abort` command in a macro. Normally, `abort` (or any command aborting with an error condition) terminates the action of the calling macro and all higher levels of nested macros; however if the `abortoff` command is executed prior to a macro containing the `abort` command, only the macro containing `abort` terminates and execution continues to the next macro. The operation of the `abortoff` command is nullified by the `aborton` command. `abortoff` is used only in macros and not entered from the keyboard.

See also: *VnmrJ User Programming*

Related: `abort` Terminate action of calling macro and all higher macros (C)
`aborton` Restore normal functioning of `abort` in a macro (C)

aborton Restore normal functioning of abort in a macro (C)

Syntax: `aborton`

Description: Nullifies the operation of a `abortoff` command and restores the normal functioning of the `abort` command. `aborton` is used only in macros and not entered from the keyboard.

See also: *VnmrJ User Programming*

Related: `abortoff` Terminate normal functioning of `abort` in a macro (C)

abs Find absolute value of a number (C)

Syntax: `abs (number) <:value>`

Description: Finds the absolute value of a number. Absolute value is a nonnegative number equal in numerical value to the given number (e.g., `abs (-6.5)` is 6.5).

Arguments: `number` is the given real number.

`value` is the return value with the absolute value of the given number. The default is to display the value in the status window.

Examples: `abs (-25)`
`abs (n) :abs_val`

See also: *VnmrJ User Programming*

AC1S-AC11S Autocalibration macros (M)

Syntax: ACnS, where n is a number from 1 to 11.

Description: Performs automatic system calibration. When finished with the calibration routines, the current probe file is updated. If the probe is new to the system (i.e., all values in the probe file are zero), system power levels are determined followed by calibration. If power levels are listed in the current probe file, these values are used. The macro AC1S determines ^1H pw90, AC5S begins ^{13}C calibration, including decoupler power calibrations. AC10S performs ^{19}F calibration, and AC11S performs ^{31}P calibration.

See also: *NMR Spectroscopy User Guide*

ACbackup Make backup copy of current probe file (M)

Syntax: ACbackup

Description: Called by the autocalibration macros **AC1S-AC11S** to back up the probe file after calibration ends. This macro is not usually called by the user.

See also: *NMR Spectroscopy User Guide*

Related: **AC1S-AC11S** Autocalibration macros (M)

acct Writes records for operator login and logoff (M)

Applicability: VnmrJ

Syntax: acct('start' | 'done')

Description: acct writes operator login and logoff records to the system adm/tmp/macrorecords.txt file used by the accounting package.

See also: *VnmrJ Installation and Administration manual*

Related:	operator	operator name (P)
	operatorlogin	Sets work space and parameters for the operator (M)
	vnmr_accounting	Open Accounting window (U)

ACreport Print copy of probe file after autocalibration (M)

Syntax: ACreport

Description: Called by the autocalibration macros **AC1S-AC11S** to print a copy of the probe file before beginning a new autocalibration run.

See also: *NMR Spectroscopy User Guide*

Related: **AC1S-AC11S** Autocalibration macros (M)

acos Find arc cosine of number (C)

Syntax: acos(value) <:n>

Description: Finds the arc cosine (also called the inverse cosine) of a number.

Arguments: value is a number in the range of ± 1.0 to $+1.0$.

n is a return argument giving the arc cosine, in radians, of value. The default is to display the arc cosine value in the status window.

Examples: acos(.5)
acos(value):acos_val

See also: *VnmrJ User Programming*

Related: **sin** Find sine value of an angle (C)

A

acosy Automatic analysis of COSY data (C)

Syntax: `acosy`

Description: Automatically analyzes a 2D COSY data set with `fn=fn1` and `sw=sw1`. In this algorithm, a fuzzy pattern recognition technique is used to detect peaks and cluster the cross peaks into groups. Symmetry measures and chemical shifts for all cross peaks are calculated. Connectivities and the correlation table are displayed on the computer screen. This method is less sensitive to the threshold and rejects most artifacts in the peak list.

See also: *NMR Spectroscopy User Guide*

Related:

<code>acosyold</code>	Automatic analysis of COSY data (C)
<code>fn</code>	Fourier number in 1st indirectly detected dimension (P)
<code>fn1</code>	Fourier number in directly detected dimension (P)
<code>ll2d</code>	Automatic and interactive 2D peak picking (C)
<code>sw</code>	Spectral width in directly detected dimension (P)
<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)

acosyold Automatic analysis of COSY data, old algorithm (C)

Syntax: `acosyold`

Description: Analyzes COSY data using an old algorithm.

See also: *NMR Spectroscopy User Guide*

Related:

<code>acosy</code>	Automatic analysis of COSY data (C)
<code>fn</code>	Fourier number in 1st indirectly detected dimension (P)
<code>fn1</code>	Fourier number in directly detected dimension (P)
<code>ll2d</code>	Automatic and interactive 2D peak picking (C)
<code>sw</code>	Spectral width in directly detected dimension (P)
<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)

acqdisp Display message on the acquisition status line (C)

Syntax: `acqdisp (message)`

Description: Displays the message specified on the acquisition status line. `acqdisp` is used primarily by the acquisition process to update the screen.

Arguments: `message` is a text string, up to 8 characters long.

See also: *NMR Spectroscopy User Guide*

acqi Interactive acquisition display process (C)

Syntax: `acqi<('par'|'disconnect'|'exit'|'standby')><:$ret>`

Description: Opens the Acquisition window for interactive locking and shimming on the lock signal, FID, or spectrum. When using a spectrometer, `acqi` normally automatically starts. On all systems, if the console has been recently rebooted, enter `su` before running `acqi`.

If `acqi` is connected to the console and you start an acquisition (`su/go/au`), `acqi` automatically disconnects.

The pulse sequence and parameter set for the FID/spectrum display can be selected by entering `gf`. Note that if clicking the FID button in `acqi` causes `acqi` to “disconnect,” the common cause is that `gf` had not been executed.

The FID display is controlled by the parameters `lsfid`, `phfid`, and `dmgf`. These display parameters are automatically sent to `acqi` when `acqi` is first invoked. These parameters may subsequently be changed and sent again to

`acqi` with the command `acqi ('par')`. If `phfid` is not set to “Not Used” for the FID display in `acqi`, a slide control will be available in `acqi` for the interactive adjustment of the `phfid` parameter. The slide will be in the IPA set of adjustments. If the parameter `dmgf` exists and is set to 'av', the FID display in `acqi` displays the square root of the sum of the squares of the real and imaginary channels.

The spectrum display is controlled by parameters `sp`, `wp`, `dmg`, `rp`, `lp`, `rfl`, `rfp`, `vs`, `vp`, `sw`, and `fn`. These parameters are automatically sent to `acqi` when `acqi` is first invoked. These parameters can subsequently be changed and sent again to `acqi` with the command `acqi ('par')`. The preparation macro `gf` also calls `acqi ('par')`, thereby causing these parameters to be sent to `acqi`. If `fn` is greater than 64K, it is lowered to 64K.

A convenient method of setting these parameters is to acquire a spectrum with `go`, then `ft` and adjust the display with the `ds` command options. Once the display is set the way you want, enter `gf`. The same display should then appear when the spectrum display is selected from `acqi`. Note that weighting parameters are not used in the `acqi` spectrum display.

The manual *NMR Spectroscopy User Guide* has a step-by-step description of using `acqi`.

Arguments: 'par' causes the current values of parameters `lsfid`, `phfid`, `dmgf`, `sp`, `wp`, `dmg`, `rp`, `lp`, `rfl`, `rfp`, `vs`, `sw`, and `fn` to be sent to `acqi`.

'disconnect' causes `acqi` to be disconnected. Clicking the Close button in `acqi` is equivalent, and puts `acqi` in the standby mode. Lock parameters, the `spin` parameter, and the shim values are sent back to the current experiment when `acqi` is “disconnected.” If the experiment has the `load` parameter set to 'y', then the shim values are not delivered to the experiment.

'exit' causes an exit from `acqi`. Clicking the exit button in the Acquisition window is equivalent.

`$ret` is a return value with the success or failure of running `acqi`. The default is a warning displayed in the status window if `acqi` fails.

'standby' starts `acqi` and puts it into the standby mode.

Examples: `acqi`
`acqi ('par')`
`acqi ('disconnect')`
`acqi ('exit')`
`acqi:$ok`

See also: *NMR Spectroscopy User Guide*

Related:	<code>Acqstat</code>	Bring up the acquisition status display (U)
	<code>dmg</code>	Display mode in directly detected dimension (P)
	<code>dmgf</code>	Absolute-value display of FID data or spectrum in <code>acqi</code> (P)
	<code>ds</code>	Display a spectrum (C)
	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>ft</code>	Fourier transform 1D data (C)
	<code>gf</code>	Prepare parameters for FID/spectrum display in <code>acqi</code> (M)
	<code>go</code>	Submit an experiment to acquisition (C)
	<code>load</code>	Load status of displayed shims (P)
	<code>lkof</code>	Track changes in lock frequency (P)
	<code>lp</code>	First-order phase in directly detected dimension (P)
	<code>lsfid</code>	Number of complex points to left-shift the np FID (P)
	<code>phfid</code>	Zero-order phasing constant for np FID (P)
	<code>rfl</code>	Ref. peak position in 1st indirectly detected dimension (P)
	<code>rfp</code>	Ref. peak frequency in directly detected dimension (P)
	<code>rp</code>	Zero-order phase in directly detected dimension (P)
	<code>sp</code>	Start of plot in directly detected dimension (P)

<code>spin</code>	Sample spin rate (P)
<code>sw</code>	Spectral width in directly detected dimension (P)
<code>vp</code>	Vertical position of the spectrum (P)
<code>vs</code>	Vertical scale (P)
<code>wp</code>	Width of plot in directly detected dimension (P)

acqmeter **Open Acqmeter window (M)**

Syntax: `acqmeter<(remote_system)>`

Description: Opens the Acqmeter window and shows a time line of lock level, temperature (VT), and/or spinner speed. When first opened, only lock level is displayed. By clicking anywhere in the lock level window with the right mouse button, a menu pops up with choices to close the lock level window, show a temperature (VT) window, show a spinner window, open a properties window, or close the Acqmeter window. Click on the choice desired in the menu with either the left or right mouse button. In the properties window, the host, font, color, and graphical mode can be changed. Continue to click in any Acqmeter window with the right mouse button to open the menu and then open or close windows, or close the Acqmeter window, as desired.

Arguments: `remote_system` is the host name of a remote machine on the same network. The default is the local machine. To activate the remote feature, the local and remote machines must be on the same Ethernet LAN (local area network) and the local machine must be able to get the Internet address of the remote machine (usually in the `/etc/hosts` file).

Examples: `acqmeter`
`acqmeter('nmr500')`

See also: *NMR Spectroscopy User Guide*

Related: `acqi` Interactive acquisition display (C)
`Acqmeter` Open Acqmeter window (U)

Acqmeter **Open Acqmeter window (U)**

Syntax: `Acqmeter <remote_system> <-f file> <&>`

Description: Opens the Acqmeter window and shows a time line of lock level, temperature (VT), and/or spinner speed. When first opened, only lock level is displayed. By clicking anywhere in the lock level window with the right mouse button, a menu pops up with choices to close the lock level window, show a temperature (VT) window, show a spinner window, open a properties window, or close the Acqmeter window. Click on the choice desired in the menu with either the left or right mouse button. In the properties window, the host, font, color, and graphical mode can be changed. Continue to click in any Acqmeter window with the right mouse button to open the menu and then open or close windows, or close the Acqmeter window, as desired.

Arguments: `remote_system` is the host name of a remote machine on the same network. The default is the local machine. To activate the remote feature, the local and remote machines must be on the same Ethernet LAN (local area network) and the local machine must be able to get the Internet address of the remote machine (usually in the `/etc/hosts` file).

`-f file` is the name of a template file in the directory `$vnmruser/vnmrsys/templates/acqstat` used to set the attributes of the Acqmeter window when it opens. This allows customizing the Acqmeter window for different users and experiments. The default name of the file is `default`.

& (ampersand) character added to the command makes `Acqmeter` into a background process. For example, if “lab” is the remote machine host name, entering the command `Acqmeter lab &` displays the acquisition status of the “lab” remote machine as a background process. To activate the remote feature, the local and remote machines must be on the same Ethernet LAN (local area network) and the local machine must be able to get the Internet address of the remote machine (usually in the `/etc/hosts` file).

Examples: `Acqmeter &`
`Acqmeter nmr400 &`
`Acqmeter gem300 -f inova500.lisa &`

See also: *NMR Spectroscopy User Guide*

Related: `acqi` Interactive acquisition display (C)
`acqmeter` Open Acqmeter window (M)

acqmode Acquisition mode (P)

Description: A global parameter specifying the normal acquisition mode for acquiring, locking, fid shimming, and prescan in VnmrJ.

Values: ' ' (empty string) normal acquisition
 'lock' lock acquisition
 'fidscan' fid shimming acquisition
 'prescan' prescan acquisition

See also: *VnmrJ Imaging, User Guide, NMR Spectroscopy User Guide*

acqstat Open Acquisition Status window (M)

Syntax: `acqstat<(remote_system)>`

Description: Opens the Acquisition Status window, which displays acquisition information such as the current acquisition task, experiment number, spinner status, and temperature status. When the host computer is attached to a spectrometer, this window should open automatically when VnmrJ is started. In the properties window, the host, font, color, and graphical mode can be changed. For a complete description of these windows, refer to the manual *NMR Spectroscopy User Guide*.

Arguments: `remote_system` is the host name of a remote machine on the same network. The default is the local machine. To activate the remote feature, the local and remote machines must be on the same Ethernet LAN (local area network) and the local machine must be able to get the Internet address of the remote machine (usually in the `/etc/hosts` file).

Examples: `acqstat`
`acqstat('u500')`

See also: *NMR Spectroscopy User Guide*

Related: `Acqstat` Open the Acquisition Status window (U)
`showstat` Display information about status of acquisition (C,U)

Acqstat Open Acquisition Status window (U)

Syntax: `Acqstat <remote_system> <-f file> <&>`

Description: Opens the Acquisition Status window, which displays acquisition information such as the current acquisition task, experiment number, spinner status, and temperature status. When the host computer is attached to a spectrometer, this

window should open automatically when VnmrJ is started. In the properties window, the host, font, color, and graphical mode can be changed. For a complete description of these windows, refer to the manual *NMR Spectroscopy User Guide*.

Arguments: `remote_system` is the host name of a remote machine on the same network. The default is the local machine. To activate the remote feature, the local and remote machines must be on the same Ethernet LAN (local area network) and the local machine must be able to get the Internet address of the remote machine (usually in the `/etc/hosts` file).

`-f file` is the name of a template file in the directory `$vnmruser/vnmrsys/templates/acqstat` used to set the attributes of the Acquisition Status window when it opens. This allows customizing the Acquisition Status window for different users and experiments. The default name of the file is `default`.

`&` (ampersand) character added to the command makes `Acqstat` into a background process. For example, if “lab” is the remote machine host name, entering the command `Acqstat lab &` displays the acquisition status of the “lab” remote machine as a background process. To activate the remote feature, the local and remote machines must be on the same Ethernet LAN (local area network) and the local machine must be able to get the Internet address of the remote machine (usually in the `/etc/hosts` file).

Examples: `Acqstat &`
`Acqstat nmr400 &`
`Acqstat gem300 -f inova500.lisa &`

See also: *NMR Spectroscopy User Guide*

Related: `Acqstat` Open the Acquisition Status window (U)
`showstat` Display information about status of acquisition (C,U)

acqstatus Acquisition status (P)

Description: Whenever `wbs`, `wnt`, `wexp`, or `werr` processing occurs, the acquisition condition that initiated that processing is available from the parameter `acqstatus`. This acquisition condition is represented by two numbers, a “done” code and an “error” code. The done code is set in `acqstatus[1]` and the error code is set in `acqstatus[2]`. Macros can take different actions depending on the acquisition condition.

The done codes and error codes are listed below and in the file `acq_errors` in `/vnmr/manual`. For example, a `werr` macro could specify special processing if the maximum number of transients is accumulated. The appropriate test in the macro would be:

```
if (acqstatus[2] = 200) then
  "do special processing, e.g. dp='y' au"
endif
```

Done codes:

11. FID complete
12. Block size complete (error code indicates `bs` number completed)
13. Soft error
14. Warning
15. Hard error
16. Experiment aborted
17. Setup completed (error code indicates type of setup completed)
101. Experiment complete
102. Experiment started

Error codes:

Warnings

- 101. Low-noise signal
- 102. High-noise signal
- 103. ADC overflow occurred
- 104. Receiver overflow occurred*

Soft errors

- 200. Maximum transient completed for single-precision data
- 201. Lost lock during experiment (LOCKLOST)

300. *Spinner errors:*

- 301. Sample fails to spin after three attempts at repositioning
- 302. Spinner did not regulate in the allowed time period (RSPINFAIL)*
- 303. Spinner went out of regulation during the experiment (SPINOUT)*
- 395. Unknown spinner device specified (SPINUNKNOWN)*
- 396. Spinner device is not powered up (SPINNOPOWER)*
- 397. RS-232 cable not connected from console to spinner (SPINRS232)*
- 398. Spinner does not acknowledge commands (SPINTIMEOUT)*

400. *VT (variable temperature) errors:*

- 400. VT did not regulate in the given time `vttime` after being set
- 401. VT went out of regulation during the experiment (VTOUT)
- 402. VT in manual mode after automatic command (see Oxford manual)*
- 403. VT safety sensor has reached limit (see Oxford manual)*
- 404. VT cannot turn on cooling gas (see Oxford manual)*
- 405. VT main sensor on bottom limit (see Oxford manual)*
- 406. VT main sensor on top limit (see Oxford manual)*
- 407. VT sc/ss error (see Oxford manual)*
- 408. VT oc/ss error (see Oxford manual)*
- 495. Unknown VT device specified (VTUNKNOWN)*
- 496. VT device not powered up (VTNOPOWER)*
- 497. RS-232 cable not connected between console and VT (VTRS232)*
- 498. VT does not acknowledge commands (VTTIMEOUT)

500. *Sample changer errors:*

- 501. Sample changer has no sample to retrieve
- 502. Sample changer arm unable to move up during retrieve
- 503. Sample changer arm unable to move down during retrieve
- 504. Sample changer arm unable to move sideways during retrieve
- 505. Invalid sample number during retrieve
- 506. Invalid temperature during retrieve
- 507. Gripper abort during retrieve
- 508. Sample out of range during automatic retrieve
- 509. Illegal command character during retrieve*
- 510. Robot arm failed to find home position during retrieve*
- 511. Sample tray size is not consistent*
- 512. Sample changer power failure during retrieve*
- 513. Illegal sample changer command during retrieve*
- 514. Gripper failed to open during retrieve*
- 515. Air supply to sample changer failed during retrieve*
- 525. Tried to insert invalid sample number*
- 526. Invalid temperature during sample changer insert*
- 527. Gripper abort during insert*
- 528. Sample out of range during automatic insert
- 529. Illegal command character during insert*
- 530. Robot arm failed to find home position during insert*
- 531. Sample tray size is not consistent*
- 532. Sample changer power failure during insert*
- 533. Illegal sample changer command during insert*
- 534. Gripper failed to open during insert*
- 535. Air supply to sample changer failed during insert*
- 593. Failed to remove sample from magnet*
- 594. Sample failed to spin after automatic insert

595. Sample failed to insert properly
 596. Sample changer not turned on
 597. Sample changer not connected to RS-232 interface
 598. Sample changer not responding*
 600. *Shimming errors:*
 601. Shimming user aborted*
 602. Lost lock while shimming*
 604. Lock saturation while shimming*
 608. A shim coil DAC limit hit while shimming*
 700. *Autolock errors:*
 701. User aborted (ALKABORT)*
 702. Autolock failure in finding resonance of sample (ALKRESFAIL)
 703. Autolock failure in lock power adjustment (ALKPOWERFAIL)*
 704. Autolock failure in lock phase adjustment (ALKPHASFAIL)*
 705. Autolock failure, lock lost in final gain adjustment (ALKGAINFAIL)*
 800. *Autogain errors.*
 801. Autogain failure, gain driven to 0, reduce **pw** (AGAINFAIL)
 Hard errors
 901. Incorrect PSG version for acquisition
 902. Sum-to-memory error, number of points acquired not equal to **np**
 903. FIFO underflow error (a delay too small?)*
 904. Requested number of data points (**np**) too large for acquisition*
 905. Acquisition bus trap (experiment may be lost)*
 1000. *SCSI errors:*
 1001. Recoverable SCSI read transfer from console*
 1002. Recoverable SCSI write transfer from console**
 1003. Unrecoverable SCSI read transfer error*
 1004. Unrecoverable SCSI write transfer error*
 1100. *Host disk errors:*
 1101. Error opening disk file (most likely a UNIX permission problem)*
 1102. Error on closing disk file*
 1103. Error on reading from disk file*
 1104. Error on writing to disk file*

See also: *NMR Spectroscopy User Guide*

Related:	react	Recover from error conditions during werr processing (M)
	werr	Specify action when error occurs (C)
	werr	When error (P)

acquire **Acquire data (M)**

Description: Macro to acquire data. It uses **execpars** to select the prep and prescan method, executes them, and then begins acquisition.

See also: *NMR Spectroscopy User Guide*

Related:	execpars	Set up the exec parameters (M)
	execprescan	Execute prescan macro (P)
	xmnext	Find next prescan or next experiment in study queue (M)
	xmwexp	Processing macro for end of acquisition in study queue (M)

actionid **Current study queue node id (P)**

Applicability: Liquids, Imaging

Description: Specifies the currently selected study queue node id.

See also: VnmrJ Imaging, User Guide, NMR Spectroscopy User Guide

Related:	<code>xmaction</code>	Perform study queue action (M)
	<code>xmnext</code>	Find next prescan or next experiment in study queue (M)
	<code>xmselect</code>	Action when study queue node is selected (M)

activestudy Active study name (P)

Applicability: Liquids, Imaging

Description: A global parameter that specifies the currently active study name. In the Walkup interface, it specifies the currently active automation run.

Values: `'s_20050601'` active study name
`'auto_2005.06.01'` active automation run name
`'null'` no active study or automation run

See also: VnmrJ Imaging, User Guide and NMR Spectroscopy User Guide

Related:	<code>acquire</code>	Acquire data (M)
	<code>autodir</code>	Automation directory absolute pathname (P)
	<code>cqinit</code>	Initialize liquids study queue (M)
	<code>studyid</code>	Study identification (P)
	<code>xmaction</code>	Perform study queue action (M)
	<code>xmselect</code>	Action when study queue node is selected (M)

add Add current FID to add/subtract experiment (C)

Syntax: (1) `add<(multiplier<,'new'>)>`
(2) `add('new')`
(3) `add('trace',index)`

Description: Adds the last displayed or selected FID to the current contents of the add/subtract experiment (exp5). The parameters `lsfid` and `phfid` can be used to shift or phase rotate the selected FID before it is combined with the data in the add/subtract experiment. A multi-FID add/subtract experiment can be created by using the `'new'` keyword. Individual FIDs in a multi-FID add/subtract experiment can subsequently be added to using the `'trace'` keyword followed by the index number of the FID.

Arguments: `multiplier` is a value that the FID is to be multiplied by before being added to the add/subtract experiment (exp5). The default is 1.0.

`'new'` is a keyword to create a new FID element in a add/subtract experiment.

`'trace'` is a keyword to use the next argument (`index`) as the number of the FID to add to in an add/subtract experiment. The default is to add to the first FID in a multi-FID add/subtract experiment.

`index` is the index number of the FID to be used as a target in a multi-FID add/subtract experiment.

Examples: `add`
`add(0.75)`
`add('new')`
`add('trace',2)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>clradd</code>	Clear add/subtract experiment (C)
	<code>lsfid</code>	Number of complex points to left-shift <code>ni</code> interferogram (P)
	<code>phfid</code>	Zero-order phasing constant for <code>np</code> FID (P)
	<code>select</code>	Select a spectrum without displaying it (C)

<code>spadd</code>	Add current spectrum to add/subtract experiment (C)
<code>sub</code>	Subtract current FID from add/subtract experiment (C)

addi Start interactive add/subtract mode (C)

Syntax: `addi`

Description: Starts the interactive add/subtract mode. Before entering `addi`, start the process with `clradd` and `spadd`, then display a second spectrum on the screen. This may involve changing experiments, selecting a second member of an array of spectra, a different trace of a 2D spectrum, or displaying a spin simulated spectrum. The Fourier numbers (`fn`) *must* be the same in the two spectra to be manipulated. The width (`sw`) of the two spectra need *not* be identical, although adding spectra of different widths will probably not be meaningful. Having selected the second spectrum and ensuring it is in `nm` mode, enter `addi` to begin the interactive process.

After `addi` is invoked, spectrum 1, the spectrum selected by the `spadd` command, appears in the center of the display. Spectrum 2, the spectrum that was active when `addi` was entered, appears on the bottom. The sum or difference of these spectra appears on top of the screen. When `addi` is first entered, this spectrum will be the sum (1 + 2) by default. The spectra is manipulated using the mouse.

The select button toggles between different modes of control.

- When the label at the screen bottom reads “active: current”, all of the parameters (except `wp`) control spectrum 2, and spectrum 2 can be phased, scaled, or shifted relative to spectrum 1.
- After clicking on select, the label at the screen bottom reads “active: addsub”, and now all of the parameters except `wp` control spectrum 1.
- Clicking select again toggles the label to read “active: result”, and now parameter changes affect only the sum or difference spectrum.

Note that `wp` always controls all spectra, because differential expansions of the two spectra are not supported. Note also that the colors of the labels change to match the colors of the different spectra.

The sum/difference spectrum displayed on the screen while `addi` is active is strictly a temporary display. Once all manipulations have been performed, and assuming the sum/difference is something you wish to perform further operations with (such as plotting), it must be saved into the add/subtract experiment (`exp5`) by clicking on save. At this point, spectrum 1, which was in the add/subtract experiment, is overwritten by the sum or difference spectrum, and `addi` ceases operation. In most cases, you will next want to enter `jexp5 ds` to display the difference spectrum on the screen, ready for further manipulation (expansion, line listing, etc.) and plotting. If you wish to continue with the add/subtract process by adding in a third spectrum, display that spectrum in the usual way and enter `addi` again.

See also: *NMR Spectroscopy User Guide*

Related:	<code>clradd</code>	Clear add/subtract experiment (C)
	<code>jexp</code>	Join existing experiment (C)
	<code>nm</code>	Select normalized intensity mode (C)
	<code>spadd</code>	Add current spectrum to add/subtract experiment (C)
	<code>spmin</code>	Take minimum of two spectra in add/subtract experiment (C)
	<code>spsub</code>	Subtract current spectrum from add/subtract experiment (C)
	<code>wp</code>	Width of plot in directly detected dimension (P)

addnucleus Add new nucleus to existing probe file (M)

Applicability: ALL

Description: Entries for nuclei not in the default probe file are appended to the end of the file. The argument should correspond to a nucleus in the nuctable.

Syntax: `addnucleus('nucleus')`

Arguments: `nucleus` — name followed by atomic number, e.g. C13 not 13C.

Examples: `addnucleus('Si29')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>addprobe</code>	Create new probe directory and probe file (M)
	<code>deletenucleus</code>	Removes nucleus entry to probe file (M)
	<code>getparam</code>	Receive parameter from probe file (M)
	<code>probe</code>	Probe type (P)
	<code>setparams</code>	Write parameter to current probe file (M)

addpar Add selected parameters to current experiment (M)

Syntax: `addpar(<'2d'|'3d'|'3rf'|'4d'|'downsamp'|'fid'|
'image'|'1l2d'|'lp'<,dim>|'oversamp'|'ss')>`

Applicability: The '3d', '3rf', '4d', 'fid', and 'image' arguments work on all systems but are only useful if system has the proper hardware.

Description: Creates selected parameters in the current experiment.

Arguments: If no argument is entered, `addpar` displays instructions for its use.

'2d', '3d', '3rf', '4d', 'downsamp', 'fid', 'image', '1l2d', 'lp', 'oversamp', and 'ss' are keywords (only one keyword is used at a time) specifying the parameters to be created:

- '2d' specifies creating `ni`, `phase`, and `sw1`, which can be used to acquire a 2D data set (functions the same as macro `par2d`).
- '3d' specifies creating `d3`, `ni2`, `phase2`, and `sw2`, which can be used to acquire a 3D data set (functions the same as macro `par3d`).
- '3rf' specifies retrieving the `ap` and `dg2` display templates for third rf channel and 3D parameters (functions the same as macro `par3rf`).
- '4d' specifies creating the acquisition parameters `d4`, `ni3`, `phase3`, and `sw3`, which can be used to acquire a 4D data set (functions the same as macro `par4d`).
- 'downsamp' specifies creating the parameters `downsamp`, `dscoef`, `ds1sfrq`, `dsfb`, and `filtfile` for digital filtering and downsampling (functions the same as macro `pards`).
- 'fid' specifies creating FID display parameters `axisf`, `crf`, `deltaf`, `dotflag`, `vpf`, and `vpfi` if the parameter set is older and lacks these parameters (functions the same as macro `fidpar`).
- '1l2d' specifies creating `th2d` and `xdiag` for the 1l2d 2D peak picking program (functions the same as macro `par1l2d`).
- 'lp' specifies creating `lpalg`, `lpopt`, `lpfilt`, `lpnupts`, `strtlp`, `lpext`, `strtext`, `lptrace`, and `lpprint` for linear prediction in the acquisition dimension (functions the same as macro `parlp`). The display template for the `dg1p` macro is also created if necessary.
- 'oversamp' specifies creating parameters `def_osfilt`, `filtfile`, `oscoef`, `osfb`, `osfilt`, `os1sfrq`, and `oversamp` for oversampling and digital filtering (functions the same as macro `paros`).

- 'ss' specifies adding parameters `ssorder`, `ssfilter`, `ssntaps`, and `sslsfrq` for time-domain solvent subtraction (functions the same as macro `parfidss`).

`dim` specifies the dimension when adding linear prediction parameters: 1 for the first implicit dimension or 2 for the second implicit dimension. Default is the acquisition dimension. Therefore, `addpar('lp')` creates the parameters listed above; `addpar('lp',1)` creates `lpalg1`, `lpopt1`, `lpfilt1`, `lpnupts1`, `strtlp1`, `lpext1`, `strtext1`, `lptrace1`, and `lpprint1`; and `addpar('lp',2)` creates `lpalg2`, `lpopt2`, `lpfilt2`, `lpnupts2`, `strtlp2`, `lpext2`, `strtext2`, `lptrace2`, and `lpprint2`. Each separate dimension of a multidimensional data set can have its own unique parameters.

Examples: `addpar`
`addpar('3d')`
`addpar('lp',1)`

See also: *NMR Spectroscopy User Guide; VnmrJ Imaging NMR*

Related:	<code>def_osfilt</code>	Default value of <code>osfilt</code> (P)
	<code>fidpar</code>	Add parameters for FID display in current experiment (M)
	<code>osfilt</code>	Oversampling filter for real-time DSP (P)
	<code>par2d</code>	Create 2D acquisition parameters (M)
	<code>par3d</code>	Create 3D acquisition parameters (M)
	<code>par3rf</code>	Get display templates for 3rd rf channel parameters (M)
	<code>par4d</code>	Create 4D acquisition parameters (M)
	<code>pards</code>	Create digital filtering and downsampling parameters (M)
	<code>parfidss</code>	Set up parameters for time-domain solvent subtraction (M)
	<code>paros</code>	Create oversampling and digital filtering parameters (M)
	<code>par112d</code>	Create parameters for 2D peak picking (M)
	<code>parlp</code>	Create parameters for linear prediction (M)

addparams Add parameter to current probe file (M)

Syntax: `addparams(param,value,nucleus<,'tmplt'><,'system'>)`

Description: Adds a new parameter and its value for a specified nucleus to the probe file or to the probe template.

Arguments: `param` is the name of the parameter to be added.

`value` is a string with the value to be written for the parameter.

`nucleus` is the nucleus to add in the probe file.

'`tmplt`' is a keyword to add the parameter to the local template. The default is the probe file.

'`system`' is a keyword to add the parameter to the system-level template or probe file, provided that you have write permission to that file. The default is to add the parameter to the local template or probe file.

Examples: `addparams('ref_pwr','53',tn)`
`addparams('ref_pwx','00',dn,'tmplt')`
`addparams('ref_pwx2','00',dn2,'tmplt','system')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>getparam</code>	Receive parameter from probe file (M)
	<code>setparams</code>	Write parameter to current probe file (M)
	<code>updateprobe</code>	Update probe file (M)

addprobe Create new probe directory and probe file (M)

Syntax: `addprobe (probe_name<, 'stdar' | 'system'><, 'stdpar'>)`

Description: Creates a new probe directory and a probe file. Default nuclei included in this file are ^1H , ^{19}F , ^{13}C , and ^{15}N . The information is saved in the user's directory `vnmrsys/probes`.

Arguments: `probe_name` is the name to be given to the probe directory and probe file.
`'stdpar'` and `'system'` are keywords for the second and third arguments:

- If the second argument is `'stdpar'`, calibration values from the standard parameter sets (`stdpar/H1.par`, `stdpar/C13.par`, etc.) will be read and written into the probe file.
- If the second argument is `'system'` and the user has write permission into the VnmrJ system probes directory (typically `/vnmr/probes`), then a system-level probe directory will be made.
- If the second argument is `'system'` and the third argument is `'stdpar'`, then both actions in the preceding bullets will occur.
- The default is the probe file is created with all parameters initialized to zero.

Examples: `addprobe('idpfg')`
`addprobe('idpfg', 'stdpar')`
`addprobe('idpfg', 'system', 'stdpar')`

See also: *NMR Spectroscopy User Guide; VnmrJ Walkup*

Related:	<code>addnucleus</code>	Add new nucleus to existing probe file (M)
	<code>deletenucleus</code>	Removes nucleus entry to probe file (M)
	<code>getparam</code>	Receive parameter from probe file (M)
	<code>probe</code>	Probe type (P)
	<code>setparams</code>	Write parameter to current probe file (M)

adept Automatic DEPT analysis and spectrum editing (C)

Syntax: `adept<(<'noll'><, 'coef'><, 'theory'>)>`

Description: Automatically analyzes a set of four DEPT spectra and edits the spectra so that the spectra is arrayed as follows:

- #4 is CH_3 carbons only
- #3 is CH_2 carbons only
- #2 is CH carbons only
- #1 is all protonated carbons

Because `adept` modifies the transformed data, it should not be repeated without retransforming the data between calls. `adept` produces a text file `dept.out` in the current experiment directory, which contains the result of the analysis.

Arguments: The following keyword arguments can be supplied in any order:

`'noll'` causes the line listing to be skipped. If `'noll'` is not supplied as an argument, `adept` first performs a line listing. In that case, the threshold parameter `th` must be set properly before starting `adept`.

`'coef'` causes the combination coefficients to be printed.

`'theory'` causes theoretical coefficients to be used. The default is optimized coefficients.

A

Examples: `adept`
`adept('coef')`
`adept('theory','noll')`

See also: *NMR Spectroscopy User Guide*

Related: `autodept` Automated complete analysis of DEPT data (M)
`Dept` Set up parameters for DEPT experiment
`deptproc` Process DEPT data (M)
`padept` Perform adept analysis and plot resulting spectra (C)
`pldept` Plot DEPT data, edited or unedited (M)
`th` Threshold (P)

aexppl Automatic plot of spectral expansion (M)

Syntax: `aexppl<(expansion_factor)>`

Description: Plots automatically expansions of given regions. Regions have to be defined first by using the `region` command or by using the cursors in `ds`.

Arguments: `expansion_factor` is a spectral expansion factor in units of Hz/mm. The default is 2 Hz/mm.

Examples: `aexppl`
`aexppl(20)`

See also: *NMR Spectroscopy User Guide*

Related: `ds` Display a spectrum (C)
`region` Divide spectrum into regions (C)

ai Select absolute-intensity mode (C)

Syntax: `ai`

Description: Selects the *absolute-intensity display mode* in which the scale is kept constant from spectrum to spectrum to allow comparison of peak heights from one spectrum to another. The alternative is the normalized-intensity display mode (`nm`) in which spectra are scaled so that the largest peak in the spectrum is `vs` mm high. The modes are mutually exclusive—the system is always in either `nm` or `ai` mode. Enter `aig?` to determine which mode is currently active.

See also: *NMR Spectroscopy User Guide*

Related: `aig` Absolute intensity group (P)
`nm` Select normalized-intensity mode (C)
`vs` Vertical scale (P)

aig Absolute-intensity group (P)

Description: Contains the result of the `ai` or `nm` command. `aig` is not set in the usual way but can be queried (`aig?`) to determine which display mode is active.

Values: 'ai' indicates the absolute-intensity display mode is active.

'nm' indicates the normalized-intensity display mode is active.

See also: *NMR Spectroscopy User Guide*

Related: `ai` Select absolute intensity mode (C)
`dmg` Display mode in directly detected dimension (P)
`nm` Select normalized-intensity mode (C)
`?` Display individual parameter value (C)

alfa **Set alfa delay before acquisition (P)**

Description: After the final event in the pulse sequence, including any receiver gate times occurring following the final pulse, acquisition occurs after a delay. This delay includes a fixed part, `alfa`, and a variable part, $1 / (\text{beta} * \text{fb})$.

- On systems with 4-pole Butterworth filters, `beta` is 2.
- On systems with 8-pole Butterworth (200-kHz) filters, `beta` is 3.8.
- On systems with 8-pole elliptical filters, `beta` is 1.29.
- On Systems with 4-pole Bessel filters, `beta` is 2.3 (only systems with 2-MHz and 5-MHz Analog-to-Digital Converter boards use this filter).

Because the total delay before acquisition is the sum of `alfa` and $1 / (\text{beta} * \text{fb})$, it is possible to shorten the delay beyond “normal” values by setting `alfa` negative (to a maximum of $1 / (\text{beta} * \text{fb})$). The macros `hoult` and `calfa` frequently result in such negative values of `alfa`.

To set `alfa` to a negative number, use either the `setvalue` command to enter a specific value of `alfa`, or use the `setlimit` command to allow entry of negative values of `alfa` directly from the keyboard.

Values: 0 to 100,000,000; in μs .

See also: *NMR Spectroscopy User Guide*

Related:	<code>calfa</code>	Recalculate <code>alfa</code> so that first-order phase is zero (M)
	<code>fb</code>	Filter bandwidth (P)
	<code>hoult</code>	Set parameters <code>alfa</code> and <code>rof2</code> according to Hoult (M)
	<code>rof2</code>	Receiver gating time following pulse (P)
	<code>setlimit</code>	Set limits of a parameter in a tree (C)
	<code>setlp0</code>	Set parameters for zero linear phase (M)
	<code>setvalue</code>	Set value of any parameter in a tree (C)

alock **Automatic lock control (P)**

Description: Governs Autolock control following the insertion of a sample with `change` or `sample`, and following initiation of an acquisition with the `go`, `ga`, or `au`. Manual adjustment of lock power, gain, and phase is possible using the `acqi` command.

Values: Possible values are 'a', 'auto', 'n', 's', 'samp', 'u', or 'y', where:

- 'a' or 'auto' selects the optimizing Autolock function, which performs a lock capture and an automatic lock power and gain adjustment before data acquisition begins (lock phase is *not* optimized).
- 'n' leaves the lock in its current state.
- 's' or 'samp' selects the optimizing Autolock function, which performs a lock capture and an automatic lock power and gain adjustment before data acquisition begins (lock phase is *not* optimized) but only if the sample has just been changed.
- 'u' turns lock off so that the experiment runs unlocked.
- 'y' turns on the software Autolock function, which searches for the correct Z0 value only.

See also: *NMR Spectroscopy User Guide*

Related:	<code>acqi</code>	Interactive acquisition display process (C)
	<code>au</code>	Submit experiment to acquisition and process data (C)
	<code>change</code>	Submit a change sample experiment to acquisition (M)
	<code>ga</code>	Submit experiment to acquisition and FT the result (C)
	<code>gf</code>	Prepare parameters for FID/spectrum display in <code>acqi</code> (M)
	<code>go</code>	Submit experiment to acquisition (C)

<code>lock</code>	Submit an Autolock experiment to acquisition (C)
<code>sample</code>	Submit change sample, Autoshim experiment to acquisition (M)

ampmode Independent control of amplifier mode (P)

Description: Gives override capability over the default selection of amplifier modes. Unless overridden, the usage of rf channels determines whether the amplifier for a channel is in pulse, CW (continuous wave), or idle mode:

- Observe channel is set to the pulse mode.
- Other used channels are set to the CW mode.
- Any unused channels are set to the idle mode.

The `ampmode` parameter can be used to override this selection.

`ampmode` does not normally exist but can be created by the user with the command `create('ampmode','flag')`.

Values: List of characters in which the mode of the first amplifier is determined by the first character, the mode of the second amplifier by the second character, and so on. For each amplifier, one of the following characters is used:

- 'c' selects CW mode.
- 'i' selects idle mode.
- 'p' selects pulse mode.
- 'd' selects default behavior.

For example, `ampmode='ddp'` selects default behavior for the first two amplifiers and forces the third channel amplifier into pulse mode. Additional filtering is usually required when an amplifier in the same band as the observe amplifier is placed in the CW mode.

See also: *VnmrJ User Programming*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>dn</code>	Nucleus for the first decoupler (P)
	<code>tn</code>	Nucleus for observe transmitter (P)

amptype Amplifier type (P)

Description: Specifies the type of amplifier on each rf channel of the spectrometer. The value is set in the Spectrometer Configuration window (opened from `config`) using the label Type of Amplifier.

For each channel, the types are Class C, Linear Full Band, Linear Low Band, Linear Broadband, or, for the fourth channel only, Shared. Selecting Shared means that the amplifier is fully configured for the third channel, and that the fourth channel shares this amplifier with the third channel.

When a type is selected for a channel, a letter (one of the values described below) is added to the value of `amptype`. For example, a system already set to Linear Full Band on the observe transmitter channel and the first decoupler channel would have `amptype='aa'`. Selecting the third channel as Linear Low Band would set `amptype='aal'`. Finally, selecting Shared for the fourth channel would set `amptype='aaln'`.

Values: 'a' indicates the channel uses a linear full-band amplifier. A full-band amplifier has two outputs: 12 MHz to ^{31}P , and $^{19}\text{F}/^{1}\text{H}$.

'b' indicates the system uses a linear broadband amplifier.

'c' indicates the system uses a class C amplifier.

'l' indicates the channel uses a linear low-band amplifier. A low-band amplifier has one output from 12 MHz to ^{31}P only.

'n' indicates the fourth channel shares a linear amplifier with the third.

See also: *NMR Spectroscopy User Guide*, *VnmrJ User Programming*

Related: `config` Display current configuration and possibly change it (M)

analyz Calculate standard peak height (M)

Syntax: `analyz ($option, $title)`

Description: Macro to calculate average peak height and standard deviation and/or average phase and standard deviation.

Arguments: `$option` = 'n' for amplitude and phase, 'a' for amplitude only, and 'p' for phase only. The `$title` option puts a title on the plot.

Examples: `analyz` – Does analysis for both amplitude and phase
`analyz ('p')` – Does analysis for phase only
`analyz ('n', 'Stability')` – Does analysis for amplitude and phase and puts title “Stability” on the plot.

analyze Generalized curve fitting (C)

Syntax: (curve fitting) `analyze ('expfit', xarray<, options>)`
 (regression) `analyze ('expfit', 'regression'<, options>)`

Description: Provides interface to curve fitting program `expfit` (using the curve fitting syntax), supplying `expfit` with input data in the form of the text file `analyze.inp` in the current experiment. `expfit` can be called from UNIX with the syntax:

```
expfit options <analyze.inp >analyze.list
```

`expfit` does a least-squares curve fitting to the data supplied in `analyze.inp`. Macros are available for the specialized uses of `analyze`, such as the 'T1' and 'kinetics' options. These macros avoid the need to select options and get the correct file format.

In the regression mode (using the regression syntax above), the type of curve fitting, ('poly1', ...) must be selected. The regression section in the manual *NMR Spectroscopy User Guide* gives the input file format and describes the menus that permit choices indirectly through menu buttons.

The text file `analyze.inp` for the options 'T1', 'T2', 'kinetics', 'contact_time', and 'regression' contains the following lines (note that (1), (2), (3), etc. do not appear in the file but are used to identify lines in the explanation):

```
(1) <text line>
(2) <text line>
(3) npeaks npairs <xscale> <yscale>
(4) <NEXT npairs1>
(5) peaks
(6) x y
(6) x y
...
(4) <NEXT npairs2>
(5) peaks
(6) x y
(6) x y
...
```

Line-by-line explanation:

(1) Optional descriptive text line, for regression only. Omit line otherwise.

(2) Optional y-axis title, for regression only. Omit line otherwise.

(3) Line containing an integer for the number of peaks (`npeaks`) followed by another integer for the number of (`x`, `y`) pairs per peak (`npairs`). If regression, the `x`-scale type and `y`-scale type are also listed.

(4) In the regression mode, a line beginning with the keyword `NEXT` is inserted at the start of each data set when the number of pairs per peak is variable. In this case, the number of (`x`, `y`) pairs for the peak (`npair1`, `npair2`, etc.) is also given on the line.

(5) Peak index.

(6) Data pairs, one to a line, are listed by peak in the following order:

```
x y    (first peak, first pair)
x y    (first peak, second pair)
...
x y    (second peak, first pair)
x y    (second peak, second pair)
...
```

In the regression mode, the line beginning with `NEXT` is inserted at the start of the data for each peak when the number of pairs per peak is variable. In this case, the header contains the maximum number of pairs for any peak.

For `'T1'`, `'T2'`, `'kinetics'`, and `'contact_time'`, information from the file `fp.out` and values of the arrayed parameter `xarray` are used to construct the file; thus, it is necessary to run `fp` prior to `analyze`.

For regression, `analyze.inp` is made by running `expl('regression')`. If the regression mode is not selected, `analyze.inp` may be slightly different.

In addition to output to the standard output, which is usually directed to `analyze.list`, `expfit` makes a file `analyze.out`, which is used by `expl` to display the results of the analysis.

User-supplied analysis programs can be called by `analyze` in place of `expfit`. Such programs should read their input from `stdin` and write the output listing to `stdout`. No `analyze.out` file needs to be generated unless display by `expl` is desired. Use the program `expfit` as a model.

Arguments: `'expfit'` is a required first argument.

`xarray` is the name of the parameter array holding `x`-values in `'T1'`, `'T2'`, `'kinetics'`, and `'contact_time'`, and is used only with these options.

`'regression'` sets regression mode and signifies generalized curve fitting with choices `'poly1'`, `'poly2'`, `'poly3'`, and `'exp'`.

`options` are any of the following keywords:

- `'T1'` sets T_1 analysis (the default).
- `'T2'` sets T_2 analysis.
- `'kinetics'` sets kinetics analysis, with decreasing peak height.
- `'increment'` sets kinetics analysis, with increasing peak height.
- `'list'` makes an extended listing for each peak.
- `'diffusion'` sets a special analysis for diffusion experiments.
- `'contact_time'` sets a special analysis for solids cross-polarization spin-lock experiments.
- `'poly1'` sets a linear fitting. It is used in regression mode only.
- `'poly2'` sets a quadratic fitting. It is used in regression mode only.
- `'poly3'` sets a cubic fitting. It is used in regression mode only.
- `'exp'` sets exponential curve fitting. It is used in regression mode only.

Examples: `analyze('expfit','d2','T1','list')`
`analyze('expfit','pad',kinetics', 'list')`
`analyze('expfit','p2','contact_time', 'list')`
`analyze('expfit','regression','poly1', 'list')`

See also: *NMR Spectroscopy User Guide*

Related: `contact_time` MAS cross-polarization spin-lock contact time (M)
`expfit` Least squares fit to polynomial or exponential curve (U)
`expl` Display exponential or polynomial curves (C)
`pexpl` Plot exponential or polynomial curves (C)
`kini` Kinetics analysis, increasing intensity (M)
`t1` T_1 exponential analysis (M)
`t2` T_2 exponential analysis (M)

ap Print out “all” parameters (C)

Applicability: `VnmrJ`

Syntax: `ap('template_name', <'filename'>)`

Description: Print a parameter list. The *User Programming* Manual describes the rules for building a template for the `ap` commands. The string parameter `ap` normally controls how the command, `ap`, displays the parameters. Use command `paramvi('ap')` to modify the `ap` parameter. The `ap` command writes the parameter list to a file if `filename` is provided as the second argument.

Arguments: `template_name` template name must be the first argument.
`filename` optional, name of file to which the parameters are written.

Examples: `ap('ap', 'apout')` — writes the parameter list using defined by the `ap` parameter to the file `apout`.
`ap('newap')`

See also: *NMR Spectroscopy User Guide; VnmrJ User Programming*

Related: `addpar` Add selected parameters to the current experiment (M)
`ap` “All” parameters display control (P)
`dg` Display group of acquisition/processing parameters (C)
`hpa` Plot parameters on special preprinted chart paper (C)
`pap` Plot out “all” parameters (C)
`paramvi` Edit a variable and its attributes with `vi` text editor (C)
`ppa` Plot a parameter list in “English” (M)

ap “All” parameters display control (P)

Description: Controls the display of the `ap` and `pap` commands to print and plot a parameter list. Use `paramvi('ap')` to modify the string value of `ap`.

See also: *NMR Spectroscopy User Guide; VnmrJ User Programming*

Related: `ap` Print out “all” parameters (C)
`dg` Display group of acquisition/processing parameters (C)
`pap` Plot out “all” parameters (C)
`paramvi` Edit a variable and its attributes with `vi` text editor (C)

apa Plot parameters automatically (M)

Syntax: `apa`

Description: Selects automatically the appropriate command on different plotter devices to plot the parameter list.

See also: *VnmrJ User Programming*

Related: **hpa** Plot parameters on special preprinted chart paper (C)
ppa Plot a parameter list in “English” (M)

aph Automatic phase adjustment of spectra (C)

Syntax: `aph<: $ok, $rp, $lp>`

Description: Automatically calculates the phase parameters **lp** and **rp** required to produce an absorption mode spectrum and applies these parameters to the current spectrum. Values calculated do *not* depend on the initial values of **lp** and **rp**.

Arguments: **\$ok** is 1 if the phase adjustment succeeds, or 0 if the adjustment fails.
\$rp is the calculated value of **rp**. If **\$rp** is requested as a return value, **rp** is returned but not applied to the current spectrum.
\$lp is the calculated value of **lp**. If **\$lp** is requested as a return value, **lp** is returned but not applied to the current spectrum.

See also: *NMR Spectroscopy User Guide*

Related: **aph0** Automatic phase of zero-order term (C)
aphx Perform optimized automatic phasing (M)
lp First-order phase in directly detected dimension (P)
rp Zero-order phase in directly detected dimension (P)

aph0 Automatic phase of zero-order term (C)

Syntax: `aph0<: $ok, $rp, $lp>`

Description: Automatically adjusts only the zero-order frequency-independent term **rp** and does not rely on the frequency-dependent term **lp** being previously adjusted. In favorable circumstances, spectra may be obtained in such a way that only **rp** is expected to change. In these cases, if **lp** has been determined for one spectrum, then **rp** only can be computer-adjusted for subsequent spectra by **aph0** (“aph-zero”). Note that **aph0** does not correctly phase an exactly on-resonance peak.

Arguments: **\$ok** is 1 if the phase adjustment succeeds, or 0 if the adjustment fails.
\$rp is the calculated value of **rp**.
\$lp is the current value of **lp**.

See also: *NMR Spectroscopy User Guide*

Related: **aph** Automatic phase adjustment of spectra (C)
aphx Perform optimized automatic phasing (M)
lp First-order phase in directly detected dimension (P)
rp Zero-order phase in directly detected dimension (P)

aphb Auto phasing for Bruker data (C)

Syntax: `aphb< (threshold) >`

Description: Phases Bruker data using the autophasing program.

Arguments: **threshold** determines if a data point is large enough to qualify it as part of a peak. If no argument is given, or if the value is equal to or less than 0, the threshold is calculated from the spectrum.

Examples: `aphb`
`aphb (2)`

See also: *NMR Spectroscopy User Guide*

Related: **aph** Automatic phase adjustment of spectra (C)
aph0 Automatic phase of zero-order term only (C)

aphx Perform optimized automatic phasing (M)

Syntax: **aphx**

Description: Optimizes parameters and arguments for the **aph** command. **aphx** first performs an **aph** then calculates a theoretical value for **lp**. If **lp** set by the **aph** is different from the calculated value by 10 per cent, the calculated value is used and an **aph0** is performed.

See also: *NMR Spectroscopy User Guide*

Related: **aph** Automatic phase adjustment of spectra (C)
aph0 Automatic phase of zero-order term only (C)
lp First order phase along directly detected dimension (P)

appdirs Starts Applications Directory Editor (M)

Applicability: ALL

Syntax: **appdirs**

Description: The **appdirs** macro brings up an editor to set the applications directories. The top section of the editor has rows consisting of a menu and two entry boxes.

Values: **Menu selections:**

Enabled — enable an application directory.

Disabled — disable an application directory.

Remove(d) — initial setting for other row and the and empty entry boxes.

Set an application directory menu to Remove(d) to completely remove it.

Fields in each row:

Applications directory path.

A comment can be added to the second entry box.

Radio-button choices:

Save as private applications directories — sets the applications directories for the current operator only.

Reset to system default applications directories — removes any private applications directories and return to the standard default set.

Save the applications directories for global use — available only to users with write permission for VnmrJ system files. A name must be provided for this choice. This will affect all users the administrator has set that name as their **appdirs** setting. The Varian default names are Experimental, Walkup, Imaging, and LcNmrMs.

Buttons:

OK — exit the editor and apply the selections made in the editor.

Cancel — exit the editor and abort the editor session, making no changes to the applications directories.

See also: *VnmrJ Installation and Administration*

Related: **exists** Checks if parameter, file, or macro exists and file type (C)

A

appmode **Application mode (P)**

Description: A global parameter that allows selection of specialized system applications modes, such as imaging, by setting the global parameters `sysmaclibpath`, `sysmenulipath`, and `syshelppath`.

For example, in `/vnmr/maclib` is a subdirectory `maclib.imaging` that contains macros used primarily with imaging applications. Similarly, in `/vnmr/menulib` is a subdirectory `menulib.imaging` for imaging-related menus. By separating the imaging macros and menus into subdirectories, access to imaging-specific macros and menus is more convenient. This separation also allows minor modifications to some macros and menus while retaining the names that are in common use or required by other VnmrJ commands.

The value of `appmode` are set from either the System settings dialog in the Utilities menu or the VnmrJ Admin interface.

Values: `'standard'` sets standard application mode.
`'imaging'` sets imaging application mode.
`'autotest'` sets autotest application mode

apptype **Application type (P)**

Description: Specifies the application type, the group of pulse sequences to which a pulse sequence belongs. It is used by the `execpars` macros to specify the actions executed by the protocol for a pulse sequence. The actions are common to the group of pulse sequences specified by the `apptype`.

Values: See the `execpars` directory in `/vnmr`.

See also: *VnmrJ Imaging, User Guide* and *NMR Spectroscopy User Guide*

Related:	<code>cqexp</code>	Load experiment from protocol (M)
	<code>execpars</code>	Set up the exec parameters (M)
	<code>execsetup</code>	Execute setup macro (P)
	<code>execprep</code>	Execute prepare macro (P)
	<code>execprescan</code>	Execute prescan macro (P)
	<code>execpreprocess</code>	Execute processing macro (P)
	<code>execplot</code>	Execute plotting macro (P)
	<code>sqexp</code>	Load experiment from protocol (M)

Apt **Set up parameters for APT experiment (M)**

Description: Converts a parameter set to the APT (attached proton test) experiment.

See also: *NMR Spectroscopy User Guide*

Related:	<code>aptaph</code>	Automatic processing for APT spectra (M)
	<code>capt</code>	Automated carbon and APT acquisition (M)
	<code>hcapt</code>	Automated proton, carbon, and APT acquisition (M)

aptaph **Automatic processing for APT spectra (M)**

Syntax: `aptaph`

Description: Automatically phases APT spectra.

See also: *NMR Spectroscopy User Guide*

Related: `Apt` Set up parameters for APT pulse sequence (M)

array **Easy entry of linearly spaced array values (M)**

Syntax: `array<(parameter<, number_steps, start, step_size)>`

Description: Arrays a parameter to the number of steps, starting value and step size given by the user. All values of the array will satisfy the limits of the parameter.

If `array` is typed with none or only some of its arguments, you enter an interactive mode in which you are asked for the missing values.

Arguments: `parameter` is the name of the parameter to be arrayed. The default is an interactive mode in which you are prompted for the parameter. Only numeric parameters can be arrayed.

`number_steps` is the number of values of the parameter. The default is an interactive mode in which you are prompted for the number of steps.

`start` is the starting value of the parameter array. The default is an interactive mode in which you are prompted for the starting value.

`step_size` is the magnitude of the difference between elements in the array. The default is an interactive mode in which you are prompted for the step size.

Examples: `array`
`array('pw')`
`array('tof', 40, 1400, -50)`

See also: *NMR Spectroscopy User Guide*

array

Parameter order and precedence (P)

Description: Whenever an array of one or more parameters is set up, the string parameter `array` tells the system the name of the parameter or parameters that are arrayed and the order and precedence in which the arraying is to take place. The parameter `array` is automatically updated when acquisition parameters are set. “Diagonal arrays” (those corresponding to using parentheses in the parameter `array`) must be entered by hand.

Values: `' '` (two single quotes with no space between) indicates no parameter is arrayed.

`'x'` indicates the parameter `x` is arrayed.

`'x, y'` indicates the parameters `x` and `y` are arrayed, with `y` taking precedence. That is, the order of the experiments is $x_1y_1, x_1y_2, \dots, x_1y_n, x_2y_1, x_2y_2, \dots, x_2y_n, \dots, x_my_n$, with a total of $m \times n$ experiments being performed.

`'y, x'` indicates the parameters `x` and `y` are arrayed, with `x` taking precedence. That is, the order of the experiments is $x_1y_1, x_2y_1, \dots, x_ny_1, x_1y_2, x_2y_2, \dots, x_my_2, \dots, x_my_n$, with total of $m \times n$ experiments being performed.

`'(x, y)'` indicates the parameters `x` and `y` are jointly arrayed. The number of elements of the parameters `x` and `y` must be identical, and the order of experiments is $x_1y_1, x_2y_2, \dots, x_ny_n$, with `n` experiments being performed.

Joint arrays can have up to 10 parameters. Regular multiple arrays can have up to 20 parameters, with each parameter being either a simple parameter or a diagonal array. The total number of elements in all arrays can be $2^{32}-1$.

See also: *NMR Spectroscopy User Guide*

Related: `array` Easy entry of linearly spaced array values (M)

arraydim

Dimension of experiment (P)

Description: After `calcdim` calculates the dimension of an experiment, the result is put into the parameter `arraydim`. If an experiment is arrayed, `arraydim` is the product of the size of the arrays.

See also: *NMR Spectroscopy User Guide*

Related: `calcdim` Calculate dimension of experiment (C)
`celem` Completed FID elements (P)

A

asin Find arc sine of number (C)

Syntax: `asin (value) <:n>`

Description: Finds the arc sine (also called the inverse sine) of a number.

Arguments: `value` is a number in the range of ± 1.0 .

`n` is a return argument giving the arc sine, in radians, of `value`. The default is to display the arc sine value in the status window.

Examples: `asin(.5)`
`asin(val):asin_val`

See also: *VnmrJ User Programming*

Related: `sin` Find sine value of an angle (C)

asize Make plot resolution along f_1 and f_2 the same (M)

Syntax: `asize`

Description: Adjusts the 2D display parameters (`sc`, `wc`, `sc2`, and `wc2`) so that the displayed resolution along both f_1 and f_2 is the same. It is not suggested for heteronuclear experiments where the chemical shift spread of one nucleus is much greater than that of the other.

See also: *NMR Spectroscopy User Guide*

Related: `sc` Start of chart (P)
`sc2` Start of chart in second direction (P)
`wc` Width of chart (P)
`wc2` Width of chart in second direction (P)

assign Assign transitions to experimental lines (M)

Syntax: (1) `assign('mark') >`
 (2) `assign(transition_number,line_number)`

Description: Assigns the nearest calculated transition to the lines from a `d11` or `n11` listing after `spin11` has placed them in `slfreq`. All lines may not be assigned and transitions must be greater than `sth`. The next `spins('iterate')` determines new parameters to minimize the differences in position of the assigned pairs.

Arguments: `'mark'` makes assign use the lines selected with the mark button in place of `d11`. The results of the `mark` operation are stored in the file `mark1d.out`, which is cleared by the command `mark('reset')`.

`transition_number` is a single calculated transition number that is assigned to a line from the `d11` listing.

`line_number` is the index of the line from the `d11` listing. Setting `line_number=0` removes an assignment from a calculated transition.

Examples: `assign`
`assign('mark')`
`assign(4,0)`

See also: *NMR Spectroscopy User Guide*

Related: `d11` Display listed line frequencies and intensities (C)
`mark` Determine intensity of the spectrum at a point (C)
`n11` Find line frequencies and intensities (C)
`slfreq` Measured line frequencies (P)
`spin11` Set up `slfreq` array (M)

`spins` Perform spin simulation calculation (C)
`sth` Minimum intensity threshold (P)

at Acquisition time (P)

Description: Length of time during which each FID is acquired. Since the sampling rate is determined by the spectral width `sw`, the total number of data points to be acquired ($2 * sw * at$) is automatically determined and displayed as the parameter `np`. `at` can be entered indirectly by using the parameter `np`.

Values: Number, in seconds. A value that gives a number of data points that is not a multiple of 2 is readjusted automatically to be a multiple of 2.

See also: *NMR Spectroscopy User Guide; VnmrJ User Programming*

Related: `np` Number of data points (P)
`sw` Spectral width in directly detected dimension (P)

atan Find arc tangent of a number (C)

Syntax: `atan(value) <:n>`

Description: Finds the arc tangent (also called the inverse tangent) of a number.

Arguments: `value` is a number between $\pi/2$ and $-\pi/2$.
`n` is a return argument giving the arc tangent, in radians, of `value`. The default is to display the arc tangent value in the status window.

Examples: `atan(.5)`
`atan(val):atan_val`

See also: *VnmrJ User Programming*

Related: `sin` Find sine value of an angle (C)

atan2 Find arc tangent of two numbers (C)

Syntax: `atan2(y,x) <:n>`

Description: Finds the arc tangent (also called the inverse tangent) of the quotient of two numbers.

Arguments: `y` and `x` are two numbers, where the quotient y/x is between $\pi/2$ and $-\pi/2$ and `x` is not equal to zero.
`n` is a return argument giving the arc tangent, in radians, of y/x . The default is to display the arc tangent value in the status window.

Examples: `atan2(1,2)`
`atan2(val):atan2_val`

See also: *VnmrJ User Programming*

Related: `sin` Find sine value of an angle (C)

atcmd Call a macro at a specified time (M)

Description: `atcmd(<('macro')><,'timespec'><,'day'><,'cancel'>)>`

Syntax: Calls a macro at the specified time. It only functions on a spectrometer. A background VnmrJ is started to execute the command. This background VnmrJ is not started in an experiment; therefore, the macro executes a `jexp` or runs commands or macros that do not need experiment parameters. It will have access to global and system global parameters.

Arguments: When called with arguments, `atcmd` updates the database with the supplied information. It does not start the process that calls the macros at the specified times. `atcmd` with no arguments starts the program that calls the macros at the specified times.

`timespec` -- has the format `hh:mm <mon tue wed thur fri sat sun>` A 24 hour clock is used -- midnight is 0:0, noon is 12:00.

`day` -- If the optional `day` field is used, the command will be repeated on that day at the appointed time. The day fields are case insensitive. For `monday`, `wednesday`, and `friday` only a single character is needed. More can be used. For `tuesday`, `thursday`, `saturday`, and `sunday`, at least two characters must be given.

`cancel` -- If the `cancel` argument is given, it will cancel all the commands that match the supplied macro. For example, if you specify `cmda` to be run at 8:00 on `mon` and 9:00 on `tue`, then `atcmd('cancel', 'cmda')` will cancel both of them. If the macro is `' '`, the cancel option will cancel all `atcmd` macros.

`list` -- The `list` argument lists the `timespec` for all the `atcmds` that match the supplied macro. If the macro is `' '`, the `list` option lists all of the `atcmd` macros and their `timespecs`. Optional arguments can be returned. The first is the number of `atcmds`. The macro and `timespec` for each `atcmd` can be returned.

When the command specified by `atcmd` is executed in background, it will be executed using the environment of the user who requested the `atcmd`. Also, the background `VnmrJ` will initially not be joined to a specific experiment.

Examples: `atcmd('echo(`good morning`)', '8:00 mon tue wed thu fri')`

Displays a welcome message every weekday at 8:00 am.

`atcmd('echo(`What are you doing here on a weekend?`)', '8:00 Sat Sun')`

Questions your intentions on the weekend.

`atcmd('startNightQueue', '22:00')`

Runs the macro `startNightQueue` at 22 hr. (10:00pm).

`atcmd('startNightQueue', 'cancel')`

Cancels the scheduled `startNightQueue` cmd

`atcmd(' ', 'cancel')`

Cancels all scheduled commands

`atcmd(' ', 'list')`

Lists all scheduled commands

atext Append string to current experiment text file (M)

Syntax: `atext(string)`

Description: Adds a line of text to the current experiment text file.

Arguments: `string` is a single line of text.

Examples: `atext('T1 Experiment')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>ctext</code>	Clear the text of the current experiment (C)
	<code>text</code>	Display text or set new text for current experiment (C)
	<code>write</code>	Write formatted text to a device (C)

attval Calculate pulse width (M)

Syntax: `attval (pw, tpwr)`

Description: Calculates the pulse width and B_1 field at every transmitter power. A low transmitter power should be used where the amplifier is not in compression. Calculation is not valid where amplifier is in compression.

Arguments: `pw` is the pulse width.
`tpwr` is the transmitter power.

Examples: `attval(7.0,59)`

atune ProTune Present (P)

Description: Hardware configuration parameter specifying if ProTune is or is not present. Parameter is set in the System Configuration window.

Arguments: `'y'` ProTune is present
`'n'` ProTune not is present

See also: *VnmrJ Installation and Administration*

Related: `wtune` Specify when to tune (P)
`tupwr` Transmitter power used in tuning (P)

au Submit experiment to acquisition and process data (M)

Syntax: `au(<'nocheck'><,<'next'><,<'wait'>>>`

Description: Performs the experiment described by the current acquisition parameters, checking the parameters `loc`, `spin`, `gain`, `wshim`, `load`, and `method` to determine the necessity to perform various actions in addition to simple data acquisition. This may involve a single FID or multiple FIDs, as in the case of arrays or 2D experiments. `au` causes the data to automatically be processed according to the following parameters:

- `wbs` specifies what happens after each block.
- `wnt` specifies what happens after each FID is collected.
- `wexp` specifies what happens when the entire acquisition is complete (which may involve several complete FIDs in the case of 1D arrays or 2D experiments).

Before starting the experiment, `au` executes the two user-created macros if they exist. The first is `usergo`, a macro that allows the user to set up general conditions for the experiment. The second is a macro whose name is formed by `go_` followed by the name of the pulse sequence (from `seqfil`) to be used (e.g., `go_s2pul`, `go_dept`). This macro allows a user to set up experiment conditions suited to a particular sequence.

Arguments: `'nocheck'` is a keyword to override checking if there is insufficient free disk space for the complete 1D or 2D FID data set to be acquired.

`'next'` is a keyword to put the experiment started with `au('next')` at the head of the queue of experiments to be submitted to acquisition.

`'wait'` is a keyword to stop submission of experiments to acquisition until `wexp` processing of the experiment, started with `au('wait')`, is finished.

Examples: `au`
`au('wait')`

See also: *NMR Spectroscopy User Guide*

Related: `auto_au` Controlling macro for automation (M)
`change` Submit a change sample experiment to acquisition (M)
`ga` Submit experiment to acquisition and FT the result (M)
`gain` Receiver gain (P)
`go` Submit experiment to acquisition (M)

A

<code>go_</code>	Pulse sequence setup macro called by <code>go</code> , <code>ga</code> , and <code>au</code> (M)
<code>load</code>	Load status of displayed shims (P)
<code>loc</code>	Location of sample in tray (P)
<code>lock</code>	Submit an Autolock experiment to acquisition (C)
<code>method</code>	Autoshim method (P)
<code>sample</code>	Submit change sample, Autoshim experiment to acquisition (M)
<code>seqfil</code>	Pulse sequence name (P)
<code>shim</code>	Submit an Autoshim experiment to acquisition (C)
<code>spin</code>	Submit a spin setup experiment to acquisition (C)
<code>spin</code>	Sample spin rate (P)
<code>su</code>	Submit a setup experiment to acquisition (M)
<code>usergo</code>	Experiment setup macro called by <code>go</code> , <code>ga</code> , and <code>au</code> (M)
<code>wbs</code>	Specify action when <code>bs</code> transients accumulate (C)
<code>wexp</code>	Specify action when experiment completes (C)
<code>wnt</code>	Specify action when <code>nt</code> transients accumulate (C)
<code>wshim</code>	Conditions when shimming is performed (P)

AuCALch3i Set up autocalibration with CH₃I sample (M)

Syntax: `AuCALch3i`

Description: Retrieves standard proton parameter set and setup for automatic calibration of proton (observe and decouple), carbon (observe and decouple), `gcal`, and C/H gradient ratio. The `AuCALch3i` macro is the same as the `AuCALch3i1` macro.

AuCALch3i1 Get autocalibration with CH₃I sample (M)

Syntax: `AuCALch3i1`

Description: Retrieves standard proton parameter set and setup for automatic calibration of proton (observe and decouple), carbon (observe and decouple), `gcal`, and C/H gradient ratio. The `AuCALch3i1` macro is the same as the `AuCALch3i` macro.

AuCALch3oh Set up autocalibration with Autotest sample (M)

Syntax: `AuCALch3oh`

Description: Retrieves standard proton parameter set and setup for automatic calibration of proton (observe), carbon (decouple), `gcal` and C/H gradient ratio. The `AuCALch3oh` macro is the same as the `AuCALch3oh1` macro.

AuCALch3oh1 Get autocalibration with Autotest sample (M)

Syntax: `AuCALch3oh1`

Description: Retrieves standard proton parameter set and setup for automatic calibration of proton (observe), carbon (decouple), `gcal` and C/H gradient ratio. The `AuCALch3oh1` macro is the same as the `AuCALch3oh` macro.

Aucalibz0 Automatic Hz to DAC calibration for Z0 (M)

Applicability: Autocalibration routine

Syntax: Called by `Augmapz0` calibration routine.

Description: Called by Augmapz0 calibration routine. Automatically calibrates lock frequency change per Z0 DAC unit change. The calibrated value is written out in the probe file as `1khzdac` parameter

See also: *System Administration*.

Related: `Augmapz0` Automatic lock gradient map generation and Z0 calibration (M)
`Aufindz0` Automatic adjustment of Z0 (M)

AuCdec Carbon decoupler calibration macro (M)

Syntax: AuCdec

Description: Used by `AuCALch3i` and `AuCALch3oh` autocalibration routines to do carbon decoupler calibrations. Calibrates high-power pulse widths and `dmf`.

See also: *System Administration*

Related: `AuCALch3i` Get autocalibration with CH₃I sample (M)
`AuCALch3oh` Get autocalibration with Autotest sample (M)
`dmf` Decoupler modulation frequency for first decoupler (P)

AuCgrad Carbon/proton gradient ratio calibration macro (M)

Syntax: AuCgrad

Description: Used by `AuCALch3i1` and `AuCALch3oh1` autocalibration routines for C/H gradient ratio calibrations.

See also: *System Administration*

Related: `AuCALch3i1` Get autocalibration with CH₃I sample (M)
`AuCALch3oh1` Get autocalibration with Autotest sample (M)

AuCobs Carbon observe calibration macro (M)

Syntax: AuCobs

Description: Used by `AuCALch3i1` autocalibration routines for carbon observe calibrations.

See also: *System Administration*

Related: `AuCALch3i1` Get autocalibration with CH₃I sample (M)

audiofilter Audio filter board type (P)

Description: Sets the type of audio filter board used where the spectral width (`sw`) is less than 100 kHz. The filter type is set in the Spectrometer Configuration window (opened from `config`) using the label Audio Filter Type.

Values: 'b' indicates the system has a 100-kHz Butterworth filter board (100 kHz Butterworth choice in the Spectrometer Configuration window).

'e' indicates the system has a 100-kHz elliptical filter board (100 kHz Elliptical choice in the Spectrometer Configuration window).

'2' indicates the system has a 200-kHz Butterworth filter board (200 kHz Butterworth choice in the Spectrometer Configuration window).

'5' indicates the system has a 500-kHz elliptical filter board (500 kHz Elliptical choice in the Spectrometer Configuration window).

See also: *System Administration*

Related: `config` Display current configuration and possibly change it (M)
`sw` Spectral width in directly detected dimension (P)

A

Aufindz0 Automatic adjustment of Z0 (M)

Syntax: Aufindz0

Description: Finds z0 by doing lock 1D spectrum. The frequency is then used along with the `lkhzdac` value in the probe file to calculate the z0 value for a given solvent and autolocking is done. This requires previous calibration of the `hzdac` value done using the [Aucalibz0](#) macro.

See also: *System Administration*

Related: [Aucalibz0](#) Automatic Hz to DAC calibration for Z0 (M)

Augcal Probe gcal calibration macro (M)

Syntax: Augcal

Description: Used by [AuCALch3i1](#) and [AuCALch3oh1](#) autocalibration routines for probe [gcal](#) calibrations.

See also: *System Administration*

Related: [AuCALch3i1](#) Get autocalibration with CH₃I sample (M)
[AuCALch3oh1](#) Get autocalibration with Autotest sample (M)
[gcal](#) Gradient calibration constant (P)

Augmap Automated gradient map generation (M)

Syntax: Augmap

Description: Automatically adjusts gradient level, offset, window, and pulse width to generate a z1–z4 gradient map using a 2-Hz D₂O sample. This macro is used by the [Aumakegmap](#) auto gradient map generation macro and is applicable only for a lock gradient map.

See also: *System Administration*

Related: [Aumakegmap](#) Auto lock gradient map generation (M)
[gsize](#) Number of z-axis shims used by gradient shimming (P)

Augmapz0 Automatic lock gradient map generation and z0 calibration (M)

Syntax: Augmapz0

Description: Using the 2-Hz D₂O sample, the `augmapz0` macro automatically creates a lock gradient map, followed by Hz to DAC calibration of Z0 for the autolocking procedure.

See also: *System Administration*

Related: [Aucalibz0](#) Automatic Hz to DAC calibration for Z0 (M)
[Aufindz0](#) Automatic adjustment of Z0 (M)

AuHdec Proton decoupler calibration (M)

Syntax: AuHdec

Description: Used by [AuCALch3i](#) autocalibration routine to do proton decoupler calibrations. Calibrates high-power pulse widths and [dmf](#).

See also: *System Administration*

Related: [AuCALch3i](#) Get autocalibration with CH₃I sample (M)
[dmf](#) Decoupler modulation frequency for first decoupler (P)

- AuHobs** **Proton observe calibration macro (M)**
 Syntax: AuHobs
 Description: Used by [AuCALch3i](#) and [AuCALch3oh](#) autocalibration routines for proton observe calibrations.
- Aumakegmap** **Auto lock gradient map generation (M)**
 Syntax: Aumakegmap (<lk or hs or H1>)
 Description: Generates z1–z4 lock gradient ('lk' argument), lock homospoil ('hs' argument), or ¹H gradient map ('H1' argument). If no argument is given, the defaults is 'lk', if gradtype='nnh' to 'hs'. The doped 2-Hz D₂O should be used for hs and lk maps. H1 map is typically done on the sample. Automatically adjusts gradient level, offset, window, and pulse width. The map name is automatically stored in the probe file.
- AuNuc** **Get parameters for a given nucleus (M)**
 Syntax: AuNuc (nucleus, solvent)
 Description: Retrieves standard parameter set for a given nucleus and adds all required parameters for Tcl/dg driven parameters. If no parameter set exists in stdpar, then carbon parameters are retrieved and tn changed.
- auto** **Prepare for an automation run (C)**
 Applicability: Systems with an automatic sample changer.
 Syntax: auto<(automation_directory)>
 Description: Prepares the automation directory for an automation run. auto aborts if the spectrometer is already in automation mode.
 Arguments: automation_directory is the name of the automation directory, either an absolute UNIX path (i.e. the first character is a "/") or a relative path (the first character is not a "/"). The default is the value of the parameter [autodir](#). If for some reason [autodir](#) is not defined, you are prompted to provide the location of the automation directory. If not given as an argument, you are prompted for the path. If the automation directory is not present, it is created with full access for all users. auto aborts if it fails to create this directory.
 Examples: auto
 auto ('/home/vnmr1/autorun_620')
 See also: *NMR Spectroscopy User Guide*, *VnmrJ User Programming*, *VnmrJ Walkup*
 Related: [auto_au](#) Controlling macro for automation (M)
 [autodir](#) Automation directory absolute pathname (P)
 [autogo](#) Start an automation run (C)
 [autoname](#) Prefix for automation data file (P)
- auto** **Automation mode active (P)**
 Applicability: Systems with an automatic sample changer.
 Description: A global variable that shows whether or not an automation run is in progress. Macros typically test this parameter because actions can differ between the automation and non-automation modes. The value of auto is not enterable by the user. An automation experiment is initiated with the [autogo](#) command. The auto parameter is only set to 'y' for those macros and commands that are run as part of an automation experiment.

Values: 'y' indicates automation mode is active.

'n' indicates automation mode is inactive

See also: *NMR Spectroscopy User Guide, VnmrJ User Programming, VnmrJ Walkup.*

Related: **auto_au** Controlling macro for automation (M)
autogo Start an automation run (C)
autora Resume suspended automation run (C)
autosu Suspend current automation run (C)

auto_au Controlling macro for automation (M)

Applicability: Systems with an automatic sample changer.

Syntax: auto_au

Description: Reads sampleinfo file (defines an automation experiment) using the **lookup** facility, sets the **solvent** and **loc** parameters based on the SOLVENT and SAMPLE# fields of sampleinfo, runs **exec** on the entry in the MACRO field, and writes the experiment text based on the TEXT field. After that, auto_au examines the value of the **wexp** parameter:

- If **wexp** is set to 'procplot', then auto_au calls **au**.
- If **wexp** is set to 'autolist', then auto_au inserts 'auto' as the first argument to **autolist** and calls **au('wait')**.
- If **wexp** is set to anything else, auto_au does not call **au**.

If no data is generated from the requested MACRO field, due to an error or some other reason, auto_au sets the STATUS field to "No Data Requested."

auto_au is used only during automation and should not be called directly. It provides a starting point for all automation experiments. As such, it is a convenient point for user customization of automation.

See also: *NMR Spectroscopy User Guide, VnmrJ User Programming, VnmrJ Walkup*

Related: **au** Submit experiment to acquisition and process data (M)
auto Prepare for an automation run (C)
autolist Set up and start chained acquisition (M)
exec Execute a VnmrJ command (C)
loc Location of sample in tray (P)
lookup Look up words and lines from a text file (C)
solvent Lock solvent (P)
wexp When experiment completes (P)

Autobackup Back up current probe file (M)

Syntax: Autobackup

Description: Makes a copy of the probe file before starting the calibrations and prints the current calibration file. Autobackup is called by the autocalibration routines **AuCALch3i1** and **AuCALch3oh1**

autodept Automated complete analysis of DEPT data (M)

Syntax: autodept

Description: Processes DEPT spectra, plots the unedited spectra, edits the spectra, plots the edited spectra, and prints out editing information.

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related:	<code>adept</code>	Automatic DEPT analysis and spectrum editing (C)
	<code>Dept</code>	Set up parameters for DEPT experiment
	<code>deptproc</code>	Process DEPT data (M)
	<code>padept</code>	Perform adept analysis and plot resulting spectra (C)
	<code>pldept</code>	Plot DEPT data, edited or unedited (M)

autodir Automation directory absolute path (P)

Applicability: Systems with an automatic sample changer or LC-NMR accessory.

Description: When using a sample changer, `autodir` is a global variable that holds the absolute path of the currently active automation directory. When VnmrJ is started, `autodir` is set to the absolute path of the last automation run.

When using the LC-NMR accessory, `autodir` specifies a directory in which experiments using a stored queue are saved.

See also: *NMR Spectroscopy User Guide*

Related:	<code>auto</code>	Set up an automation directory (C)
	<code>autoname</code>	Prefix for automation data file (P)
	<code>globalauto</code>	Automation directory name (P)
	<code>walkup</code>	Walkup automation (M)

autogo Start automation run (C)

Applicability: Systems with an automatic sample changer.

Syntax: `autogo<(file<, automation_directory>)>`

Description: Starts an automation run. The `autogo` parameter cannot be entered while the spectrometer is in automation mode. You must have an `enter` queue prepared to start an automation run. The queue is checked to verify that it was prepared using the `enter` command (`autogo` aborts if an error in the format is found.) Your automation directory is also checked for the presence of a non-empty `enter` queue (`autogo` aborts if the current queue in the automation directory is present and not empty). Finally, `autogo` checks the automation directory and runs the `auto` command if this directory is not present or another problem is found. When `autogo` completes, the system is in automation mode and your automation run starts.

Arguments: `file` is the file name of your `enter` queue. The default is that the system prompts you for the location of the `enter` queue.

`automation_directory` is the pathname of the automation directory. The default is the current value of the parameter `autodir`.

Examples: `autogo`
`autogo('MySamples')`
`autogo('MySamples', '/home/vnmr1/AutoRun_621')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>auto</code>	Set up an automation directory (C)
	<code>autodir</code>	Automation directory absolute path (P)
	<code>autoname</code>	Prefix for automation data file (P)
	<code>enter</code>	Enter sample information for automation run (C)

autolist Set up and start chained acquisition (M)

Syntax: `autolist(<options,>experiment1<, experiment2<, ...>)`

Description: Sets up parameters for chained experiments by executing the experiments given as arguments and then starting a chained acquisition. Note that the macro **au** is executed as part of **autolist** and should not be included in the arguments to **autolist**.

Arguments: **options** is one or more of the following keywords:

- 'auto' is a keyword to add 'wait' to the **au** call (e.g., `au('wait', 'next')`).
- 'start' is a keyword to make the first experiment in the list as one that needs to be acquired rather than processed.

experiment1, **experiment2**, ... are experiments written as strings (e.g., 'dept' or 'c13'). **experiment1** is the current experiment and, when it finishes, the macro **procplot** is called to process the data. If **experiment2** is listed, that experiment is executed and then the macro **au('next')** is performed. For subsequent experiments, the text, **solvent** and **temp** are used from the preceding experiment. Also, the **wexp** parameter is reset to 'autolist' with the first experiment removed.

Examples: `autolist('h1', 'c13', 'dept')`
`autolist('h1', 'hcosy')`

See also: *NMR Spectroscopy User Guide*

Related:	auto_au	Controlling macro for automation (M)
	au	Submit experiment to acquisition and process data (M)
	hc	Automated proton and carbon acquisition (M)
	hcapt	Automated proton, carbon, and APT acquisition (M)
	hccorr	Automated proton, carbon, and HETCOR acquisition (M)
	hcosy	Automated proton and COSY acquisition (M)
	procplot	Automatically process FIDs (M)
	solvent	Lock solvent (P)
	temp	Sample temperature (P)
	wexp	When experiment completes (P)

autoname **Create path for data storage (C)**

Applicability: Automation

Syntax: `autoname:$path`
`autoname(name_template):$path`
`autoname(name_template,sample_info_file):$path`
`autoname(name_template,sample_info_file,`
`<'keepspace'|'replacespace'):$path`
`autoname(name_template,sample_info_file,`
`<,'excluded_suffixes'<,'keepspace'|'replace`
`space'):$path`

Description: The **autoname** command determines the path for data storage during an automation run and uses the value of a naming template (the **autoname** parameter by default) and the contents of a sample info file (default is **sampleinfo** in the current experiment) to determine this path. The path name is stored in the return argument or displayed on line 3 if no return argument is present.

The name is prefaced with using the value of the parameter **autodir** or **userdir**+ '/data/' if **autodir** is equal to ''.

The default **excluded_suffix** is **.fid**.

Arguments: No argument provided. The command uses the default **autoname** parameter and **sampleinfo** in the current experiment directory for the path to the

sample info file. If the autoname parameter does not exist or is set to "", the default template is %SAMPLE#: %%PEAK#: %.

name_template (no quotes) is string that contains keywords separated by substitution specifiers to represent the data storage path. Substitution specifiers in this template are either a percent sign (%) or a dollar sign (\$). The keywords are obtained from the sample_info_file file, if it exists, using % substitution specifiers or VNMR parameters using \$ substitution specifiers.

A template is passed directly using:

```
autoname ('$owner$/$sample$') : $path.
```

Percent sign (%) substitution specifier is used with the autoname command to scan the sample_info_file for the text specific by keyword between the first percent sign in the template string and the next percent sign. The text specified by the keyword between the % substitution specifiers is passed to \$path.

The following percent substitutions (% keywords) for time and date are obtained from the system clock, not from the sample info file:

<i>Keyword</i>	<i>Format</i>	<i>Description</i>
%DATE%	YYYYMMDD	4 digit year 2 digit month 2 digit day
%TIME%	HHMMSS	2 digit each for hours, minutes, and seconds
%YR%	YYYY	4-digit year
%YR2%	YY	2-digit year
%MO%	MM	2-digit month
%DAY%	DD	2-digit day
%HR%	HH	2-digit hour
%MIN%	MM	2-digit month
%SEC%	SS	2-digit second

The following are some of the percent substitutions (% keywords) are obtained from the second argument, sample_info_file.

<i>Keyword</i>	<i>Description</i>
%USER%	user name
%MACRO%	macro name
%SAMPLE%	sample name
%SOLVENT%	solvent name

String parameters cannot not contain any of the following characters: ' ', '!', '"', '\$', '&', '\', ", '(', ')', '*', ';', '<', '>', '?', '\\', '[', ']', '^', '~', '{', '}', '|', ':', '\0'

Version number is specified by %Rn% where n is an integer from 0 to 9 (default 2), as follows:

<i>n=</i>	<i>Description</i>
0	no revision digits are appended (all names must be uniquely constructed without these revision digits).
1 to 9	revision number is padded with leading zeroes to form an n-digit number. If more places are needed than specified, more zeroes are used.

>9 (more than one digit)	Rnn is still used as a search string in the sampleinfo file. %Rn% must be specified at the end of the name_template string. The revision digits are always appended except if %R0% is used.
no %Rn%	default of %R2% is used

Specify the starting number to be used when constructing the version number by appending a colon : and start number after Rn.

The default starting value is 1. A zero is not allowed.

Dollar sign (\$) substitution specifiers works in manner analogous to the percent substitution specifier, except that the text between the dollar signs is interpreted as the name of a VNMR parameter. The value of this parameter is substituted for the substitution specifier.

Numeric parameters are represented as a string and truncated to an integer value. The template, pw=\$pw\$usec, with vnmr parameter pw having a value of 12.3 produces pw=12usec01 which is appended to .fid and passed to \$path. The 01 following usec is added by the %R2% default setting.

sample_info_file (no quotes) is the name of a text file to read for the % substitutions passed to autoname. The file must exist.

Using the keyword 'replacespaces' uses underscores (_) in place of spaces ' ' in the resulting path name or the keyword 'keepspace' retains spaces in the resulting path name.

The keyword, 'keepspace' or 'replacespaces' is an optional argument (includes quotes). The argument is accepted as the third or fourth argument.

Solaris and Linux operating systems default to replacespaces.

A comma separated list of excluded suffixes the new path name will not use or match is specified if the third keyword is not 'keepspace' or 'replacespaces'.

Examples: Using a \$ substitution specifier:

```
autoname (pw=$pw$usec) : $path
```

A \$ substitution specifier, pw=\$pw\$usec, is the name_template and a relative path. The vnmr parameter, pw, has a value of 12.3 and the resulting filename is: pw=12usec01.fid. The path name is prefaced with the value of the parameter autmdir if the name template generates a relative pathname.

Examples: Using \$ substitution specifiers and a comma separated list of suffixes:

```
autoname ('$seqfil$_$tn$_', '/vnmr/
conpar', '.img') : $path
```

The \$ substitution specifier is; \$seqfil\$_\$tn\$_ the dummy info filename is; '/vnmr/conpar', and the comma separated list of excluded suffixes is .img. The path name is prefaced with seqfil_tn_index. Each time a file is written to the directory the command changes the index by one (see %Rn% above). The suffix is both .fid and .img. The file is named gems_H1_03.img if target directory contains gems_H1_01.fid and gems_H1_02.img.

See also: *NMR Spectroscopy User Guide, VnmrJ User Programming, VnmrJ Walkup*

Related:	autoname	Temple determining the path where is data stored (P)
	svfname	Determines the name used to store data (C)
	svfname	Specifies the filename template (P)

autoname **Prefix for automation data file (P)**

Applicability: Automation

Description: The `autoname` template determines the resulting path where the data is stored for an entry in the automation run and uses the contents of a sample info file (the name by default is "sampleinfo" in the current experiment) to determine this path. The path name is stored in the return argument and displayed on line 3 if no return argument is present.

See also: *NMR Spectroscopy User Guide*, *VnmrJ User Programming*, *VnmrJ Walkup*

Related: `autoname` Determines path for data storage during an automation run (C).

autora Resume suspended automation run (C)

Applicability: Systems with an automatic sample changer.

Syntax: `autora`

Description: Resumes a previously suspended automation run. No matter what caused the interruption (including `autosca`, power failure, or system boot-up), the system examines the condition of the automation file and resumes acquisition for all experiments that have not finished. If `autora` is executed while an automation run is in progress, it has no effect.

See also: *NMR Spectroscopy User Guide*

Related: `autosca` Suspend current automation run (C)

autosca Suspend current automation run (C)

Applicability: Systems with an automatic sample changer.

Syntax: `autosca`

Description: Suspends the automation mode at the conclusion of the current experiment and changes the system to the manual mode. The currently running experiment is not interrupted.

See also: *NMR Spectroscopy User Guide*

Related: `autora` Resume suspended automation run (C)

autoscale Resume autoscaling after limits set by scalelimits macro (M)

Syntax: `autoscale`

Description: Returns to autoscaling in which the scale limits are determined by the `expl` command such that all the data in the `expl` input file is displayed.

See also: *NMR Spectroscopy User Guide*

Related: `expl` Display exponential or polynomial curves (C)
`scalelimits` Set limits for scales in regression (M)

autostack Automatic stacking for processing and plotting arrays (M)

Syntax: `autostack`

Description: When processing and plotting arrayed 1D spectra, VnmrJ automatically determines whether the stacking mode is horizontal, vertical or diagonal from the number of traces and the number of lines in the spectrum. If this automatic function is not desirable (or makes an undesirable decision), it can be overridden by placing the `stack` macro in the experiment startup macro or by calling `stack` before processing (or reprocessing) a spectrum. `autostack` switches back to automatic determination of the stack mode by destroying the `stackmode` parameter.

See also: *NMR Spectroscopy User Guide*

Related: **proarray** Process arrayed 1D spectra (M)
plarray Plot arrayed 1D spectra (M)
stack Fix stacking mode for processing / plotting arrayed spectra (M)
stackmode Stacking control for processing (P)

autotest Open Auto Test Window (C)

Syntax: `autotest`

Description: Opens the Auto Test window.

See also: *AutoTest Software* manual.

autotime Displays approximate time for automation (M)

Syntax: `autotime (<automation directory>)`

Description: Displays approximate time for each experiment and for each location in an automation run. If no argument is given, time is calculated for the current automation run (`enterQ`).

See also: *NMR Spectroscopy User Guide*

Related: **explist** Display approximate time for current experiment chain (M)

av Set abs. value mode in directly detected dimension (C)

Syntax: `av`

Description: Selects the absolute-value spectra display mode by setting the parameter **dmg** to the string value 'av'. In the *absolute-value display mode*, each real point in the displayed spectrum is calculated as the square root of the sum of the squares of the real and imaginary points comprising each respective complex data point. All information, including noise, is always positive, and the relationship between signal and noise is linear.

For multidimensional data, `av` has no effect on data prior to the second Fourier transform. If **pmode** = 'full', `av` acts in concert with commands **ph1**, **av1**, or **pwrl** to yield the resultant contour display for the 2D data.

See also: *NMR Spectroscopy User Guide*

Related: **av1** Set abs. value mode in 1st indirectly detected dimension (C)
av2 Set abs. value mode in 2nd indirectly detected dimension (C)
dmg Display mode in directly detected dimension (C)
dmgfi Absolute-value display of FID data or spectrum in `acqi` (P)
ft Fourier transform 1D data (C)
ft1d Fourier transform along f_2 dimension (C)
ft2d Fourier transform 2D data (C)
pa Set phase angle mode in directly detected dimension (C)
pa1 Set phase angle mode in 1st indirectly detected dimension (C)
ph Set phased mode in directly detected dimension (C)
ph1 Set phased mode in 1st indirectly detected dimension (C)
pmode Processing mode for 2D data (P)
pwrl Set power mode in 1st indirectly detected dimension (C)
wft Weigh and Fourier transform 1D data (C)
wft1d Weigh and Fourier transform of 2D data (C)
wft2d Weigh and Fourier transform 2D data (C)

av1 Set abs. value mode in 1st indirectly detected dimension (C)Syntax: `av1`

Description: Selects the absolute-value spectra display mode along the first indirectly detected dimension by setting the parameter `dmg1` to the value 'av1'. If the parameter `dmg1` does not exist, `av1` creates it and set it to 'av1'.

In the *absolute-value display mode*, each real point in the displayed trace is calculated as the square root of the sum of the squares of the real and imaginary points comprising each respective complex data point. For hypercomplex data, the real-real and imaginary-real points from each respective hypercomplex data point are used in the summation. In this mode, all information, including noise, is always positive; and the relationship between signal and noise is linear.

The `av1` command is only needed if mixed-mode display is desired. If the parameter `dmg1` does not exist or is set to the null string, the display mode along the first indirectly detected dimension defaults to the display mode of the directly detected dimension (characterized by the parameter `dmg`). For the contour display of multidimensional data, the result of `av1` is the same as for traces provided that `pmode='partial'` or `pmode=' '` (two single quotes with no space between).

See also: *NMR Spectroscopy User Guide*

Related: `av` Set abs. value mode in directly detected dimension (C)
`dmg1` Data display mode in 1st indirectly detected dimension (P)

av2 Set abs. value mode in 2nd indirectly detected dimension (C)Syntax: `av2`

Description: Selects absolute-value spectra display mode for the second indirectly detected dimension by setting the parameter `dmg2` to the value 'av2'. If `dmg2` does not exist or is set to the null string, `av2` creates `dmg2` and set it equal to 'av2'.

In the *absolute-value display mode*, all information, including noise, is positive; and the relationship between signal and noise is linear. Each real point in the displayed trace is calculated as the square root of the sum of the squares of the real and imaginary points comprising each respective complex data point. For hypercomplex data, the real-real and imaginary-real points from each respective hypercomplex data point are used in the summation.

The `av2` command is only needed if mixed-mode display is desired. If the parameter `dmg2` does not exist or is set to the null string, the display mode along the second indirectly detected dimension defaults to the display mode of the directly detected dimension (characterized by the parameter `dmg`). For the contour display of multidimensional data, the result of `av2` is the same as for traces provided that `pmode='partial'` or `pmode=' '` (two single quotes with no space between).

See also: *NMR Spectroscopy User Guide*

Related: `av` Set abs. value mode in directly detected dimension (C)
`dmg2` Data display mode in 2nd indirectly detected dimension (P)

averag Calculate average and standard deviation of input (C)Syntax: `averag(number1,number2,...):average,sd,
number_arguments,sum_numbers,sum_squares`

Description: Finds average, standard deviation, and other characteristics of a set of numbers.

Arguments: `number1,number2,...` is a finite set of numbers.

`average` is the average of the numbers.

`sd` is the standard deviation of the numbers.

`number_arguments` is the number of `number1, number2, ...` arguments.

`sum_numbers` is the sum of the numbers

`sum_squares` is the sum of squares of the numbers.

Examples: `averag(3.4, 4.3, 3.5, 5.4) : r1, r2`

See also: *VnmrJ User Programming*

awc

Additive weighting const. in directly detected dimension (P)

Description: Adds the current value of `awc` to each value of the weighting function along the directly detected dimension. This dimension is often referred to as the f_2 dimension in 2D data sets, the f_3 dimension in 3D data sets, and so forth. `awc` is applied *after* the sinebell and exponential function, but *before* the Gaussian function. This allows using `gf` as a Gaussian apodization even when `awc` is non-zero. Typical value of `awc` is 'n'.

See also: *NMR Spectroscopy User Guide*

Related: `awc1` Additive weighting const. in 1st indirectly detected dimension (P)
`awc2` Additive weighting const. in 2nd indirectly detected dim. (P)
`gf` Gaussian function in directly detected dimension (P)

awc1

Additive weighting const. in 1st indirectly detected dimension (P)

Description: Adds the current value of `awc1` to each value of the weighting function along the first indirectly detected dimension. This dimension is often referred to as the f_1 dimension of a multidimensional data set. `awc1` is analogous to the parameter `awc`. The “conventional” parameters (`lb`, `gf`, etc.) operate on the detected FIDs, while this “2D” parameter is used during processing of the interferograms.

See also: *NMR Spectroscopy User Guide*

Related: `awc` Additive weighting const. in directly detected dimension (P)

awc2

Additive weighting const. in 2nd indirectly detected dimension (P)

Description: Adds the current value of `awc2` to each value of the weighting function along the second indirectly detected dimension. This dimension is often referred to as the f_2 dimension of a multidimensional data set. `awc2` is analogous to the parameter `awc`. The value of `awc2` can be set with `wti` on the 2D interferogram data.

See also: *NMR Spectroscopy User Guide*

Related: `awc` Additive weighting const. in directly detected dimension (P)
`wti` Interactive weighting (C)

axis

Provide axis labels and scaling factors (C)

Syntax: `axis('fn' | 'fn1' | 'fn2')`
`<:$axis_label,$freq_scaling,$scaling_factor>`

Description: Displays or returns values of the axis labels and scaling factors to the calling macro. See the macro `r1` for an example of using this command.

Arguments: `'fn' | 'fn1' | 'fn2'` is the Fourier number parameter for the axis of interest.

`$axis_label` is the axis label (e.g., ppm, kHz, cm, or ppm(sc)).

`$freq_scaling` is the divisor needed to convert from units of Hz to the units defined by the `axis` parameter with any scaling. `axis` uses the current value

of the **axis** parameter for that dimension and also checks for axis scaling using the corresponding **scalesw**, **scalesw1**, or **scalesw2** parameter.

\$scaling_factor is a second scaling factor, determined solely by the **scalesw** type of parameter. This last scaling factor is independent of the value of the **axis** parameter.

Examples: `axis('fn')`
`axis('fn1'):$lab,$fr,$scl`

See also: *VnmrJ User Programming*

Related:	axis	Axis label for displays and plots (P)
	rl	Set reference line (M)
	scalesw	Scale spectral width in directly detected dimension (P)
	scalesw1	Scale spectral width in 1st indirectly detected dimension (P)
	scalesw2	Scale spectral width in 2nd indirectly detected dimension (P)

axis **Axis label for displays and plots (P)**

Applicability: Certain arguments work only if system has the proper hardware.

Description: Specifies the units for the axis display and plot.

For 1D experiments, **axis** uses a single letter that includes 'h' for Hz, 'p' for ppm, and 'k' for kHz (e.g., **axis**='h').

For 2D experiments, **axis** uses two letters, with the first letter describing the detected spectral axis (f_2), and the second letter describing the indirectly detected axis (f_1). Thus **axis**='ph' is appropriate for a homonuclear 2D-J experiment, with a referenced ppm scale along the spectral axis and an axis in Hz ('h') along the J-axis. **axis**='pp' is appropriate for COSY or NOESY experiments.

For 3D experiments, **axis** uses three letters with the first letter describing the detected spectral axis (f_3), the second letter describing the first indirectly detected axis (f_1), and the third letter specifying the second indirectly detected axis (f_2).

The special letter d is used to reference the indirectly detected axis to the parts per million of the decoupler channel, as appropriate for heteronuclear chemical shift correlation experiments, which would typically have **axis**='pd'. The letter n is used to suppress the axis display on one or both axes (e.g., **axis**='nn', **axis**='pn').

For systems with multiple decouplers, the characters '1', '2', and '3' can be used to reference an axis relative to the frequency of that decoupler. Setting **axis**='p1' is effectively the same as **axis**='pd'.

Values: '1' sets the axis label for units of ppm relative to the first decoupler.
 '2' sets the axis label for units of ppm relative to the second decoupler.
 '3' sets the axis label for units of ppm relative to the third decoupler.
 'c' sets the axis label for units of centimeters.
 'd' sets the axis label for units of ppm relative to the first decoupler.
 'h' sets the axis label for units of hertz.
 'k' sets the axis label for units of kilohertz.
 'm' sets the axis label for units of millimeters.
 'n' sets no axis label display.
 'p' sets the axis label for units of ppm relative to the observe transmitter.
 'u' sets the axis label for units of micrometers.

See also: *NMR Spectroscopy User Guide*

Related:	axis	Provide axis labels and scaling factors (C)
	axisf	Axis label for FID displays and plots (P)

`dscale` Display scale below spectrum or FID (C)
`pscale` Plot scale below spectrum or FID (C)

axisf **Axis label for FID displays and plots (P)**

Description: Specifies the units for the FID axis display and plot. To create the FID display parameters `axisf`, `dotflag`, `vpf`, `vpfi`, `crf`, and `deltaf` (if the parameter set is older and lacks these parameters), enter `addpar('fid')`.

Values: 's' sets the axis label for units of seconds.

'm' sets the axis label for units of ms.

'u' sets the axis label for units of μ s.

'n' sets no axis label display.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to the current experiment (M)
`axis` Axis label for displays and plots (P)
`dscale` Display scale below spectrum or FID (C)
`pscale` Plot scale below spectrum or FID (C)

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bandinfo	Shaped pulse information for calibration (M)
banner	Display message with large characters (C)
bc	1D and 2D baseline correction (C)
beepoff	Turn beeper off (C)
beepon	Turn beeper on (C)
bigendian	Determine system byte order (C)
binom	Set up parameters for BINOM pulse sequence (M)
bioref	Bio-NMR Referencing (P)
bootup	Macro executed automatically (M)
box	Draw a box on a plotter or graphics display (C)
boxes	Draw boxes selected by the mark command (M)
bpa	Plot boxed parameters (M)
br24	Set up parameters for BR24 pulse sequence (M)
bs	Block size (P)

bandinfo **Shaped pulse information for calibration (M)**

Applicability: Information only useful on systems capable of shaped pulse generation.

Syntax: `bandinfo<(shape,width<,ref_power>):duration,power`

Description: Displays a table containing the duration and the predicted 90° pulse power setting for the pulse shape and bandwidth given by the arguments. No parameter settings are changed. The necessary data is contained in the `shapeinfo` file in the `shapelib` subdirectory.

Arguments: If `bandinfo` is run without arguments, prompts operator for input
`shape` is the name of the shape. The default is system prompts for a name.
`width` is the bandwidth, in Hz, desired for the pulse.
`ref_power` is value of `tpwr` to which `pw90` is set. The default is 55 dB.
`duration` is the duration, in μ s, of the pulse.
`power` is the predicted 90° pulse power setting.

Examples: `bandinfo`
`bandinfo('sinc',10):pw,tpwr`

See also: *User Programming*

Related: `pulseinfo` Shaped pulse information for calibration (M)
`pw90` 90° pulse width (P)
`tpwr` Observe transmitter power level with linear amplifiers (P)

banner **Display message with large characters (C)**

Syntax: `banner(message<,color>)`

Description: Displays text as large-size characters on the graphics windows.

Arguments: `message` is the text to be displayed. If the text includes a single quotation mark ('), it must be preceded by a backslash (\ '). Multiline displays are available by

B

inserting two backslashes (\\) between lines. Any undefined characters are displayed as a “bug” shape.

`color` is the color of text on a color display: 'red', 'yellow', 'green', 'cyan', 'blue', 'magenta', and 'white'. The default is 'yellow'.

Examples: `banner('banner sample')`
`banner('Don\'t Touch', 'blue')`

See also: *User Programming*

bc **1D and 2D baseline correction (C)**

Description: Makes 1D or 2D baseline correction using a spline or a second to twentieth order polynomial fitting of predefined baseline regions. `bc` defines every other integral (those integrals that disappear when `intmod='partial'`) as baseline and attempts to correct these points to zero.

1D baseline correction

Syntax: `bc<(n|'unbc'<,nsubregion<,minpoints<,minregion>>>)>`

Description: Performs a 1D baseline correction. The nonintegrated parts of the spectrum (i.e., every odd region between integral reset points, or the integral gaps with `intmod='partial'`) are divided into baseline subregions. The number of baseline subregions in each area are adjusted as possible, so that the subregions are more or less equal in size. Finally, the “center of gravity” (midpoint in *x* and average of the *y* values in the region) for each of the subregions is calculated.

Arguments: *n* is an integer from 1 to 20 for the baseline correction step. A polynomial of the (*n*-1)th order is calculated “through” the “baseline points” using the Chebychev least-squares fitting algorithm, and that polynomial function is subtracted from the spectrum. The coefficients of the polynomial are written into the file `cureexp+ '/bc.out'`. The default is 1 (a spline fit).

'unbc' is a keyword to make `bc` read in the coefficients from the file written by the previous `bc` operation and reverse that operation. This option is only functional for polynomials with two or more coefficients performing baseline correction operations on 1D spectra or individual 2D traces (i.e., baseline corrections cannot be undone with the default spline correction).

`nsubregion` defines the number of subregions (minimum 3, maximum 400). By default, the total number of subregions is 20 (if *fn*<2048), 40 (if *fn*=2048 or *fn*=4096), or 80 (if *fn*>4096).

`minpoints` sets the minimum number of data points required in an integral gap for `bc` to regard it as baseline. Use this to exclude small, nonintegrated areas between close signals. The default is *fn*/1000 (but at least 3).

`minregion` defines the minimum number of subregions assigned to each baseline area. The default is 1.

Examples: `bc`
`bc(3)`
`bc('unbc')`
`bc(1,200,8,2)` gives a spline correction using 200 baseline subregions, a gap of 8 data points between two (even) integral regions is regarded as baseline, and each baseline area is split into at least two subregions.

2D baseline correction

Syntax: `bc(trace_direction<,num_coeff><,trace_start<,>,trace_end>)`

Description: 2D baseline correction can be performed on three types of 2D data:

- f2 spectra (`trace_direction='f2'`) after the first half of a 2D FT (`wft1da`).
- f2 traces (`trace_direction='f2'`) after a full 2D FT (`wft2da`).
- f1 traces (`trace_direction='f1'`) after a full 2D FT (`wft2da`).

Arguments: `trace_direction` specifies the direction, 'f1' or 'f2', along which the 2D baseline correction is to take place.

`num_coeff` is the number of coefficients, from 1 to 20, used in the fitting procedure. The default value is 1, which gives a spline fit. A value of 2 gives a linear baseline fit ($a + bx$), a value of 3 gives a quadratic fit ($a + bx + cx^2$), etc. The maximum value (20) gives a 19th-order polynomial fit with 20 coefficients.

`trace_start` is the trace number for the spectrum on which the 2D baseline correction is to start. It must lie within the appropriate range or an error results.

`trace_end` is the trace number for the spectrum on which the 2D baseline correction is to end. It must lie within the appropriate range or an error results.

Examples: `bc('f1')`
`bc('f2',3)`
`bc('f2',3,10,60)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dc</code>	Calculate spectral drift correction (C)
	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>intmod</code>	Integral display mode (P)
	<code>trace</code>	Mode for 2D data display (P)
	<code>wft1da</code>	Weight and Fourier transform phase-sensitive data (M)
	<code>wft2da</code>	Weight and Fourier transform phase-sensitive data (M)

beepoff **Turn beeper off (C)**

Description: Turns off the beeper sound so that the system does not use sound to warn the user when errors occur. The default is the beeper is turned on.

See also: *User Programming*

Related: `beepon` Turn beeper on (C)

beepon **Turn beeper on (C)**

Syntax: `beepon`

Description: Turns on the beeper sound so that the user hears a sound when errors occur. The default is the beeper is turned on.

See also: *User Programming*

Related: `beepoff` Turn beeper off (C)

bigendian **Determine system byte order (C)**

Syntax: `bigendian:$type`

Description: The bigendian command determines the system byte order for storing numbers. One architecture is Big Endian, used by Sun computers with the "Sparc" CPU'S. The other architecture is Little Endian, used by most PCs.

Return values to argument `$type`:

- 1 if it is a "Big Endian" system.
- 0 if it is a "Little Endian" system.

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This command should rarely be used. Its only current use is when imaging .fdf files are created. The .fdf file headers can specify whether the data is stored as big or little endian.

binom **Set up parameters for BINOM pulse sequence (M)**

Description: Sets up a binomial water suppression pulse sequence.

See also: *NMR Spectroscopy User Guide*

bioref **Bio-NMR Referencing (P)**

Applicability: All

Syntax: `bioref='<y or n>'`

Description: Flag, global or local, for Bio-NMR Referencing. Setting the flag (`bioref='y'`) sets the system to bio-NMR referencing (based on `nuctables/nuctabrefBio`) rather than standard IUPAC / organic chemistry referencing (based on `nuctables/nuctabref`). Bio-NMR referencing uses DSS for nuclei such as ^{13}C and liquid NH_3 for ^{15}N .

Creating `bioref` as a local parameter (`create('bioref','flag')` creates a local flag) permits its use for a specific case. The parameter can be created as a local parameter and saved with a standard parameter set (`stdpar/N15`) to enable bio-NMR referencing for a specific nucleus. The local value of the parameter takes precedence over the global parameter.

`create('bioref','flag','global')` — creates a global flag.
`setenumerals('bioref',2,'y','n','global')` — sets the possible values of a string parameter in a parameter tree.

Examples: `bioref='y'` sets referencing to use `nuctables/nuctabrefBio`

Related: `create` Create new parameter in a parameter tree (C)

bootup **Macro executed automatically (M)**

Syntax: `bootup<(foreground)>`

Description: Executed automatically when VnmrJ is started up. The `bootup` macro displays a message, looks for a macro `login` in the user's local `maclib` directory and executes it (if found), starts `Acqstat` and `acqi` (`acqi` is not run if system is configured as a workstation), and then starts the menu system. This set of actions can be modified on a per user basis by constructing custom `bootup` or `login` macros in the user's `maclib` directory. A custom `login` macro is preferred because all custom `bootup` macros are overridden whenever a new VnmrJ release is installed.

Arguments: `foreground` is 0 if VnmrJ is being run in the foreground or nonzero if being run in the background. This argument is passed to the `login` macro.

See also: *User Programming*

Related: `acqi` Interactive acquisition display process (C)
 `Acqstat` Bring up the acquisition status display (U)

box **Draw a box on a plotter or graphics display (C)**

Syntax: `box(<'keywords',>x1mm,x2mm,y1mm,y2mm
 <,'nolimit'>)<:r1,r2>`

Description: Draws a box on a plotter or a graphics display.

Arguments: 'keywords' identifies the output device ('graphics' | 'plotter'), drawing mode ('xor' | 'normal'), and drawing capability ('newovly' | 'ovly' | 'ovlyC').

- 'graphics' | 'plotter' is a keyword for the output device. The default is 'plotter'. The output selected is passed to subsequent **pen**, **move**, or **draw** commands and remains active until a different output is specified.
- 'xor', 'normal' is a keyword for the drawing mode when using the 'graphics' output device. The default is 'normal'. In the 'xor' mode, if a line is drawn such that one or more points of the line are in common with a previous 'xor' line, the common points are erased. In the normal mode, the common points remain. The mode selected is passed to subsequent **pen**, **move**, and **draw** commands and remains active until a different mode is specified.
- 'newovly', 'ovly' and 'ovlyC' are keywords that specify an interactive drawing capability that is slightly slower than the 'xor' mode but more consistent in color. 'newovly' clears any previous draws, boxes, and writes made with the 'ovly' modes and draws the figure. 'ovly' draws without clearing so that multi-segment figures can be created. 'ovlyC' clears without drawing.

x1mm is the left edge of the box, x2mm is the right edge, y1mm is the bottom, and y2mm is the top. The location of the edges are given in plotter units (mm on most plots) and are scaled in mm for the graphics display. (If units are in Hz or ppm, you can use the **hztomm** command to convert units.)

'nolimit' allows the box to extend outside the limits determined by the parameters **sc**, **wc**, **sc2**, and **wc2**.

r1, r2 return the location of the upper left corner of the box.

Examples: `box('plotter', 20, 100, 40, 150)`
`box(25, 105, 45, 155, 'nolimit') : r1, r2`

See also: *NMR Spectroscopy User Guide*

Related:	gin	Return current mouse position and button values (C)
	hztomm	Convert positions from Hz or ppm to plotter units (C)
	sc	Start of chart (P)
	sc2	Start of chart in second direction (P)
	wc	Width of chart (P)
	wc2	Width of chart in second direction (P)
	wcmax	Maximum width of chart (P)

boxes **Draw boxes selected by the mark command (M)**

Syntax: `boxes<('graphics' | 'plotter')>`

Description: Draws boxes on a plotter or a graphics display with the location of the edges given in Hz. The data to make the boxes is stored in the `mark2d.out` file produced by the **mark** command. If there is no data in `mark2d.out`, a box is drawn from the current cursor positions. The **boxes** command also numbers the boxes above the upper left corner.

Arguments: 'graphics' | 'plotter' is a keyword to send output to the graphics display or to the plotter, respectively. The default is 'graphics'.

Examples: `boxes`
`boxes('plotter')`

B

See also: *NMR Spectroscopy User Guide*

Related: **mark** Determine intensity of spectrum at a point (C)

bpa Plot boxed parameters (M)

Syntax: **bpa**:*\$sc2_minimum*

Description: Plots a box around the entire chart (assuming blank paper) and then plots “chemist-style” parameters in boxes along the lower edge of the chart. **bpa** is the same as **ppa**, but with a different layout. Both **ppa** and **bpa** behave somewhat naively if the pulse sequence is more complex, but they were designed primarily for chemists, not for spectroscopists.

Arguments: *sc2_minimum* returns the minimum value for **sc2** to plot a scale properly. To use the command **pir**, **vp** has to be set to a non-zero value.

See also: *NMR Spectroscopy User Guide*

Related: **apa** Plot parameters automatically (M)
pap Plot out “all” parameters (C)
pir Plot integral amplitudes below spectrum (C)
ppa Plot a parameter list in “English” (M)
sc2 Start of chart in second direction (P)
vp Vertical position of spectrum (P)

br24 Set up parameters for BR24 pulse sequence (M)

Applicability: Systems with solids hardware.

Description: Converts a FLIPFLOP, MREV8, or S2PUL parameter set into a BR24 solids line-narrowing multiple-pulse sequence.

See also: *User Guide: Solid-State NMR*

Related: **cylbr24** Set up parameters for cycled BR24 pulse sequence (M)
flipflop Set up parameters for FLIPFLOP pulse sequence (M)
mrev8 Set up parameters for MREV8 pulse sequence (M)
s2pul Set up standard two-pulse sequence (M)

bs Block size (P)

Description: Directs the acquisition computer, as data are acquired, to periodically store a block of data on the disk, from where it can be read by the host computer.

CAUTION: If **bs='n'**, block size storage is disabled and data are stored on disk only at the end of the experiment. If the experiment is aborted prior to termination, data will be lost.

Values: 1 to 32767 transients, 'n'

See also: *NMR Spectroscopy User Guide*

Related: **wbs** Specify action when **bs** transients accumulate (C)
wbs When block size (P)

C

<code>c13</code>	Automated carbon acquisition (M)
<code>c13p</code>	Process 1D carbon spectra (M)
<code>calcdim</code>	Calculate dimension of experiment (C)
<code>calfa</code>	Recalculate alfa so that first-order phase is zero (M)
<code>calibflag</code>	Correct systematic errors in DOSY experiments (P)
<code>calibrate</code>	Start a dialog for autocalibration routines (M)
<code>callacq</code>	Utility macro to call Acq command (M)
<code>capt</code>	Automated carbon and APT acquisition (M)
<code>Carbon</code>	Set up parameters for ¹³ C experiment (M)
<code>cat</code>	Display one or more text files in text window (C)
<code>cattn</code>	Coarse attenuator type (P)
<code>cd</code>	Change working directory (C)
<code>cdc</code>	Cancel drift correction (C)
<code>cdept</code>	Automated carbon and DEPT acquisition (M)
<code>cdump</code>	Prints the current graphics screen (M)
<code>celem</code>	Completed FID elements (P)
<code>center</code>	Set display limits for center of screen (C)
<code>centersw</code>	Move cursor to center of spectrum (M)
<code>centersw1</code>	Move cursor to center of spectrum in 1st indirect dimension (M)
<code>centersw2</code>	Move cursor to center of spectrum in 2nd indirect dimension (M)
<code>cexp</code>	Create an experiment (M)
<code>cf</code>	Current FID (P)
<code>cfpmult</code>	Calculate first-point multiplier for 2D experiments (M)
<code>change</code>	Submit a change sample experiment to acquisition (M)
<code>checkstring</code>	Find and replace unwanted characters (C)
<code>chiliConf</code>	Control flag set by ecc_on and ecc_off (P)
<code>Cigar2j3j</code>	Convert the parameter to a CIGAR2j3j experiment (M)
<code>cla</code>	Clear all line assignments (M)
<code>cla</code>	Calculated transition number (P)
<code>clamp</code>	Calculated transition amplitude (P)
<code>cleanexp</code>	Remove old files and directories from an experiment (M)
<code>clear</code>	Clear a window (C)
<code>cleardosy</code>	Delete temporarily saved data in current sub experiment (M)
<code>clfreq</code>	Calculated transition frequency (P)
<code>clindex</code>	Index of experimental frequency of a transition (P)
<code>clradd</code>	Clear add/subtract experiment (C)
<code>color</code>	Select plotting colors from a graphical interface (M)
<code>combiplate</code>	View a color map for visual analysis of VAST microtiter plate (U)
<code>combishow</code>	Display regions (red, green, and blue) in CombiPlate window (M)
<code>compressfid</code>	Compress double-precision FID data (M,U)
<code>config</code>	Display current configuration and possibly change it (M)
<code>confirm</code>	Confirm message using the mouse (C)
<code>Console</code>	System console type (P)

C

<code>contact_time</code>	MAS cross-polarization spin-lock contact time (M)
<code>continueMovie</code>	Continue movie in either forward or backward direction (C)
<code>convert</code>	Convert data set from a VXR-style system (M,U)
<code>convertbru</code>	Convert Bruker data (M,U)
<code>copy</code>	Copy a file (C)
<code>cos</code>	Find cosine value of an angle (C)
<code>Cosy</code>	Convert the parameter to a COSY experiment (M)
<code>cosyps</code>	Set up parameters for phase-sensitive COSY pulse sequence (M)
<code>cp</code>	Copy a file (C)
<code>cp</code>	Cycle phase (P)
<code>cpmgt2</code>	Set up parameters for CPMGT2 pulse sequence (M)
<code>cpos_cvt</code>	Convert data set from a VXR-style system (M,U)
<code>cptmp</code>	Copy experiment data into experiment subfile (M)
<code>cpx</code>	Create pbox shape file (M)
<code>cqexp</code>	Load experiment from protocol (M)
<code>cqfindz0</code>	Run an experiment to find the value of z0 (M)
<code>cqgmap</code>	Perform gradient shimming utility functions (M)
<code>cqinit</code>	Initialize liquids study queue (M)
<code>cqpars</code>	Create study queue parameters for liquids (M)
<code>cqplot</code>	Macro to perform generic 2D plot (M)
<code>cqprotocol</code>	Macro to create protocols (M)
<code>cqreset</code>	Reset study queue parameters (M)
<code>cqsavestudy</code>	Macro to save study queue parameters (M)
<code>cqwtmenu</code>	Macro to set weighting functions from a panel (M)
<code>cr</code>	Cursor position in directly detected dimension (P)
<code>crl</code>	Cursor position in 1st indirectly detected dimension (P)
<code>cr2</code>	Cursor position in 2nd indirectly detected dimension (P)
<code>crcom</code>	Create user macro without using text editor (M)
<code>create</code>	Create new parameter in a parameter tree (C)
<code>createqcomp</code>	Create qcomp parameter (M)
<code>crf</code>	Current time-domain cursor position (P)
<code>crl</code>	Clear reference line in directly detected dimension (M)
<code>crl1</code>	Clear reference line in 1st indirectly detected dimension (M)
<code>crl2</code>	Clear reference line in 2nd indirectly detected dimension (M)
<code>crmode</code>	Current state of the cursors in df, ds, or dcon1 programs (P)
<code>crof2</code>	Recalculate rof2 so that lp = 0 (M)
<code>cryo_noisetest</code>	Run Cold Probe conditioning experiments (M)
<code>cryoclient</code>	Start the CryoBay Monitor program (M, U)
<code>ct</code>	Completed transients (P)
<code>ctext</code>	Clear the text of the current experiment (C)
<code>curexp</code>	Current experiment directory (P)
<code>curscan</code>	Scan currently in progress (P)
<code>curwin</code>	Current window (P)
<code>cutoff</code>	Data truncation limit (P)
<code>cyclenoe</code>	Set up parameters for CYCLENOE pulse sequence (M)
<code>cylbr24</code>	Set up parameters for cycled BR24 pulse sequence (M)

cylmrev	Set up parameters for cycled MREV8 pulse sequence (M)
cz	Clear integral reset points (C)

c13 Automated carbon acquisition (M)

Syntax: `c13<(solvent)>`

Description: Prepares parameters for automatically acquiring a standard ^{13}C spectrum. The parameter **wexp** is set to 'procplot' for standard processing. If **c13** is used as the command for automation via the **enter** command, the **au** is supplied automatically and should not be entered on the MACRO line of the **enter** program. However, it is possible to customize the standard **c13** macro on the MACRO line by following it with additional commands and parameters. For example, `c13 nt=1` uses the standard **c13** setup but with only one transient.

Arguments: **solvent** is the name of the solvent. In automation mode the solvent is supplied by the **enter** program. The default is 'CDC13'.

Examples: `c13`
`c13 ('DMSO')`

See also: *NMR Spectroscopy User Guide*

Related:	au	Submit experiment to acquisition and process data (M)
	c13p	Process of 1D carbon spectra (M)
	enter	Enter sample information for automation run (C)
	procl1d	Processing macro for simple (non-arrayed) 1D spectra (M)
	procplot	Automatically process FIDs (M)
	wexp	When experiment completes (P)

c13p Process 1D carbon spectra (M)

Syntax: `c13p`

Description: Processes non-arrayed 1D carbon spectra using a set of standard macros. **c13p** is called by the **procl1d** macro, but can also be used directly. Fully automatic processing (up to a point where a spectrum could be plotted) is provided: Fourier transformation (using pre-set weighting functions), automatic phasing (**aphx** macro), automatic integration (**integrate** macro if required only), vertical scale adjustment (**vsadjc** macro), avoiding excessive noise (**noislm** macro), threshold adjustment (**thadj** macro), and referencing to the TMS signal if present (**setref** macro then **tmsref** macro).

See also: *NMR Spectroscopy User Guide*

Related:	aphx	Perform optimized automatic phasing (M)
	c13	Automated carbon acquisition (M)
	integrate	Automatically integrate 1D spectrum (M)
	noislm	Limit noise in spectrum (M)
	procl1d	Processing macro for simple (non-arrayed) 1D spectra (M)
	setref	Set frequency referencing for proton spectra (M)
	thadj	Adjust threshold (M)
	tmsref	Reference spectrum to TMS line (M)
	vsadjc	Adjust vertical scale for carbon spectra (M)

calcdim Calculate dimension of experiment (C)

Syntax: `calcdim`

C

Description: Calculates the dimension of an experiment and puts the result into the parameter `arraydim`. If an experiment is arrayed, `arraydim` is the product of the size of the arrays.

See also: *NMR Spectroscopy User Guide*

Related: `arraydim` Dimension of experiment (P)

calfa Recalculate alfa so that first-order phase is zero (M)

Syntax: `calfa`

Description: Based upon the current `alfa` and `lp` values, `calfa` calculates a new value for `alfa` so that the first-order phase parameter `lp` is rendered approximately 0. When digital filtering is active (`dsp= 'r'` or `dsp= 'i'`), `calfa` also adjusts `rof2` as well as `alfa`. For `calfa` to work properly, a trial spectrum must be obtained and phased to pure absorption. This spectrum provides `calfa` with the current `alfa` and `lp` values. `calfa` pertains to processing 2D data. Unless `lp` is approximately 0, `fpmult` will affect both the `dc` offset and the curvature of the spectrum.

See also: *NMR Spectroscopy User Guide*

Related:

<code>alfa</code>	Set <code>alfa</code> delay before acquisition (P)
<code>cfpmult</code>	Calculate first-point multiplier for 2D experiments (M)
<code>crof2</code>	Recalculate <code>rof2</code> so that <code>lp</code> = 0 (M)
<code>dc</code>	Calculate spectral drift correction (C)
<code>dsp</code>	Type of DSP for data acquisition (P)
<code>fpmult</code>	First-point multiplier for <code>np</code> FID data (P)
<code>hoult</code>	Set parameters <code>alfa</code> and <code>rof2</code> according to Hoult (M)
<code>lp</code>	First-order phase in directly detected dimension (P)
<code>rof2</code>	Receiver gating time following pulse (P)

calibflag Correct systematic errors in DOSY experiments (P)

Syntax: `calibflag`

Description: Corrects systematic errors in DOSY experiments.

Values: `'y'` corrects systematic deviations in DOSY analysis.

`'n'` omits gradient correction in DOSY analysis.

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)

calibrate Start a dialog for autocalibration routines (M)

Syntax: `calibrate`

Description: Starts a dialog for autocalibration routines.

callacq Utility macro to call Acq command (M)

Syntax: `callacq(arg_string)`

Description: Utility macro to construct a string to pass to `psg` via the `Acq ( )` command. This macro should be used only by users with advanced knowledge. A well-constructed argument string is required. The motivation for this macro is to make the `'go'` macro re-entrant, while still synchronizing with `VnmrJ`.

Arguments: `arg_string` is a character string constructed from a macro.

Examples: `callacq($callback)`

Related:	<code>go</code>	Submit experiment to acquisition (M)
	<code>reqparcheck</code>	Flag which enables/disables required parameters (P)
	<code>reqparclear</code>	Clears the parameters in required parameter list (M)
	<code>reqparlist</code>	List of required parameters (P)
	<code>reqpartest</code>	Tests whether required parameters are set (M)

capt Automated carbon and APT acquisition (M)

Syntax:	<code>capt<(solvent)></code>	
Description:	Prepares parameters for automatically acquiring a standard ^{13}C spectrum, followed by an APT experiment. In non-automation mode, the carbon and APT spectra are acquired in the experiment in which <code>capt</code> is entered. Following acquisition completes, the commands <code>rttmp('C13')</code> and <code>rttmp('apt')</code> can be used for further processing of the carbon and APT spectra, respectively.	
Arguments:	<code>solvent</code> is name of the solvent used. In automation mode, the <code>enter</code> program supplies name. In non-automation mode, the default is ' <code>cdc13</code> '.	
Syntax:	<code>capt au</code> <code>capt('dmsol')</code>	
See also:	<i>NMR Spectroscopy User Guide</i>	
Related:	<code>Apt</code>	Prepare parameters for APT experiment (M)
	<code>c13</code>	Automated carbon acquisition (M)
	<code>enter</code>	Enter sample information for automation run (C)
	<code>rttmp</code>	Retrieve experiment subfile (M)

Carbon Set up parameters for ^{13}C experiment (M)

Description:	Set up parameters for ^{13}C experiment

cat Display one or more text files in text window (C)

Syntax:	<code>cat(file1<,file2,...>)</code>	
Description:	Displays the contents of one or more text files on the text window. It pauses after the window has filled and waits for the user to indicate whether it should display more or should terminate.	
Arguments:	<code>file1, file2, ...</code> are the names of the files to be displayed.	
Examples:	<code>cat('/vnmr/manual/cat')</code> <code>cat('/vnmr/manual/cat', '/vnmr/manual/cattn')</code>	
See also:	<i>NMR Spectroscopy User Guide</i>	

cattn Coarse attenuator type (P)

Applicability:	Systems with a coarse attenuator.
Description:	Identifies the type of coarse attenuator if this attenuator is present on the current rf channel. The value of <code>cattn</code> is set in the Spectrometer Configuration window (opened by entering <code>config</code>) using the label Coarse Attenuator.
Values:	0 for no coarse attenuator, as in the case with class C amplifiers (Not Present choice in Spectrometer Configuration window). 79 for standard systems (79 dB choice in Spectrometer Configuration window).

127 for imaging attenuator (63.5 dB SIS choice in Spectrometer Configuration window).

63 for deuterium decoupler channel.

See also: *VnmrJ Installation and Administration*

Related: **config** Display current configuration and possibly change it (M)
fatten Fine attenuator (P)
tpwr Observe transmitter power level with linear amplifiers (P)

cd Change working directory (C)

Syntax: `cd<(directory)>`

Description: Changes current working directory to another directory.

Arguments: `directory` is the name of the directory that becomes the new current working directory. The change is made only if the directory name already exists and the user has permission to be in the directory. If no argument is included, `cd` changes the current working directory to the user's home directory.

Examples: `cd`
`cd(userdir+'/expl')`
`cd('/home/george/vnmrsys')`

See also: *NMR Spectroscopy User Guide*

Related: **pwd** Display current working directory (C)

cdc Cancel drift correction (C)

Syntax: `cdc`

Description: Turns off the drift correction started by the **dc** command and resets the spectral drift correction parameters **lvl** (level) and **tlt** (tilt) to zero.

See also: *NMR Spectroscopy User Guide*

Related: **dc** Calculate spectral drift correction (C)
dcg Drift correction group (P)
lvl Zero-order baseline correction (P)
tlt First-order baseline correction (P)

cdept Automated carbon and DEPT acquisition (M)

Syntax: `cdept<(solvent)>`

Description: Prepares parameters for automatically acquiring a standard ^{13}C spectrum, followed by a DEPT experiment. In non-automation mode, the carbon and DEPT spectra are acquired in the experiment in which `cdept` was entered. Following the completion of the acquisition, the **rttmp** ('C13') and **rttmp** ('dept') commands can be used for further processing of the carbon and DEPT spectra, respectively.

Arguments: `solvent` is name of the solvent used. In automation mode, the **enter** program supplies name. In non-automation mode, the default is 'cdc13'.

Examples: `cdept au`
`cdept('DMSO')`

See also: *NMR Spectroscopy User Guide*

Related: **adept** Automatic DEPT analysis and spectrum editing (C)
c13 Automated carbon acquisition (M)
dept Prepare parameters for DEPT experiment (M)

`enter` Enter sample information for automation run (C)
`rttmp` Retrieve experiment subfile (M)

`cdump` Prints the current graphics screen (M)

Syntax: `cdump('filename')`

Description: `cdump` takes the current display and sends it to the current printer. If an optional `filename` is passed as an argument, the current display will be saved in the print subdirectory of the user's `vnmr.sys` directory. This directory will be created if it does not already exist. If the `filename` passed to the `cdump` macro is an absolute pathname, i.e., it starts with a '/' character, that pathname will be used.

If the current display is saved as a file, the format of the file is specified by the `printformat` parameter. It can be set to the following values. `as` for PostScript formatted output.

`japed` for Joint Photographic Experts Group JFIF formatted output.

`nag` for Portable Network Graphics formatted output.

`celem` Completed FID elements (P)

Description: Indicates the current number of completed FIDs in an experiment. When `go` or `au` is entered, `celem` is set to 0. As each FID acquisition is completed, `celem` is updated to reflect this. This parameter is most useful in conjunction with `wbs`, `wnt`, `wexp`, and `werr` processing commands.

See also: *NMR Spectroscopy User Guide*

Related:

<code>arraydim</code>	Dimension of experiment (P)
<code>au</code>	Submit experiment to acquisition and process data (C)
<code>go</code>	Submit experiment to acquisition (C)
<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
<code>wbs</code>	Specify action when <code>bs</code> transients accumulate (C)
<code>werr</code>	Specify action when error occurs (C)
<code>wexp</code>	Specify action when experiment completes (C)
<code>wnt</code>	Specify action when <code>nt</code> transients accumulate (C)

`center` Set display limits for center of screen (C)

Description: Sets parameters `sc` and `wc` (horizontal control) and parameters `sc2` and `wc2` (vertical control) to produce a display (and subsequent plot) in the center portion of the screen (and page). For 2D data, space is left for the scales.

See also: *NMR Spectroscopy User Guide*

Related:

<code>full</code>	Set display limits for a full screen (C)
<code>fullt</code>	Set display limits for full screen with room for traces (C)
<code>left</code>	Set display limits for left half of screen (C)
<code>right</code>	Set display limits for right half of screen (C)
<code>sc</code>	Start of chart (P)
<code>sc2</code>	Start of chart in second direction (P)
<code>wc</code>	Width of chart (P)
<code>wc2</code>	Width of chart in second direction (P)

`centersw` Move cursor to center of spectrum (M)

Description: Sets cursor position parameter `cr` in the directly detected dimension for the center of the spectrum.

See also: *NMR Spectroscopy User Guide*

Related: `centersw1` Move cursor to center of spectrum in 1st indirect dimension (M)
`centersw2` Move cursor to center of spectrum in 2nd indirect dimension (M)
`cr` Cursor position in directly detected dimension (P)

centersw1 Move cursor to center of spectrum in 1st indirect dimension (M)

Description: Sets cursor position parameter `cr1` in the first indirectly detected dimension to the center of the spectrum.

See also: *NMR Spectroscopy User Guide*

Related: `centersw` Move cursor to center of spectrum (M)
`cr1` Cursor position in 1st indirectly detected dimension (P)

centersw2 Move cursor to center of spectrum in 2nd indirect dimension (M)

Description: Sets cursor position parameter `cr2` in the second indirectly detected dimension to the center of the spectrum.

See also: *NMR Spectroscopy User Guide*

Related: `centersw` Move cursor to center of spectrum (M)
`cr2` Cursor position in 2nd indirectly detected dimension (P)

cexp Create an experiment (M)

Syntax: `cexp(<experiment_dir,>experiment_number)`

Description: Creates an experiment as a temporary workspace that can hold a complete 1D, 2D, or 3D data set. Up to 9999 experiments can be created. Experiment 5 is special because it is the add-subtract experiment. `cexp` creates the appropriate `jexpxxx` macro so that the newly created experiment can be joined.

Arguments: `experiment_dir` specifies the path of the directory in which the particular experiment is to be created. If `experiment_dir` is not entered, the default is the user directory specified by `userdir`.

`experiment_number` specifies the number, from 1 to 9999, of the experiment to be created.

Examples: `cexp(3)`
`cexp('/data',2)`

See also: *NMR Spectroscopy User Guide*

Related: `delexp` Delete an experiment (C)
`jexp` Join existing experiment (C)
`userdir` User directory (P)

cf Current FID (P)

Description: Specifies which FID to operate on when working with multi-FID data. All subsequent operations such as Fourier transformation are applied to the selected data block.

When an experiment acquires `nf` number of data segments through explicit acquisition, `cf` indicates the `cf`th FID to use. For example, in the COSY-NOESY experiment with `nf=2`, `cf=1` would select the COSY part of the experiment, and `cf=2` would select the NOESY part.

Values: 1 through the value of parameter `nf`.

See also: *NMR Spectroscopy User Guide*

Related: **nf** Number of FIDs (P)

cfpmult Calculate first-point multiplier for 2D experiments (M)

Description: Calculates an **fpmult** value for the dataset, which is then used by **wft2da**. For 2D experiments, such as NOESY, run **cfpmult** on the transformed first increment, prior to entering **wft2da**, to minimize “f₂ ridges” in the final 2D spectrum. To do this manually for a 2D dataset, enter **fpmult=1.0 wft (1) cdc** in the command line and note whether the spectrum (essentially the baseline) moves up or down when **dc** is typed. Vary the value of **fpmult** until the dc correction (jump in the baseline) is as small as possible. With care, **fpmult** can be set to two decimal places. Typical values for **fpmult** range from 1.00 to 2.00. The default value is 1.0.

This calculation only needs to be performed for cosine-type experiments, such as NOESY, where both the t₂ FID and the t₁ interferogram decay. **cfpmult** might give incorrect values for first increments of experiments having baseline distortions (e.g., water suppression with 11-echo or 1331); in such cases, manual optimization of **fpmult** is more suitable.

When processing 2D data, unless the parameter **lp** is approximately 0, **fpmult** affects both the dc offset and the curvature of the spectrum. See the entries for **alfa** and **calfa** for more information.

See also: *NMR Spectroscopy User Guide*

Related:	alfa	Set alfa delay before acquisition (P)
	calfa	Recalculate alfa so that first-order phase is zero (M)
	crof2	Recalculate rof2 so that lp = 0 (M)
	dc	Calculate spectral drift correction (C)
	fpmult	First point multiplier for np FID data (P)
	lp	First-order phase in directly detected dimension (P)
	wft2da	Weight and Fourier transform phase-sensitive data (M)

change Submit a change sample experiment to acquisition (M)

Applicability: Systems with automatic sample changer.

Description: Removes the sample currently in the probe and loads the sample currently in sample location **loc**. **change** runs in the acquisition computer and is inoperative if **loc** is 0 and/or **traymax** is 'n' or 0. **change** also sets all hardware according to the current parameters.

See also: *NMR Spectroscopy User Guide*

Related:	au	Submit experiment to acquisition and process data (C)
	ga	Submit experiment to acquisition and FT the result (C)
	go	Submit experiment to acquisition (C)
	loc	Location of sample in tray (P)
	lock	Submit an autolock experiment to acquisition (C)
	sample	Submit change sample, Autoshim experiment to acquisition (M)
	shim	Submit an Autoshim experiment to acquisition (C)
	spin	Submit a spin setup experiment to acquisition (C)
	su	Submit a setup experiment to acquisition (M)
	traymax	Sample changer tray size (P)

checkstring Find and replace unwanted characters (C)

Syntax: `checkstring(' $VALUE', variable):variable`

C

Description: `checkstring` is used panel to check and replace user-entered strings like `samplename`, `notebook`, or `page` for Unix-unfriendly characters:
 "" (blank space) , ; : * ! ? (" ") [" "] { " " } < " "> ~ # \$ & /
 Data may be saved to unexpected directories (or not at all) with Save Data Setup (used for automatic saving of NMR data) if operating system special characters are used within a filename.
 An error/warning message is issued and the respective character(s) is/are replaced with an underscore, `_`. Multiple consecutive characters are replaced by one single underscore. Example: `samplename = 'special type of (new) sample'` becomes `'special_type_of_new_sample'`.

chiliConf Control flag set by `ecc_on` and `ecc_off` (P)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Control flag set by `ecc_on` and `ecc_off` macros

Values: `E` — enable PSG control of ECC
`n` — disable PSG control of ECC

Related: `ecc_on` Turns on eddy current compensation for Cold Probes (M)
`ecc_off` Turns off eddy current compensation for Cold Probes (M)

Cigar2j3j Convert the parameter to a CIGAR2j3j experiment (M)

Syntax: Convert the parameter to a CIGAR2j3j experiment.

c1a Clear all line assignments (M)

Syntax: `c1a`

Description: Clears the line assignment parameters `clindex` and `slfreq` for spin simulation iteration, which matches simulated spectra to actual data.

See also: *NMR Spectroscopy User Guide*

Related: `assign` Assign transitions to experimental lines (M)
`d1a` Display line assignments (M)
`clindex` Index of experimental frequency of a transition (P)
`slfreq` Measured line frequencies (P)

c1a Calculated transition number (P)

Description: A global arrayed parameter that stores the transition number of calculated transitions of the spin simulation program when they are above a threshold set by `sth`. In the iterative mode, the `c1a` value of an assigned transition is associated with an experimental frequency whose index is the `clindex` value.

See also: *NMR Spectroscopy User Guide*

Related: `clamp` Calculated transition amplitude (P)
`clfreq` Calculated transition frequency (P)
`clindex` Index of experimental frequency of a transition (P)
`sth` Minimum intensity threshold (P)

clamp **Calculated transition amplitude (P)**

Description: A global arrayed parameter that stores the transition amplitude of calculated transitions of the spin simulation program when they are above a threshold set by the parameter `sth`. Enter `dla('long')` to display `clamp`.

See also: *NMR Spectroscopy User Guide*

Related: `cla` Calculated transition number (P)
`clfreq` Calculated transition frequency (P)
`clindex` Index of experimental frequency of a transition (P)
`dla` Display line assignments (C)
`sth` Minimum intensity threshold (P)

cleanexp **Remove old files and directories from an experiment (M)**

Syntax: `cleanexp<(file1<,file2<,...>>)>`

Description: Removes experiment subfiles from chained experiments that exist in an experiment directory. `cleanexp` only cleans the currently active experiment.

Arguments: `file1`, `file2`, ... are specific experiment subfiles to be removed. If no argument is given, all files in `curexp/subexp` are removed.

Examples: `cleanexp`
`cleanexp('H1','relayh')`

See also: *NMR Spectroscopy User Guide*

Related: `curexp` Current experiment directory (P)
`hccorr` Automated proton, carbon, and HETCOR acquisition (M)
`hcosy` Automated proton and COSY acquisition (M)

clear **Clear a window (C)**

Syntax: `clear<(window_number)>`

Description: Clears one of the four windows on the GraphOn terminal (status, input, graphics, text) or one of the two windows on the Sun (text and graphics).

Arguments: `window_number` is the number (1 to 4) of the window to be cleared:

- 1 clears the status window (GraphOn only)
- 2 clears the graphics window
- 3 clears the input window (GraphOn only)
- 4 clears the text window (the default value).

Examples: `clear`
`clear(2)`

See also: *User Programming*

cleardosy **Delete temporarily saved data in current sub experiment (M)**

Syntax: `cleardosy`

Description: Deletes any copies of DOSY data temporarily saved in the current sub experiment.

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)

C

clfreq **Calculated transition frequency (P)**

Description: A global arrayed parameter that stores the transition frequency of calculated transitions of the spin simulation program when they are above a threshold set by the parameter **sth**. Enter **dla** to display **clfreq**.

See also: *NMR Spectroscopy User Guide*

Related: **cla** Calculated transition number (P)
clamp Calculated transition amplitude (P)
clindex Index of experimental frequency of a transition (P)
dla Display line assignments (M)
sth Minimum intensity threshold (P)

clindex **Index of experimental frequency of a transition (P)**

Description: A global arrayed parameter where each value contains the index of an experimental frequency assigned to the associated calculated transition for use in iterative spin simulation. Use **assign** to make the assignments. A value of zero indicates no assignment.

See also: *NMR Spectroscopy User Guide*

Related: **assign** Assign transitions to experimental lines (M)
cla Clear line assignments (M)
cla Calculated transition number (P)
dla Display line assignments (M)

clradd **Clear add/subtract experiment (C)**

Description: Deletes the add/subtract experiment (exp5).

See also: *NMR Spectroscopy User Guide*

Related: **add** Add current FID to add/subtract experiment (C)
sub Subtract current FID from add/subtract experiment (C)

color **Select plotting colors from a graphical interface (M)**

Description: Displays a window with color palettes for selecting colors for plotting the background of the display screen, spectrum, integral, FID, etc.

See also: *NMR Spectroscopy User Guide*

Related: **pl** Plot spectra (C)
setcolor Set colors for graphics window and for plotters (C)

combiplate **View a color map for visual analysis of VAST microtiter plate (U)**

Syntax: (From UNIX) **combiplate**

Description: Opens the CombiPlate window, which provides a map of microtiter plate, allowing data to be viewed from individual sample wells. The window enables viewing integral region intensities by colors and color densities.

See also: *NMR Spectroscopy User Guide*

Related: **combishow** Display regions as red, green, and blue in CombiPlate window (M)
dlivast Produce text file and process last wells (M)

combishow **Display regions (red, green, and blue) in CombiPlate window (M)**

Syntax: **combishow**(r,g,b)

Description: Displays integral regions shown on the spectrum as red (r), green (g), and blue (b) in the CombiPlate window. CombiPlate reads the regions automatically. 1, 2, or 3 integral regions can be designated. At least one integral region must be specified. Combishow displays spectra associated with individual wells.

See also: *NMR Spectroscopy User Guide*

Related: `combiplate` View a color map for visual analysis of VAST microtiter plate (U)
`dlivast` Produce text file and process last wells (M)

compressfid Compress double-precision FID data (M,U)

Syntax: `compressfid(<inFIDdir,>outFIDdir)`
 (From UNIX) `compressfid -i inFIDdir -o outFIDdir -f`
 (From UNIX) `compressfid -e exp_number -o outFIDdir -f`

Description: Compresses double-precision FID data to single-precision and updates the parameter `dp` in the file `procpa`. `compressfid` can be run through a macro interface in VnmrJ or directly at the UNIX level. In entering FID directory names, leave off the `.fid` directory extension.

Arguments: `inFIDdir` is the double-precision FID directory to be compressed. If `inFIDdir` is not entered, the default FID directory is `curexp/acqfil`.
`outFIDdir` is the FID directory to receive the output.
`exp_number` is the number of the experiment that contains the FID data.
`-i` specifies that the next argument is the input FID directory.
`-o` specifies that the next argument is the output FID directory.
`-e` specifies that the next argument is the number of the experiment that contains the FID data. The `-e` and the `-i` options are mutually exclusive.
`-f` specifies that any existing directory with the name `outFIDdir.fid` is to be overwritten. Note that the macro interface always overwrites any preexisting directory with the name specified by `outFIDdir.fid`.

Examples: `compressfid('/vnmr/fidlib/fid1d',`
`'testfid1d')compressfid('testfid1d')`
 (From UNIX) `compressfid -e 5 -o testfid1d -f`
 (From UNIX) `compressfid -i /vnmr/fidlib/fid1d -o`
`testfid1d -f`

See also: *NMR Spectroscopy User Guide*

Related: `dp` Double precision (P)

config Display current configuration and possibly change it (M)

Syntax: `config <('display')>`

Description: Displays the current system configuration parameters in a window (called the Spectrometer Configuration window). The values of the configuration parameters can be changed if `config` is entered from the console without any arguments and the user has write access to the directories `/vnmr` and `/vnmr/conpar`. If so, the user can interactively make changes to the choices in the window.

If the user does not meet the conditions above, or if the VnmrJ administrator enters the command `config('display')`, instead of the interactive mode, the user is restricted to the display mode, where system information is listed in the Process tab -> Text page.

If `config` is entered without any arguments, or if Utilities->System Settings is selected, the program checks if the user is logged in as the administrator. If so,

it runs in interactive mode; if not, it runs in display mode. By entering `config('display')`, `vnmr1` can run in the display mode instead of interactively.

In the interactive mode, a separate panel displays the options with the current choice appearing to the right. Position the mouse over the choice to be modified, then use the left button to cycle through each choice or use the right button to display a menu of all possible choices.

The Use Console Data button sets parameter values in the Spectrometer Configuration window using information captured during console startup.

This button makes `config` capture from the system all values shown in the Spectrometer Configuration window except Sample Changer, Sample Changer Serial Port, Rotor Synchronization, Frequency Overrange, and Upper Limit of decoupler power. For the Gradients entry, `config` recognizes the Performa I and Performa II modules but not other gradients. For the VT Controller entry, if VT is found, `config` does not change the value set, and if VT is not found, `config` changes the value to Not Present.

The EXIT, and SAVE button writes a new `conpar` configuration file before leaving. The QUIT, no SAVE button terminates the session with no modifications to the `conpar` file, but remember that the parameters are always set. These two buttons require use of the left button on the mouse. In the display mode, the current choices are displayed in the text window.

To send output to the printer, enter the sequence of commands `printon config('display') printoff`.

Commands for working with parameters (such as `create`, `destroy`, `exists` and `setvalue`) have an option to select which parameter tree the parameter is in. The `systemglobal` tree is the internal name for `/vnmr/conpar`, and it can be used to search for, modify, or create a parameter in `conpar`. But note that any changes made, either directly (e.g., by typing `vttype=0`) or by using `create` and similar commands, only affect parameters in memory. To permanently change parameters:

- For parameters in `config`, enter the change in the Spectrometer Configuration window and then quit using the Exit & Save button.
- For other parameters, after creating or changing the parameter, enter `fsave('/vnmr/conpar','systemglobal')`.

Both methods, usually restricted to `vnmr1` only, overwrite `conpar`.

The Spectrometer Configuration labels listed below can be changed in the interactive mode. For each label, the choices available and a short description of the label is provided. Shown in parentheses is the associated parameter, which you should refer to for further information.

- System Type: Spectrometer or Data Station. Sets the basic type of system (`system`).
- Console: or Imager. Sets the type of system console (`Console`). When `go`, `au`, or `ga` is entered, the value set is copied to the current experiment as the `console` parameter (lowercase c).
- Proton Frequency: 085, 100, 200, 300, 400, 500, 600, 700, 750, 800, 900, 3T, and 4T. Sets the resonant frequency, in MHz or tesla, of ^1H as determined by magnet field strength (`hlfreq`).
- Sample Changer: None, Carousel, SMS 50 Sample, SMS 100 Sample, VAST, NMS, LC-NMR, 768 AS. Sets the type of sample changer. Set to none if a sample changer is not present or is to be disabled (`traymax`).
- Sample Changer Comm Port: Not Used, Port A, Port B, Ethernet. Sets the serial port used to connect the sample changer. Select Not Used if no sample changer is present (`smsport`).

- Shimset: Varian 13 Shims, Varian 14 Shims, Oxford 15 Shims, Oxford 18 Shims, Varian 18 Shims, Varian 20 Shims, Varian 23 Shims, Varian 26 Shims, Varian 28 Shims, Varian 29 Shims, Varian 35 Shims, Varian 40 Shims, Ultra 18 Shims, Ultra 39 Shims, and Whole Body Shims. Sets type of shim sets on system (`shimset`).
- Audio Filter Type: 100 kHz Elliptical, 100 kHz Butterworth 200 kHz Butterworth, 500 kHz Elliptical. If the spectral width (sw) is less than 100 kHz, sets type of audio filters used (`audiofilter`).
- VT Controller: Not Present, Present. Sets whether a variable temperature controller is present or not on the system (`vttype`).
- Maximum DMF: 9900, 32700, 2.0e6. Sets maximum frequency, in Hz, for decoupler modulation (`parmax [11]`).
- Max. Spectral Width: 100 kHz, 200 kHz, 500 kHz, 2 MHz, 5 MHz. Sets maximum spectral width available to a system (`parmax [5]`).
- AP Interface Type: Type 1, Type 2, Type 3, N/A. Sets type of AP bus interface board in the system.
- Fifo Loop Size: 63, 1024, 2048. Sets size of FIFO loop, which depends on the type of controller board in the system.
- Rotor Synchronization: Not Present, Present. Sets whether system supports the solids rotor synchronization module (`rotorsync`).
- Lock Frequency: (frequency entered directly). Sets lock frequency of the system. **To observe NMR signals, the lock frequency value must be set correctly** (`lockfreq`).
- IF Frequency: 10.5 MHz, 20.0 MHz.
- Number of RF Channels: 1, 2, 3, 4, 5. Selects which rf channel is listed in the Configure panel that appears in the lower section of the Spectrometer Configuration window (`numrfch`).
- Gradients: Not Present, Present. Sets whether system has optional gradients for the X, Y, or Z axis. If present, the gradients are listed in the Configure panel in lower section of Spectrometer Configuration window (Gradients is not associated with any parameter).
- Configure: RF Channel 1 (Obs), RF Channel 2 (Dec), RF Channel 3 (Dec2), RF Channel 4 (Dec 3), RF Channel 5 (Dec4), Gradients. Sets which labels appear in the Configure panel in lower section of Spectrometer Configuration window (Configure is not associated with any parameter).
- Type of RF: U+ Direct Synthesis, U+ H1 Only, Direct Synthesis, Broadband, Fixed Frequency, Deuterium Decoupler, SIS Modulator. Sets type of frequency generation on the current rf channel (`rftype` and `rfchtype`).
- Synthesizer: Not Present, PTS 160, PTS 200, PTS 250, PTS, 320, PTS 500, PTS 620, PTS 1000. Sets type of PTS frequency synthesizer on the current rf channel (`ptsval`).
- Latching: Not Present, Present. On systems equipped with a special version of the PTS frequency synthesizer, sets how frequency values are sent on the current rf channel (`latch`).
- Frequency Overrange: Not Present, 10000 Hz, 100000 Hz. On systems equipped with a special version of the PTS frequency synthesizer, sets the presence of a signal phase stability option on the current rf channel (`overrange`).

- Step Size: 0.1 Hz, 0.2 Hz, 1 Hz, 100 Hz. Sets frequency step size on current rf channel. (`parstep[7]`, `parstep[8]`, `parstep[16]`, `parastep[20]`).
- Coarse Attenuator: Not Present, 63 dB, 79 dB, 63.5 dB (SIS). Sets range of coarse attenuator if this attenuator is present on the current rf channel (`cattn`).
- Upper Limit: (number entered directly). Sets upper limit of the coarse attenuator if this attenuator is present on the current rf channel (`parmax[17]`, `parmax[9]`, `parmax[18]`, `parmax[21]`).
- Fine Attenuator: Not Present, Present. Sets whether a fine attenuator is present or not on the current rf channel (`fattn`).
- Waveform Generator: Not Present, Present. Sets whether a waveform generator board is present or not on current rf channel (`rfgw`).
- Type of Amplifier: Class C, Linear Full Band, Linear Low Band, Shared, Linear Broadband. (Shared is fourth channel only.) Sets type of amplifier on the current rf channel (`amptype`).
- X Axis, Y Axis, Z Axis: None, WFG + GCU, Performa I, Performa II/III, Performa II/III+WFG, Performa XYZ, Performa XYZ+WFG, SIS (12 bit), Homospoil. On systems with gradients, sets type of gradient for each axis. The value is set separately for each axis (`gradtype`).
- Gradient Coil. Detects the gradient coil configuration file that defines the current installed gradient coil (`sysgcoil`).

Arguments: 'display' is a keyword that the system administrator can use to make config run in the display mode rather than the interactive mode.

Examples: `config`
`config('display')`

See also: *VnmrJ Installation and Administration*

Related:	<code>amptype</code>	Amplifier type (P)
	<code>audiofilter</code>	Audio filter type (P)
	<code>cattn</code>	Coarse attenuator (P)
	<code>Console</code>	System console type (P)
	<code>fattn</code>	Fine attenuator (P)
	<code>fifolpsize</code>	FIFO loop size (P)
	<code>gradtype</code>	Gradients for X, Y, and Z axes (P)
	<code>hlfreq</code>	Proton frequency of spectrometer (P)
	<code>latch</code>	Frequency synthesizer latching (P)
	<code>lockfreq</code>	Lock frequency (P)
	<code>numrfch</code>	Number of rf channels (P)
	<code>overrange</code>	Frequency synthesizer overrange (P)
	<code>parmax</code>	Parameter maximum values (P)
	<code>parmin</code>	Parameter minimum values (P)
	<code>parstep</code>	Parameter step size values (P)
	<code>ptsval</code>	PTS frequency synthesizer value (P)
	<code>rfchtype</code>	Type of rf channel (P)
	<code>rftype</code>	Type of rf generation (P)
	<code>rfgw</code>	RF waveform generator (P)
	<code>rotorsync</code>	Rotor synchronization (P)
	<code>shimset</code>	Type of shim set (P)
	<code>sysgcoil</code>	System gradient coil (P)
	<code>system</code>	System type (P)
	<code>traymax</code>	Sample changer tray slots (P)
	<code>vttype</code>	Variable temperature controller present (P)

confirm Confirm message using the mouse (C)

Syntax: `confirm(message) : response`

Description: Displays a dialog box with the specified message and two buttons: Confirm and Cancel. Clicking on the buttons with the mouse produces a return value.

Arguments: `message` is a single-line muticharacter string to be shown in the dialog box.
`response` is 1 if the user clicks the left button of the mouse on the Confirm button or presses the Return key; `response` is 0 if the user clicks the mouse on the Cancel button.

Examples: `confirm('Are you sure you want pw>100?'):$response`

See also: *User Programming*

Console System console type (P)

Description: A global parameter that sets the type of system console The value is usually set using the Console label in the Spectrometer Configuration window (opened from `config`).

When `go`, `au`, or `ga` is entered, the value of the Console parameter is copied from the systemglobal parameter tree to the current experiment and named as the `console` parameter (lowercase c). If `console` does not exist in an old parameter set, `rt` via `fixpar` creates it and sets it to ' '. Both `console` and `Console` are type acquisition. Macros can use `Console` and `console` to take conditional action based on spectrometer type.

See also: *VnmrJ Installation and Administration*

Related:	<code>au</code>	Submit experiment to acquisition and process data (M)
	<code>config</code>	Display current configuration and possibly change it (M)
	<code>fixpar</code>	Correct parameter characteristics in experiment (M)
	<code>ga</code>	Submit experiment to acquisition and FT the results (M)
	<code>rt</code>	Retrieve FIDs (M)
	<code>go</code>	Submit experiment to acquisition (M)
	<code>system</code>	System type (P)

contact_time MAS cross-polarization spin-lock contact time (M)

Applicability: Systems with solids module.

Description: Processes data obtained using an array of values for a pulse-length parameter. It runs the UNIX program `expfit`, which does an exponential curve fitting that determines the value of Tch and $T1rho$. The output is matched to the equation

$$I = [S0 - (S0 - S_{inf}) * \exp(-T/Tch)] * \exp(-T/T1rho) + S_{inf}$$

where Tch is the time constant of a spin-locked cross-polarization process, and $T1rho$ is relaxation time of ^{13}C polarization in the proton rotating field.

The required input is file `fp.out` from the program `fp` and the values of the arrayed parameter. The output table is file `analyze.list` in the current experiment. The file `analyze.out` is used by the `expl` to display the results.

See also: *User Guide: Solid-State NMR*

Related:	<code>expfit</code>	Least-squares fit to polynomial or exponential curve (U)
	<code>expl</code>	Display polynomial/exponential curves (C)
	<code>fp</code>	Find peak heights (C)

continueMovie Continue movie in either forward or backward direction (C)

Syntax: `continueMovie(rate)`

Description: Like `startMovie`, but `continueMovie` can play a movie forward or backward, and, instead of always starting from the beginning, it starts from the beginning if movie has not started yet, or continues from where it was stopped (by `stopMovie`). Movie direction is controlled by parameter `aipMovieSetting[3]=1` or `-1`.

Arguments: `aipMovieRate`, or a number for the rate

See also: `startMovie`, `stopMovie`, `resetMovie`.

convert Convert data set from a VXR-style system (M,U)

Syntax: `convert(VXR_file)`
(From UNIX) `cpos_cvt VXR_file`

Description: Converts data stored on a VXR-style system (VXR, XL, or Gemini) to the format used in software. The macro `convert` loads the data from `VXR_file` into the current experiment and converts it to the new format. The UNIX command `cpos_cvt` writes the converted data in a subdirectory of the current working directory, using the original name of the data set.

Arguments: `VXR_file` is the name of a VXR-style file to be converted to VnmrJ style

See also: *NMR Spectroscopy User Guide*

Related: `cpos_cvt` Convert data set from a VXR-style system (C,U)
`decomp` Decompose a VXR-style directory (C)

convertbru Convert Bruker data (M,U)

Syntax: (From UNIX) `convertbru file <options>`
`convertbru(file<,options>)`

Description: A C-language program for converting 32-bit Bruker AMX data and 24- and 32-bit Bruker AM data into a 32-bit format compatible with the Varian `sread` program. After converting the Bruker data into the new format, the converted data can be read into VnmrJ using `sread` and can then be processed normally. The parameters `proc` and `proc1` are set appropriately by `sread`, so that `wft` or `wft2da` correctly processes the data.

Bruker AM parameters are converted to Varian parameters as shown in the table "AM Parameter Conversion." Bruker parameter names that do not conflict with a Varian parameter name are converted under the original name: `td`, `fw`, `ds`, `o1`, `o2`, `ns`, `te`, `id`, `sfo1`, `sfo2`, and `ro`. Parameters `proc` and `proc1` are set to 'rft' for all spectra (assuming TPPI data in both dimensions).

AM Parameter Conversion

<i>Bruker</i>	<i>Varian</i>	<i>Bruker</i>	<i>Varian</i>
sweeps completed	<code>ct</code>	<code>sp</code>	<code>satdly</code>
<code>td</code>	<code>np</code>	<code>dp</code>	<code>dpwr</code>
<code>dw</code>	<code>dw</code>	<code>te</code>	<code>temp=te-273</code>
<code>fw</code>	<code>fb=1.1*sw/2</code>	<code>id</code>	<code>sw1=1/id</code>
<code>ds</code>	<code>ss</code>	<code>sfo1</code>	<code>sfrq=sfo1+o1</code>
<code>sw</code>	<code>sw</code>	<code>sfo2</code>	<code>dfrq=sfo2+o2</code>
experiments done	<code>ni</code>	<code>p#</code>	<code>p#</code>
<code>o1</code>	<code>tof</code>	<code>d#</code>	<code>d#</code>
<code>o2</code>	<code>dof</code>	<code>s#</code>	<code>s#</code>
<code>rd</code> (or <code>d1</code> if <code>rd=0</code>)	<code>rd</code>	<code>ro</code>	<code>spin</code>
<code>pw</code> (or <code>p0</code> if <code>pw=0</code>)	<code>pw</code>	<code>rg</code>	<code>gain</code>

<i>Bruker</i>	<i>Varian</i>	<i>Bruker</i>	<i>Varian</i>
p1	pw90	date	date
de	de	time	time
ns	nt		

Bruker AMX parameters are converted to Varian parameters as shown in the table “AMX Parameter Conversion.” All Bruker parameters are converted under their original names if the name doesn't conflict with the name of a Varian parameter. Arrayed Bruker parameters like P and D are converted to the names P# and D#, where # is the index into the array.

Because `sread` is limited to 8-character parameter names, the parameters `rouwd1#` and `rouwd2#` are converted to `rtwd1#` and `rtwd2#`.

The parameter `proc` is set to 'ft' when the Bruker parameter `aq_mod` is 1, and `proc` is set to 'rft' when `aq_mod` is 2. `procl` is always set to `rft`, assuming TPPI in `t1`.

If there is a file named `info` in the directory with the Bruker data, it is read in and put into the text file for the converted data set.

AMX Parameter Conversion

<i>Bruker</i>	<i>Varian</i>	<i>Bruker</i>	<i>Varian</i>
ns (from acqu)	nt	te	temp=te-273
ns (from acqu)	ct	sfo1	sfrq=sfo1
td (from acqu)	np	sfo2	dfrq=sfo2
td (from acqu2s)	ni	o1	tof
sw_h	sw	o2	dof
sw_h	dw=1.0e6/sw	ro	spin
sw_h (from acqu2s)	sw1	rg	gain
fw	fb=1.1*sw/2	date	date
ds	ss	date	time
rd (or d1 if rd=0)	rd	nucleus	tn
de	de	decnuc	dn
pw (or p0 if pw=0)	pw	pulprog	pslabel
p1	pw90	pulprog	seqfil

Arguments: `file` is the input file name. For AMX data, `file` should be the name of the directory that contains the `acqu`, `acqu2s`, and `fid` or `ser` files. For AM data, `file` should be the name of the file containing the AM data. The `file` argument is not required to have a `.bru` extension, but if it does, the `.bru` extension is removed before creating the output file. Unless the `-cfile` option is present, the output file will have the same name as the input file, but with a `.cv` extension, and will be written into the current working directory.

options for AMX and AM data are the following, which can be entered in any order as long as `file` comes first (options are usually not necessary, but can be used to override the default actions of `convertbru`):

- `-bam` or `-bamx` specifies whether input is AM or AMX data. The default is determined from name of the input file given.
- `-cfile` specifies that the output file is given the name specified by `file` and is written with `.cv` appended to the name

- `-dxxx`, where `xxx` is the decoupler frequency (it must be a value between 10.0 and 640.0 MHz). The default is to read from data set.
- `-f` specifies that old output file is to be overwritten. The default is to not overwrite old files.
- `-olsb` or `-omsb` specifies whether the data has the least- or most-significant byte first. For AM data, the default is determined from data set. For AMX data, the default is `-olsb`.
- `-pxxx`, where `xxx` is the number of 24- or 32-bit words to skip before converting data. This option is for use with `-t` option to skip the header in AM data without converting it. Typical header sizes are 216 or 256 words. The default is 0.
- `-s3` or `-s4` specifies if AM data is 24-bit (3-byte) or 32-bit (4-byte). All AMX data is 32-bit. The default is determined from the data set.
- `-tall`, `-thdr`, or `-tdata` specifies whether `convertbru` should convert the header and the data, just the header, or just the data. The default is `-tall`.

Examples: Convert AM data from a UNIX shell (in all these examples, the file name is arbitrarily named `br_data`):

- `convertbru br_data` determines the file format and converts the header and data in the file `br_data`.
- `convertbru br_data -d250.0 -cout` determines the file format, converts the header and data in the `br_data`, sets the decoupler frequency to 250.0 MHz, and writes to an output file named `out.cv` in the current working directory.
- `convertbru br_data -thdr` determines file format and converts only the header in the file `br_data`.
- `convertbru br_data -tdata -p256 -s3 -omsb` converts only the data in `br_data` after skipping the 256-word header. The data is converted assuming it is 24-bit AM data words with the most-significant byte first.

Convert AM data from VnmrJ:

- `convertbru('br_data', '-tdata', '-p256', '-s3', '-omsb')` converts only the data in `br_data` after skipping the 256-word header. The data is converted assuming it is 24-bit AM data words with the most-significant byte first.

Convert AMX data from a UNIX shell:

- `convertbru br_data -f` converts `acqus` and `acqu2s` files to ASCII, if needed, and then converts data and overwrites the existing `br_data.cv` file.

Convert AMX data from VnmrJ:

- `convertbru('br_data', '-f')` converts `acqus` and `acqu2s` files to ASCII, if needed, and then converts data and overwrites the existing `br_data.cv` file.
- `convertbru('br_data', '-c/home/vnmr1/bdata/data1')` converts `acqus` and `acqu2s` files to ASCII, if needed, and then converts the data and writes it to `/home/vnmr1/bdata/data1.cv`.

See also: *NMR Spectroscopy User Guide*

Related: [readbrutape](#) Read Bruker data files from 9-track tape (U)

`sread` Read converted data into VnmrJ (C)
`wft2da` Weight and Fourier transform phase-sensitive data (M)

copy **Copy a file (C)**

Syntax: `copy(<'-r',>from_file,to_file)<:$res>`

Description: Makes a copy of a file and is identical to the `cp` command. All arguments are passed. Command will abort with no return value if an illegal file name is used.

Arguments: `'-r'` — keyword requesting a recursive copy (i.e., copy a directory).

`from_file` — name of the file (or directory if `'-r'` used) to be copied.

`to_file` — name of the copy of the file (or directory). If the `from_file` argument has an extension (e.g., `.fid`), be sure the `to_file` argument has the same extension.

`:$res` — variable to hold the result of the copy process.

1 is returned if the copy is successful.

0 is returned if the copy failed.

Examples: `copy(' -r', '/home/vnmr1/vnmrsys/seqlib', '/vnmr/seqlib')`

`copy('/home/vnmr1/vnmrsys/seqlib/d2pul', \`
`'/vnmr/seqlib/d2pul')`

See also: *NMR Spectroscopy User Guide*

Related: `cp` Copy a file (C)

cos **Find cosine value of an angle (C)**

Syntax: `cos(angle)<:n>`

Description: Finds the cosine of an angle.

Arguments: `angle` is the angle, given in radians.

`n` is the return value with the cosine of `angle`. The default is to display the cosine value in the status window.

Examples: `cos(.5)`
`cos(val):cos_val`

See also: *User Programming*

Related: `sin` Find sine value of an angle (C)

Cosy **Convert the parameter to a COSY experiment (M)**

Description: Convert the parameter to a COSY experiment.

See also: *NMR Spectroscopy User Guide*

Related: `cosyps` Set up parameters for phase-sensitive COSY pulse sequence (M)
`Dqcosy` Set up parameters for double-quantum filtered COSY (M)
`relayh` Set up parameters for RELAYH pulse sequence (M)

cosyps **Set up parameters for phase-sensitive COSY pulse sequence (M)**

Description: Sets up a phase-sensitive COSY (homonuclear correlation) experiment.

See also: *NMR Spectroscopy User Guide*

Related: `Cosy` Set up parameters for COSY pulse sequence (M)

C

Dqcosy Set up parameters for double-quantum filtered COSY (M)
relayh Set up parameters for RELAYH pulse sequence (M)

cp Copy a file (C)

Syntax: `cp (<'-r' , >from_file, to_file) <:$res>`

Description: Makes a copy of a file and is identical to the **copy** command. All arguments are passed. Command will abort with no return value if an illegal file name is used.

Arguments: **'-r'** is a keyword requesting a recursive copy (i.e., copy a directory).

`from_file` is the name of the file (or directory if **'-r'** used) to be copied.

`to_file` is the name of the copy of the file (or directory). If the `from_file` argument has an extension (e.g., `.fid`), be sure the `to_file` argument has the same extension.

`$res` variable to hold the result of the copy process.

1 is returned if the copy is successfully

0 is returned if the copy failed

Examples: `cp ('/home/vnmr1/vnmrsys/seqlib/d2pul', \`
`'/vnmr/seqlib/d2pul')`
`cp ('-r', '/home/vnmr1/vnmrsys/seqlib', '/vnmr/seqlib')`

See also: *NMR Spectroscopy User Guide*

Related: **copy** Copy a file (C)

cp Cycle phase (P)

Description: Sets the values that real-time variable `oph` is calculated as, either 0,1,2,3 (`cp= 'y'`) or 0 (`cp= 'n'`). The only circumstance where setting `cp= 'n'` may be useful is when displaying an FID with **acqi**. If there is an imbalance between the two receiver channels, the FID displayed for **acqi** may show alternating dc levels. The standard **gf** macro that prepares parameters for the FID display in **acqi** automatically handles this issue.

Values: **'y'** makes `oph` calculate as 0,1,2,3; this is the typical value.

'n' makes `oph` calculate as 0.

See also: *User Programming*

Related: **acqi** Interactive acquisition display process (C)
go Submit experiment to acquisition (C)
gf Prepare parameters for FID/spectrum display in **acqi** (M)

cpmgt2 Set up parameters for CPMGT2 pulse sequence (M)

Description: Macro to set up a CPMGT2 (Carr-Purcell Meiboom-Gill T_2) experiment.

See also: *NMR Spectroscopy User Guide*

Related: **t2** T_2 exponential analysis (M)

cpos_cvt Convert data set from a VXR-style system (M,U)

Syntax: (From UNIX) `cpos_cvt VXR_file`
`convert (VXR_file)`

Description: Converts data stored on a VXR-style system (Gemini, VXR, or XL) to the format used in VnmrJ software. `cpos_cvt` writes the converted data in a subdirectory of the current working directory, using the original name of the

data set. The command `convert` loads the data from `VXR_file` into the current experiment and converts it to the new format.

Arguments: `VXR_file` is the file name in the VXR-style format to be converted to the VnmrJ style.

Related:	<code>convert</code>	Convert data set from a VXR-style system (C,U)
	<code>decomp</code>	Decompose a VXR-style directory (C)
	<code>rt</code>	Retrieve FIDs (C)

cptmp **Copy experiment data into experiment subfile (M)**

Syntax: `cptmp<(file)>`

Description: Copies the data (parameters, FID, and transformed spectrum) from the current experiment into a subdirectory inside `curexp+ '/subexp'`.

Arguments: `file` is the name of the subfile to receive the data. The default is to take the name from the transmitter nucleus (if `seqfil = 's2pul'`) or to use the pulse sequence name.

Examples: `cptmp`
`cptmp('cosy')`

Related:	<code>curexp</code>	Current experiment directory (P)
	<code>rttmp</code>	Retrieve experiment data from experiment subfile (M)
	<code>seqfil</code>	Pulse sequence name (P)
	<code>svtmp</code>	Move experiment data into experiment subfile (M)

cpx **Create pbox shape file (M)**

Syntax: `cpx<(ref_pw90,ref_pwr)>` or `cpx<('g')>`

Description: Calls UNIX command `Pbox`, which generates the specified pulse shape or decoupling/spin locking pattern, as defined by the `shapelib/Pbox.inp` file.

Arguments: `ref_pw90` is the reference 90° pulse width
`ref_pwr` is the reference power level.
`'g'` is a keyword that is required only when generating gradient shapes and if the file type is not specified otherwise.

Examples: `cpx`
`cpx('g')`
`cpx(pw90*compH, tpwr)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>Pbox</code>	Pulse shaping software (U)

cqexp **Load experiment from protocol (M)**

Applicability: Liquids

Description: Macro to load an experiment from a protocol.

Syntax: `cqexp(experiment <, apptype>)`

The first argument is the experiment name, and the second argument is the apptype. If the apptype is not specified, the previous apptype is used.

Examples: `cqexp('Proton', 'stdld')`

Related: [apptype](#) Application type (P)
[execpars](#) Set up the exec parameters (M)

cqfindz0 Run an experiment to find the value of z0 (M)

Applicability: Liquids

Description: A macro to run a deuterium experiment to find the correct value of z0 for a given solvent. It requires an entry in the probe file for the number of deuterium Hz per DAC. Run the appropriate probe calibration for 1k Hz per DAC to set the value in the probe file. The macro may be accessed through the Find z0 button available on several panels.

Related: [solvent](#) Lock solvent (P)
[z0](#) Z0 field position (P)

cqgmap Perform gradient shimming utility functions (M)

Applicability: Liquids

Description: Macro runs gradient shimming utility functions.

Related: [gmapshim](#) Run gradient autoshimming, set parameters, map shims (M)

cqinit Initialize liquids study queue (M)

Applicability: Liquids

Description: Initializes the liquids study queue.

Related: [cqreset](#) Reset study queue parameters (M)
[sqfilemenu](#) Study queue file menu commands (M)

cqpars Create study queue parameters for liquids (M)

Applicability: Liquids

Description: A macro to create study queue parameters for the Walkup interface.

See also: VnmrJ Walkup

Related: [fixpar](#) Correct parameter characteristics in experiment (M)

cqplot Macro to perform generic 2D plot (M)

Applicability: Liquids

Description: A macro to perform generic 2D plotting, including 1D experiment traces. Usually called by other macros, and not used from the command line.

Related: [plot](#) Automatically plot spectra (M)
[plot2D](#) Plot results of 2D peak picking (C)
[plt2Darg](#) Plot 2D arguments (P)

cqprotocol Macro to create protocols (M)

Applicability: Liquids

Description: A macro to create protocols for liquids applications. Called by the *Make protocols dialogs* in the Utilities menu.

cgreset Reset study queue parameters (M)

Applicability: Liquids

Description: Reset liquids study queue parameters. Usually called by other macros when starting a new study.

Related: `cqinit` Initialize liquids study queue (M)
`sqfilemenu` Study queue file menu commands (M)

cgsavestudy Macro to save study queue parameters (M)

Applicability: Liquids

Description: A macro to save study parameters in the liquids study queue. Usually called by other macros when starting a new study.

Related: `studypar` Study parameters (P)
`xmsubmit` Submit sample(s) to the study queue (M)
`xmendq` End a chained study queue (M)

cgtwmenu Macro to set weighting functions from a panel (M)

Applicability: Liquids, Imaging

Description: A macro to set weighting functions from a panel. It is used for both 1D and 2D weighting parameters. Called by processing parameter panels.

cr Cursor position in directly detected dimension (P)

Description: Contains the current cursor position. The `rl` macro uses `cr` to set the reference line.

See also: *NMR Spectroscopy User Guide*

Related: `centersw` Move cursor to center of spectrum (M)
`crf` Current time-domain cursor position (P)
`crl` Clear ref. line in directly detected dimension (M)
`delta` Difference of two frequency cursors (P)
`rl` Set reference line in directly detected dimension (M)

crl Cursor position in 1st indirectly detected dimension (P)

Description: Contains the current cursor position along the first indirectly detected dimension. Analogous to the `cr` parameter except that `crl` applies to the first indirectly detected dimension of a multidimensional data set. The `rl1` macro uses `crl` to set the reference line along this dimension.

See also: *NMR Spectroscopy User Guide*

Related: `centersw1` Move cursor to center of spectrum in 1st indirect dimension (M)
`cr` Cursor position in directly detected dimension (P)
`cr2` Cursor position in 2nd indirectly detected dimension (P)
`rl1` Set ref. line in 1st indirectly detected dimension (M)

C

cr2 Cursor position in 2nd indirectly detected dimension (P)

Description: Contains the current cursor position along the second indirectly detected dimension. Analogous to the **cr** parameter except that **cr2** applies to the second indirectly detected dimension of a multidimensional data set. The **r12** macro uses **cr2** to set the reference line along this dimension.

See also: *NMR Spectroscopy User Guide*

Related:

centersw2	Move cursor to center of spectrum in 2nd indirect dimension (M)
cr	Cursor position in directly detected dimension (P)
cr1	Cursor position in 1st indirectly detected dimension (P)
r12	Set ref. line in 2nd indirectly detected dimension (M)

crcom Create user macro without using text editor (M)

Syntax: `crcom(file,actions)`

Description: Creates a macro file in the user's macro library (maclib) with the contents given in the **actions** argument.

Arguments: **file** is the file name of the user macro to be created. If a macro of the same name already exists, the user is asked whether or not to overwrite it.

actions is a string containing the actions making up the user macro. The string cannot include a carriage return. If a single quote is needed within the string, it must be preceded by a backslash (see second example below).

Examples: `crcom('plot','pl pscale pap page')`
`crcom('lds','load=\'y\' su load=\'n\'')`

See also: *User Programming*

create Create new parameter in a parameter tree (C)

Syntax: `create(parameter<,type<,tree>>)`

Description: Creates a parameter in one of the parameter trees. A *parameter tree* is a UNIX file containing the attributes of parameters as formatted text. Refer to the command **paramvi** for a description of the file contents.

Arguments: **parameter** is the name of the parameter to be created.

type is the type of values in the parameter to be created and can be one of the following values (default is 'real'):

- 'real' is a value with no limits on range and can be positive or negative.
- 'string' is a value composed of characters. Entry of strings can be limited to selected words by enumerating the possible values with the command **setenumerat**. For example, the enumerated values of **intmod** are 'off', 'partial', and 'full'. Therefore, **intmod** can be set only to one of these three string values, such as **intmod='full'**.
- 'delay' is a value from 0 to 8190, in unit of seconds.
- 'frequency' is a positive real number value.
- 'flag', like 'string', is a value composed of characters. Entry of flags can be limited to selected characters by enumerating the possible values with the command **setenumerat**. For example, the enumerated values of **dmm** are 'c', 'f', 'g', 'm', 'p', 'r', 'u', 'w', and 'x'. Therefore, **dmm** can only be set to a combinations of these nine characters, such as **dmm='ccw'**. If enumerated values are not set, the 'string' and 'flag' types are identical.
- 'pulse' is a value from 0 to 8190, in units of μ s.

- 'integer' is a value composed of integers (0, 1, 2, 3, ...).
- tree is one of the following types of parameter trees (default is 'current'):
- 'current' contains parameters that are adjusted to set up an experiment. The parameters are from the file `curpar` in the current experiment.
 - 'global' contains user-specific parameters from the file `global` in the `vnmr/sys` directory of the present UNIX user.
 - 'processed' contains parameters with which the data was obtained. These parameters are from the file `propar` in the current experiment.
 - 'systemglobal' contains instrument-specific parameters from the text file `/vnmr/conpar`. Most of these parameters are defined using the `config` program. All users have the same `systemglobal` tree. Note that `conpar` is not written out when you exit; the only time `conpar` is ever modified is by the `config` program. Thus, any changes you make to `conpar` using `create` (or `destroy`, `setvalue`, etc.) are not permanent. To permanently create a parameter in `conpar`, you must use a text editor to change `/vnmr/conpar`.

Examples: `create('a')`
`create('b', 'string')`
`create('c', 'real', 'global')`

See also: *User Programming*

Related:	<code>destroy</code>	Destroy a parameter (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>fread</code>	Read parameters from file and load them into a tree (C)
	<code>fsave</code>	Save parameters from a tree to a file (C)
	<code>paramvi</code>	Edit a parameter and its attributes using <code>vi</code> text editor (M)
	<code>prune</code>	Prune extra parameters from current tree (C)
	<code>setenumerals</code>	Set values of a string variable in a tree (C)
	<code>setgroup</code>	Set group of a parameter in a tree (C)
	<code>setprotect</code>	Set protection mode of a parameter (C)

createqcomp Create qcomp parameter (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Macro to create the `qcomp` parameter with the appropriate attributes. `qcomp` is created as a flag parameter in the global tree.

crf Current time-domain cursor position (P)

Description: Contains current time-domain cursor position. To create `crf` and the other FID display parameters `axisf`, `dotflag`, `vpf`, `vpfi`, and `deltaf` (if the parameter set is older and lacks these parameters), enter `addpar('fid')`.

Values: Number, in seconds.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>cr11</code>	Clear ref. line in 1st indirectly detected dimension (C)
	<code>deltaf</code>	Difference of two time cursors (P)
	<code>fidpar</code>	Add parameters for FID display in current experiment (M)

C

cr1 Clear reference line in directly detected dimension (M)

Description: Clears frequency referencing along the directly detected dimension by setting the reference parameters **rfl** and **rfp** to zero. **cr1** also resets the referencing parameters **refpos** and **reffrq**.

See also: *NMR Spectroscopy User Guide*

Related:

cr11	Clear ref. line in 1st indirectly detected dimension (C)
cr12	Clear ref. line in 2nd indirectly detected dimension (C)
r1	Set ref. line in directly detected dimension (M)
reffrq	Reference frequency of reference line (P)
refpos	Position of reference frequency (P)
rfl	Ref. peak position in directly detected dimension (P)
rfp	Ref. peak frequency in directly detected dimension (P)

cr11 Clear reference line in 1st indirectly detected dimension (M)

Description: Clears frequency referencing along the first indirectly detected dimension by setting the reference parameters **rfl1** and **rfp1** to zero. **cr11** also resets the referencing parameters **refpos1** and **reffrq1**.

See also: *NMR Spectroscopy User Guide*

Related:

cr1	Clear ref. line in directly detected dimension (C)
r11	Set ref. line in 1st indirectly detected dimension (M)
reffrq1	Ref. frequency of reference line in 1st indirect dimension (P)
refpos1	Position of reference frequency in 1st indirect dimension (P)
rfl1	Ref. peak position in 1st indirectly detected dimension (P)
rfp1	Ref. peak frequency in 1st indirectly detected dimension (P)

cr12 Clear reference line in 2nd indirectly detected dimension (M)

Description: Clears frequency referencing along the second indirectly detected dimension by setting the reference parameters **rfl2** and **rfp2** to zero. **cr12** also resets the referencing parameters **refpos2** and **reffrq2**.

See also: *NMR Spectroscopy User Guide*

Related:

cr1	Clear ref. line in directly detected dimension (C)
r12	Set ref. line in 2nd indirectly detected dimension (M)
reffrq2	Ref. frequency of reference line in 2nd indirect dimension (P)
refpos2	Position of reference frequency in 2nd indirect dimension (P)
rfl2	Ref. peak position in 2nd indirectly detected dimension (P)
rfp2	Ref. peak frequency in 2nd indirectly detected dimension (P)

crmode Current state of the cursors in df, ds, or dcon1 programs (P)

Description: Stores the current state (box mode or cursor mode) of cursors in the **df**, **ds**, or **dcon1** interactive display programs. **crmode** is mostly used by programmable menus to determine the status of the cursors. It is stored in the file **vnmrsys/global**.

Values: 'b' signifies the box mode, 'c' signifies the cursor mode.

See also: *User Programming*

Related:

dcon1	Interactive 2D data display (C)
df	Display a single FID (C)
ds	Display a spectrum (C)

crof2 Recalculate rof2 so that lp = 0 (M)

Syntax: `crof2<(alfa)>`

Description: Recalculates a new value for `rof2` (receiver gating time following a pulse) based upon the current `rof2` and `lp` (first-order phase) values, so that `lp` is rendered approximately 0. For `crof2` to work properly, a trial spectrum must be obtained and phased to pure absorption. This spectrum provides the current `rof2` and `lp` values for `crof2`. The value of the `alfa` delay is left constant, provided `rof2` does not become less than 1 μ s.

`crof2` pertains to processing 2D data. Unless `lp` is approximately 0, `fpmult` affects both the dc offset and the curvature of the spectrum.

Arguments: `alfa` specifies a value for the `alfa` delay before acquisition.

Related:	<code>alfa</code>	Set <code>alfa</code> delay before acquisition (P)
	<code>cfpmult</code>	Calculate first point multiplier for 2D experiments (P)
	<code>fpmult</code>	First point multiplier for np FID data (P)
	<code>lp</code>	First-order phase along directly detected dimension (P)
	<code>rof2</code>	Receiver gating time following a pulse (P)

cryo_noisetest Run Cold Probe conditioning experiments (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Runs the probe conditioning experiments and analyzes the noise using the `cnd` macro. Measures the hydrogen-induced noise and provides an efficient remedy.

Values: NOBURN – waits the operator input period of time between tests.
No arguments – macro will prompt for a time in minutes.

cryoclient Start the CryoBay Monitor program (M, U)

Applicability: Systems with Cold Probes and CryoBay Monitor software.

Description: Starts the CryoBay Monitor software in a separate window. This program is a CORBA client that requires an active CORBA server running on the CryoBay PC.

See also: *Cryogenic Systems Installation and Operation*

ct Completed transients (P)

Description: Stores a nonuser-enterable informational parameter that changes during the course of an experiment to reflect the number of completed transients. During most experiments, an accurate transient counter is displayed in the acquisition status window, updated every five seconds.

The value of `ct` is displayed in the acquisition parameter group by the `dg` command and is only updated when data processing occurs on the FID. In an experiment that is accumulating and not processed until the acquisition is complete, `ct` always indicates 0 until the end of the acquisition.

See also: *NMR Spectroscopy User Guide*

Related: `dg` Display parameters of acquisition/processing group (C)

ctext Clear the text of the current experiment (C)

Description: Clears the text from the current experiment text file (a block of text that may be used to describe the sample and experiment).

See also: *NMR Spectroscopy User Guide*

Related: `atext` Append string to the current experiment text (M)
`text` Display text or set new text for current experiment (C)

curexp Current experiment directory (P)

Description: Contains the full UNIX path to the currently active experiment. This parameter is useful when accessing text files generated by various commands (e.g., `cat (curexp+ ' /fp.out ' )`).

See also: *NMR Spectroscopy User Guide*

Related: `systemdir` VnmrJ system directory (P)
`userdir` VnmrJ user directory (P)

curscan Scan currently in progress (P)

Applicability: Systems with LC-NMR accessory.

Description: Keeps track of which “scan” is currently in progress. If `curscan` does not exist, the `parlc` macro can create it.

See also: *NMR Spectroscopy User Guide*

Related: `parlc` Create LC-NMR parameters (M)

curwin Current window (P)

Description: An arrayed global parameter. The first value is the index of the selected window pane in the graphics window. The second value is the number of window pane rows. The third value is the number of columns.

See also: *NMR Spectroscopy User Guide*

Related: `fontselect` Open FontSelect window (C)
`jwin` Activate current window (M)
`mapwin` List of experiment numbers (P)
`setgrid` Activate selected window (M)
`setwin` Activate selected window (C)

cutoff Data truncation limit (P)

Description: Defines the distance above and below the current vertical position `vp` at which spectra and integrals are truncated. By arraying `cutoff` to have two different values, the truncation limits above and below the current vertical position can be controlled independently (e.g., `cutoff=50` truncates data at `vp+50` mm and `vp-50` mm, and `cutoff=50, 10` truncates data at `vp+50` mm and `vp-10` mm). `cutoff='n'` disables the action of `cutoff`.

`cutoff` is not active during interactive spectral displays (i.e., for the `ds` command), but is active during non-interactive spectral displays and plots (for the `dss` and `pl` commands).

Values: 'n', number in mm.

See also: *NMR Spectroscopy User Guide*

Related: `ds` Display a spectrum (C)
`dss` Display stacked spectra (C)
`pl` Plot spectra (C)
`vp` Vertical position of spectrum (P)

- cyclenoe** **Set up parameters for CYCLENOE pulse sequence (M)**
 Applicability: Systems in which the observe channel is equipped with direct synthesis rf and a linear amplifier.
 Description: Sets up a difference NOE experiment.
- cy1br24** **Set up parameters for cycled BR24 pulse sequence (M)**
 Applicability: Systems with solids module.
 Description: Sets up a BR24 sequence with quadrature detection and prepulse for solids multiple-pulse line narrowing.
 See also: *User Guide: Solid-State NMR*
 Related: [br24](#) Set up parameters for BR24 pulse sequence (M)
- cylmrev** **Set up parameters for cycled MREV8 pulse sequence (M)**
 Applicability: Systems with a solids module.
 Description: Sets up a MREV8 sequence with quadrature detection and prepulse for solids multiple-pulse line narrowing.
 See also: *User Guide: Solid-State NMR*
 Related: [mrev8](#) Set up parameters for MREV8 pulse sequence (M)
- cz** **Clear integral reset points (C)**
 Syntax: `cz<(frequency1,frequency2,...)>`
 Description: Removes currently defined integral reset points.
 Arguments: `frequency1,frequency2,...` are reset points corresponding to specified frequencies to be removed. The default is remove all reset points.
 Examples: `cz`
 `cz(800,600,250,60)`
 See also: *NMR Spectroscopy User Guide*
 Related [dli](#) Display listed integral values (C)
 [dlni](#) Display listed normalized integral values (C)
 [nli](#) Find normalized integral values (C)
 [z](#) Add integral reset point at the cursor position (C)

E

e	Eject sample (M)
eaddr	Display Ethernet address (M,U)
ecc_on	Turns on eddy current compensation for Cold Probes (M)
ecc_off	Turns off eddy current compensation for Cold Probes (M)
echo	Display strings and parameter values in text window (C)
edit	Edit a file with user-selectable editor (M)
eject	Eject sample (M)
elist	Display directory on remote VXR-style system (M,U)
email	Email address (P)
enter	Enter sample information for automation run (M,U)
enterdialog	Start a dialog window using enterexp file (M)
eread	Transfer file from remote source (M,U)
ernst	Calculate the Ernst angle pulse (C)
errlog	Display recent error messages (C)
errloglen	Number of lines in error message display (P)
ewrite	Transfer file to remote destination (M,U)
exec	Execute a command (C)
execpars	Set up the exec parameters (M)
execplot	Execute plotting macro (P)
execprep	Execute prepare macro (P)
execprescan	Execute prescan macro (P)
execproc	Execute processing macro (P)
execprocess	Execute processing macro (P)
execsetup	Execute setup macro (P)
exists	Checks if parameter, file, or macro exists and file type (C)
exit	Call the vnmr _{exit} command (M)
exp	Find exponential value of a number (C)
expactive	Determine if experiment has active acquisition (C)
expfit	Make least-squares fit to polynomial or exponential curve (U)
expl	Display exponential or polynomial curves (C)
expladd	Add another diffusion analysis to current display (M)
explib	Display experiment library (M)
explist	Display current experiment chain and approx. time for each (M)
explog	Display log file for experiment (M)
exptime	Display experiment time (C)

e **Eject sample (M)**

Description: Ejects the sample from the probe by turning on the eject air and the slow drop air. The **e** macro functions the same as the **eject** macro.

E

See also: *NMR Spectroscopy User Guide*

Related: **eject** Eject sample (M)
i Insert sample (M)
insert Insert sample (M)

eaddr Display Ethernet address (M,U)

Description: Displays the name of the local host and its hardware Ethernet address. The 48-bit address is presented in octal, decimal, and hexadecimal formats.

See also: *NMR Spectroscopy User Guide*

Related: **dnode** Display list of valid limNET nodes (M,U)

ecc_on Turns on eddy current compensation for Cold Probes (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Turns on eddy current compensation

Related: **ecc_off** Turns off eddy current compensation for Cold Probes (M)

ecc_off Turns off eddy current compensation for Cold Probes (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Turns off eddy current compensation.

Related: **ecc_on** Turns on eddy current compensation for Cold Probes (M)

echo Display strings and parameter values in text window (C)

Syntax: `echo(<' -n' ,>string1,string2, ....)>`

Description: Displays strings and parameter values in the text window similar to the UNIX echo command.

Arguments: ' -n ' is a keyword that suppresses advancing to the next line. The default is to advance to the next line.

`string1,string2,...` are one or more strings (surrounded with single quote marks) or parameters. The format used for numbers is identical to the %g format described for the **write** command.

Examples: `echo`
`echo('This is a string')`
`echo('Pulse Width is: ',pwr)`
`echo(' -n ', 'No new line')`

See also: *User Programming*

Related: **write** Write formatted text to a device (C)

edit Edit a file with user-selectable editor (M)

Syntax: `edit(file)`

Description: Opens a file for editing using a text editor. The default editor is vi. To select another editor, set the UNIX environmental variable `vimreditor` to the name of the editor (change the line `setenv vimreditor old_editor` in `.login` to become `setenv vimreditor new_editor`, e.g., `setenv vimreditor emacs`) and make sure a script with the prefix `vimr_` followed

by the name of the editor (e.g., `vnmr_emacs`) is placed in the `bin` subdirectory of the system directory. The script file makes adjustments for the type of graphic interface in use.

Scripts provided with VnmrJ include `vnmr_vi` and `vnmr_textedit`. To create other scripts, see the `vnmr_vi` script for non-window editor interfaces and the `vnmr_textedit` script for window-based editor interfaces.

Arguments: `file` is the name of the file you wish to edit.

Examples: `edit('myfile')`

See also: *User Programming*

Related:	<code>paramedit</code>	Edit a parameter and its attributes with user-selected editor (C)
	<code>paramvi</code>	Edit a parameter and its attributes with <code>vi</code> editor (M)
	<code>macroedit</code>	Edit a user macro with user-selectable editor (C)
	<code>macrovi</code>	Edit a user macro with <code>vi</code> editor (C)
	<code>menuvi</code>	Edit a menu with the <code>vi</code> editor (M)
	<code>textvi</code>	Edit text file of current experiment with <code>vi</code> editor (M)

eject **Eject sample (M)**

Syntax: `eject`

Description: Ejects the sample from the probe by turning on the eject air and the slow drop air. The `e` macro functions the same as the `e` macro.

See also: *NMR Spectroscopy User Guide*

Related:	<code>e</code>	Eject sample (M)
	<code>i</code>	Insert sample (M)
	<code>insert</code>	Insert sample (M)

elist **Display directory on remote VXR-style system (M,U)**

Syntax: `elist(remote_node,remote_directory)`
(From UNIX) `elist remote_node remote_directory`

Description: Lists directory contents on a remote VXR-style (Gemini, VXR-4000, or XL) system.

Arguments: `remote_node` is the name of the remote VXR-style system.
`remote_directory` is the name of the directory on the remote system.

Examples: `elist('gemini','fidlib')`
(From UNIX) `elist gemini fidlib`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dnode</code>	Display list of valid limNET nodes (M,U)

email **Email address (P)**

Applicability: *VnmrJ Walkup*

Description: A global parameter set to the email address of an operator. It is used to send an email message to an operator when an experiment or sample is complete. The parameter is set from the operator email field in the VnmrJ Adm interface.

See also: *VnmrJ Installation and Administration, VnmrJ Walkup*

Related:	<code>operatorlogin</code>	Sets workspace and parameters for the operator (M)
	<code>prescan</code>	Study queue prescan (P)

E

enter **Enter sample information for automation run (M,U)**

Applicability: Systems with an automatic sample changer.

Syntax: `enter<(file<,configuration_file>)>`
(From UNIX) `enter <file> <configuration_file>`

Description: Enables entry of sample information for automation runs, including the sample location, user information, solvent used, experiment or experiments to run, and arbitrary text information. `enter('abc')` creates a directory named `abc`. In this directory is a file named `abc`, which contains experiment information.

Arguments: `file` is the name of the file to be edited. The default is that `enter` prompts for this information. If the file already exists, new entries are appended to it.

`configuration_file` is the name of a user-supplied file that customizes `enter` for local use. Several configuration files are provided:

- `enter.conf` is used when defining an experiment when an automation run is not currently active.
- `auto.conf` is used when defining an experiment for a current automation run. The `walkup` macro is provided for this style of entering samples.
- `gilson.conf` is used with the VAST accessory.

Examples: (From VnmrJ or UNIX) `enter`
(From VnmrJ) `enter('mysamples')`
(From UNIX) `enter MySamples`
(From VnmrJ) `enter('mysamples','auto.conf')`

See also: *NMR Spectroscopy User Guide; User Programming, VnmrJ Walkup*

Related:	<code>auto</code>	Set up an automation directory (C)
	<code>autogo</code>	Start an automation run (C)
	<code>autoname</code>	Prefix for automation data file (P)
	<code>autora</code>	Resume a suspended automation run (C)
	<code>autosa</code>	Suspend current automation run (C)
	<code>printer</code>	Printer device (P)
	<code>status</code>	Display status of all experiments (C)
	<code>walkup</code>	Walkup automation (M)

enterdialog **Start a dialog window using enterexp file (M)**

Applicability: Systems with automation.

Syntax: `enterdialog`

Description: Internal macro used by `enter` to start a dialog window using the `enterexp` file in the `dialoglib` directory.

See also: *NMR Spectroscopy User Guide; User Programming, VnmrJ Walkup*

Related: `enter` Enter sample information for automation run (M,U)

eread **Transfer file from remote source (M,U)**

Applicability: Systems with limNET protocol software installed.

Syntax: (From VnmrJ) `eread(local_file,remote_node,remote_file)`
(From UNIX) `eread local_file remote_node remote_file`

Description: Copies a remote file to the local host. It will not overwrite a preexisting file.

Arguments: `local_file` is the file name of the local host. If `local_file` is not a dot file (i.e., starts with “.”), `eread` uses the “I1” and “I2” values of the remote file to create an extension and then append it to the local file name.

`remote_node` is a symbolic node name for a specified node file. Use the command `dnode` to list nodes defined on your system. The names of the remote computers or “nodes” available to the limNET protocol are contained in the file `/vnmr/nodes`. *Note that this is not the same file as the name of the remote computers available to the Internet protocol (IP), which are contained in the file `/etc/hosts`.* Each user only needs to know the “names” of relevant nodes.

`remote_file` is the name of file to be transferred from the remote host.

Examples: (From VnmrJ) `eread('osv700','VXR4000','dsk1.osv700')`
(From UNIX) `eread osv700 VXR4000 dsk1.osv700`

See also: *NMR Spectroscopy User Guide*

Related: `dnode` Display list of valid limNET nodes (M,U)
`ewrite` Transfer file to remote destination (M,U)

ernst Calculate the Ernst angle pulse (C)

Syntax: `ernst(t1_estimate<,90_pulse_width>)`

Description: Calculates the optimum (“Ernst”) pulse width according to the formula

$$pw = \cos^{-1}(\exp^{-(at+dl)/t1\_estimate}) \bullet (pw90/360)$$

The new `pw` value is entered in the parameter table.

Arguments: `t1_estimate` is an estimate of the T_1 for a peak of interest.

`90_pulse_width` is a 90° pulse width determined by the parameter `pw90`. The default is the current value of parameter `pw90` if `pw90` exists.

Examples: `ernst(5)`
`ernst(3,12.6)`

See also: *NMR Spectroscopy User Guide*

Related: `pw` Pulse width (P)
`pw90` 90° pulse width (P)

errlog Display recent error messages (C)

Description: Displays in the text window the most recent error messages. The global parameter `errloglen` controls the number of lines displayed. If `errloglen` is not defined, `errlog` displays 10 lines by default.

See also: *NMR Spectroscopy User Guide*

Related: `acqstatus` Acquisition status (P)
`errloglen` Number of lines in error message display (P)

errloglen Number of lines in error message display (P)

Description: Sets the number of lines in the display of error messages by `errlog`.

Values: Integer, default is 10.

See also: *NMR Spectroscopy User Guide*

Related: `errlog` Display recent error messages (P)

E

ewrite **Transfer file to remote destination (M,U)**

Applicability: Systems with limNET protocol software installed.

Syntax: (From VnmrJ) `ewrite(local_file,remote_node,remote_file)`
(From UNIX) `ewrite local_file remote_node remote_file`

Description: Takes a preexisting local file and copies it to a remote host. The file cannot preexist on the remote host.

Arguments: `local_file` is the file name of the local host.

`remote_node` is a symbolic node name for a specified node file. Use the command `dnode` to list nodes defined on your system. The names of the remote computers or “nodes” available to the limNET protocol are contained in the file `/vnmr/nodes`. *Note that this is not the same file as the name of the remote computers available to the Internet Protocol (IP), which are contained in the file `/etc/hosts`.* Each user only needs to know the “names” of relevant nodes.

`remote_file` is the name of file to be transferred from the remote host.

Examples: (From VnmrJ) `ewrite('osv700','VXR4000','dsk1.osv700')`
(From UNIX) `ewrite osv700 VXR4000 dsk1.osv700`

See also: *NMR Spectroscopy User Guide*

Related: `dnode` Display list of valid limNET nodes (M,U)
 `eread` Transfer file from remote source (M,U)

exec **Execute a command (C)**

Syntax: `exec(command_string)`

Description: Executes the command given by the string argument.

Arguments: `command_string` is a character string constructed from a macro.

Examples: `exec($cmdstr)`
`exec(parstyle)`

See also: *User Programming*

execpars **Set up the exec parameters (M)**

Description: Set up the exec parameters as listed in `/vnmr/execpars`.

See also: *User Programming*

Related: `apptype` Application type (P)
 `execplot` Execute plotting macro (P)
 `execprep` Execute prepare macro (P)
 `execprescan` Execute prescan macro (p)
 `execproc` Execute processing macro (P)
 `execsetup` Execute setup macro (P)

execplot **Execute plotting macro (P)**

Description: Defines which plotting macro to use to plot this experiment.

See also: *User Programming*

Related: `apptype` Application type (P)
 `plot` Automatically plot spectra (M)

execprep Execute prepare macro (P)

Description: Defines which prepare macro to use to prescan this experiment.

See also: *User Programming*

Related: `apptype` Application type (P)
 `acquire` Acquire data (M)
 `plot` Automatically plot spectra (M)

execprescan Execute prescan macro (P)

Description: Defines which prescan macro to use to prescan this experiment.

See also: *User Programming*

Related: `apptype` Application type (P)
 `acquire` Acquire data (M)

execproc Execute processing macro (P)

Description: Defines which processing macro to use to process this experiment.

See also: *User Programming*

Related: `apptype` Application type (P)
 `acquire` Acquire data (M)

execprocess Execute processing macro (P)

Description: Defines which processing macro to use to process this experiment.

See also: *User Programming*

execsetup Execute setup macro (P)

Description: Defines which setup macro to use to prescan this experiment.

See also: *User Programming*

Related: `apptype` Application type (P)
 `cqexp` Load experiment from protocol (M)
 `sqexp` Load experiment from protocol (M)

exists Checks if parameter, file, or macro exists and file type (C)

Syntax: `exists(name, 'keyword'):$res1, $res2`
 `exists(name, 'keyword'<, argument>):$res1, $res2`

Description: Checks for the existence of a parameter, file, command, parameter file, or a macro from within a macro. The command can be used to check if a file is an ASCII text file, a directory, or to search the application directories for a file or directory.

Arguments: `$res1`— results from `exists` are returned to the `$` variable.

`$res2` — optional: returns the absolute path to the file, command, macro, etc. The `exists` command does not pass anything to the optional second argument if it does not find the specified file, command, macro, etc.

`name` — the name of a parameter, file, command, or macro.

<i>keyword</i>	<i>description and returned values</i>
'maclib'	Macros reside in applications directories, or <code>appdirs</code>. Typical directories are the users <code>vnmr/sys/maclib</code> directory and <code>/vnmr/maclib</code>. The <code>appdirs</code> are searched in order then macros are executed. <code>Exists</code> returns the following to <code>\$res1</code>: 0 — if the macro is not found in any of the <code>appdirs</code> 1, 2, or larger integer — indicates it was found in the first, second, third, etc. <code>appdir</code>. Name of any <code>appdir</code> (<code>shapelib</code>, <code>manual</code>, <code>probes</code>, <code>shims</code>) directory or directory within <code>appdir</code> and be used for the keyword <code>maclib</code>.
'command'	The <code>command</code> keyword is similar to the <code>maclib</code> keyword, except that it firsts checks to see if the name represents a built-in <code>Vnmr</code> command. <code>Exists</code> returns the following to <code>\$res1</code>: 0 — if the name is neither a built-in command nor a macro. 1 — if the name represents a built-in command. 2, 3, 4, or 5 — if name is a macro.
'ascii'	Checks if the file specified by name is an ASCII text file. <code>Exists</code> returns the following to <code>\$res1</code>: 0 — if the file is not an <code>ascii</code> file. 1 — if the file is an <code>ascii</code> file.
'parlib'	Checks for the file specified by name is in <code>parlib</code> using the path defined by applications directories or <code>appdirs</code> for <code>parlib</code>. A <code>.par</code> is appended to the name if it is not found and the search repeated if the file is not found on the first pass. <code>Exists</code> returns the following to <code>\$res1</code>: 0 — if the file is not found. 1 — if the file is found. Optional: result returned to <code>\$res2</code>. Return the absolute path of the parameter set if it is found.
'psglib'	Checks for the file specified by name is in <code>psglib</code> using the path defined by applications directories or <code>appdirs</code> for <code>psglib</code>. A <code>.c</code> is appended to the name if it is not found and the search repeated if the file is not found on the first pass. <code>Exists</code> returns the following to <code>\$res1</code>: 0 — if the file is not found. 1 — if the file is found. Optional: result returned to <code>\$res2</code>. Return the absolute path of the file set if it is found.

The following keywords accept an argument

<i>argument</i>	<i>description and returned values</i>
'file'	Checks if the file specified by name exists. <code>Exists</code> returns the following to <code>\$res1</code>: 0 — if the file does not exist. 1 — if the file exists.
'perm'	<code>perm</code> is a combination of one or more of the following: r — read w — write e — execute Access permission can be checked by passing one, two, or three characters in a single argument.

<i>keyword</i>	<i>description and returned values</i>
'parameter'	Checks if the parameter file specified by name exists. Exists returns the following to \$res1: 0 — if the parameter file does not exist. 1 — if the parameter file exists.
'tree'	tree is one of the following: current (default if no argument is supplied), global, processed, or systemglobal.
'directory'	Checks for the existence of the specified directory in the applications directories. Exists returns the following to \$res1: 0 — if the directory does not exist. 1 — if the directory exists.
'errval'	An error value to return to \$res1 if the directory does not exist.

Examples: `exists('ni','parameter'):$twod`
`exists('/vnmr/conpar','file','rw')`
`exists('wft','command'):$num`

Using `exists` from within a macro to search the `bin` directory in the applications directories for the file `myprog` and, if found, return the path to the `$myprogPath` argument:

```
exists($myprog,'bin'):$e,$myprogPath
  if ($e) then
    shell($myprogPath):$res
  else
    write('line3','%s: Program %s has not been
installed',$0,$myprog)
  endif
```

Using `exists` from within a macro to search for files in the top-level of the `appdirs`.

```
exists('pulsecal','')
```

The search for `pulsecal` starts at the top-level of all `appdirs`.

Using `exists` from within a macro to search multi-level directories:

```
exists(probename,'probes/'+probe)
```

The first argument is set to `' '` which forces `exists` to check for directories in the `appdirs`.

```
exists('nomacro','maclib',-1):$ok
```

Sets `$ok` to `-1` instead of `0` if `nomacro` does not exist in any of the applications directories. This feature can be applied to interface controls to make a button either not appear or appear grayed out if a macro (or file) does not exist.

See also: *User Programming*

Related:	<code>appdirs</code>	Starts Applications Directory Editor (M)
	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>hidecommand</code>	Execute macro instead of command with same name (C)
	<code>which</code>	Display which macro or command is used (M)

E

exit **Call the vnmrexit command (M)**

Description: Calls the **vnmrexit** command to exit from VnmrJ. As a macro, **exit** provides a user some flexibility in defining other things to do when exiting.

CAUTION: When you exit from the VnmrJ user interface on your X display system, whether you are using an X terminal or a Sun computer, and whether you are using OpenWindows, CDE, or Motif, you must first exit from any copy of VnmrJ running on your system. Failure to do this can cause current parameter values and even current data to be lost.

exp **Find exponential value of a number (C)**

Syntax: `exp (value) <:n>`

Description: Finds the exponential value (base *e*) of a number.

Arguments: `value` is a number.

`n` is the return value giving the exponential value of `value`. The default is to display the exponential value in the status window.

Examples: `exp (.5)`
`exp (val) :exp_val`

See also: *User Programming*

Related	atan	Find arc tangent of a number (C)
	cos	Find cosine value of an angle (C)
	ln	Find natural logarithm of a number (C)
	sin	Find sine value of an angle (C)
	tan	Find tangent value of an angle (C)

expactive **Determine if experiment has active acquisition (C)**

Syntax: (1) `expactive <(exp_number)> <: $answer>`
(2) `expactive ('auto') <: $mode>`
(3) `expactive ('current') <: $exp> <, $user>`

Description: Determines whether an acquisition is active or pending in an experiment.

Arguments: `exp_number` is the number, from 1 to 9999, of the experiment to be checked. The default is the current experiment.

`$answer` is a return value: -1 if an acquisition is not possible (e.g., the system is a data station), 0 if no acquisition active in the requested experiment, 1 if an acquisition active in that experiment, and 2 or larger if an acquisition is queued in the requested experiment (subtract 1 from the value to determine its position in the acquisition queue). With no return argument, the result displays on line 3.

`'auto'` is a keyword to check if the system is in automation mode.

`$mode` is a return value: 1 if the system is in automation mode, or 0 if otherwise. With no return argument, the result is displayed on line 3.

`'current'` is a keyword that determines whether an active experiment has an active acquisition command running. An experiment is still considered active if it holds up additional acquisitions during its `wexp` processing by the `'wait'` flag. If `expactive ('current')` does not have a return argument, results are displayed on line 3.

`$exp` is a return value indicating the current active experiment number: -1 if no acquisition is possible, or 0 if no acquisition is active.

`$user` is a return value indicating the user who started the acquisition. If the system is running in automation mode, `$user` is set to "auto." If no acquisition is running, `$user` is set to "nobody."

Examples: `expactive`
`expactive(3)`
`expactive(2):$active`
`expactive('auto'):$automode`

expfit Make least-squares fit to polynomial or exponential curve (U)

Syntax: (From UNIX) `expfit options <analyze.inp >analyze.list`

Description: Makes a least-squares curve fitting to the data supplied in the file `analyze.inp`. For the specialized uses of `analyze`, VnmrJ macros (e.g., `t1`, `t2`, `kind`) are available that provide the correct file format and avoid the need for the user to select options.

In the regression mode, the type of curve fitting, (`'poly1'`, ...) must be selected. For regression (generalized curve fitting), the regression section in the manual *NMR Spectroscopy User Guide* shows the input file format and describes the menus that permit option choices indirectly through menu buttons.

The following text file is an example of the file `analyze.inp` (for options T1, T2, kinetics, contact_time, and regression). (1), (2), etc. do not actually appear in the file but are used to identify lines in the description presented below the file.

```
(1) time
(2)   <amp>
(3)   2  4  linear linear

(4)   NEXT  4
(5)   1
(6)   1  1
      2  4
      3  9
      4  16
(4)   NEXT  3
(5)   2
(6)   2  5
      3  10
      4  17
```

This file contains the following information:

- (1) Optional x-axis title.
- (2) Optional y-axis title, for regression only.
- (3) Line containing an integer for the number of peaks, followed by another integer for the number of pairs per peak. If regression, the x-scale type and y-scale type are also listed.
- (4) In the regression mode, a line beginning with the keyword NEXT is inserted at the start of each data set when the number of pairs per peak is variable, followed by an integer for the number of pairs for the peak.
- (5) An integer that indexes the peaks.
- (6) Data pairs, one to a line, listed by peak.

For options T1, T2, kinetics, and contact_time, information from the file `fp.out` and from the array `xarray` are used to construct this file; therefore, it is necessary to run `fp` prior to `analyze`. For regression, this file is made by running `expl('regression')`.

For diffusion, contact_time, and, if not in regression mode, `poly1` and `poly2`, the `analyze.inp` file is slightly different:

- (1) List of n x-y data pairs
- (2) <text line>

```
(3)  <x-values>  <y-values>
(4)  x    y
      . . .
```

(1) Title line.

(2) Descriptive text line.

(3) Number of x values and y values.

(4) Data pairs, one to a line, are listed by peak in the following order:

```
x    y    (first peak, first pair)
x    y    (first peak, second pair)
...
x    y    (second peak, first pair)
...
```

expfit also makes a file `analyze.out` that is used by `expl` to display the results of the analysis in addition to output to the standard output, which is usually directed to `analyze.list`.

Arguments: options can be any of the following:

`T1` sets T_1 analysis. This value is the default.

`T2` sets T_2 analysis.

`kinetics` sets kinetics analysis with decreasing peak height.

`increment` sets kinetics analysis with increasing peak height.

`list` sets an extended listing for each peak.

`diffusion` sets a special analysis for diffusion experiments.

`contact_time` sets a special analysis for solids cross-polarization spin-lock experiments.

`regression` sets regression mode, providing generalized curve fitting with choices `poly1`, `poly2`, `poly3`, and `exp`:

- `poly0` calculates the mean.
- `poly1` sets a linear fitting.
- `poly2` sets a quadratic fitting.
- `poly3` sets a cubic curve fitting.
- `exp` sets an exponential curve fitting.

Examples: (From UNIX) `expfit d2 T1 list <analyze.inp >analyze.out`
 (From UNIX) `expfit regression exp list <analyze.inp >analyze.out`

See also: *NMR Spectroscopy User Guide*

Related:	<code>analyze</code>	Generalized curve fitting (C)
	<code>expl</code>	Display exponential or polynomial curves (C)
	<code>fp</code>	Find peak heights (C)
	<code>kind</code>	Kinetics analysis, decreasing intensity (M)
	<code>t1</code>	T_1 exponential analysis (M)
	<code>t2</code>	T_2 exponential analysis (M)

expl Display exponential or polynomial curves (C)

Syntax: `expl<(<options,>line1,line2,...)>`

Description: Displays exponential curves resulting from T_1 , T_2 , or kinetic analyses. Also displays polynomial curves from diffusion or other types of analysis. The parameters `sc`, `wc`, `sc2`, and `wc2` control the size of the display.

In general, the first time `expl` is displayed, it calculates appropriate limits for the two axes. A subsequent call to `expl`, while a previous `expl` is displayed on the graphics screen, uses the axis scaling that displayed `expl`. To have the new `expl` recalculate its own axis limits and not use those currently displayed, call the `autoscale` macro before executing `expl`. Alternately, the axis limit for the `expl` display can be specified using the `scalelimits` macro.

Arguments: options can be any of the following:

- 'regression' is a keyword signifying the beginning of generalized curve fitting. `expl` displays the data in the file `regression.inp` as unconnected points and also uses `regression.inp` to create the file `analyze.inp`, which serves as input to `analyze` for curve fitting.
- 'linear', 'square', and 'log' are keywords for display of the data points against a square or logarithmic axis scale, with the exception of the results from regression. The first keyword controls the x-axis scale, the second the y-axis. The default is 'linear'.
- 'link' is a keyword to link the data points rather than a display of the theoretical curve.
- 'nocurve' is a keyword to produce a plot of data points only.
- 'tinysymbol' is a keyword to display small-scale data point symbols.
- 'nosymbol' is a keyword to produce a plot of the curve only.
- 'noclear' is a keyword to not erase the graphics screen before drawing the plot. This prevents the graphics screen from being cleared of data.
- 'oldbox' is a keyword to plot an additional curve on an existing plot. Only the first data set in the file `analyze.out` is plotted. The box and scale description is derived from the file `expl.out` in the current experiment. When the 'oldbox' option is used, a second argument is necessary to identify the curve number and data point symbol to represent the data. This second argument is a number from 1 to 6.
- 'file' is a keyword that, when followed by a file name, makes that file replace the file `analyze.out` as the input to `expl`.

`line1, line2, ...` specify the curves to be displayed. The default is to display the first eight curves (if that many exist) along with data points.

Examples: `expl`
`expl(1,3,6)`
`expl('oldbox',5)`
`expl('regression')`
`expl('regression',4,5)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>analyze</code>	Generalized curve fitting (C)
	<code>autoscale</code>	Resume autoscaling after limits set by <code>scalelimits</code> (M)
	<code>expfit</code>	Make least squares fit to polynomial or exponential curve (C)
	<code>pexpl</code>	Plot exponential or polynomial curves (C)
	<code>sc</code>	Start of chart (P)
	<code>sc2</code>	Start of chart in second direction (P)
	<code>scalelimits</code>	Set limits for scales in regression (M)
	<code>wc</code>	Width of chart (P)
	<code>wc2</code>	Width of chart in second direction (P)

expladd **Add another diffusion analysis to current display (M)**

Applicability: Systems with the diffusion option.

E

Syntax: `expladd(integral_region)`

Description: Adds results of another diffusion analysis to the currently displayed results.

Arguments: `integral_region` specifies the number of the region whose results are to be added to the existing graph.

Examples: `expladd(1)`

See also: *NMR Spectroscopy User Guide*

Related: `expl` Display exponential or polynomial curves (C)
`pexpl` Plot exponential or polynomial curves (C)
`pexpladd` Add another diffusion analysis to current plot (M)

explib Display experiment library (M)

Description: Displays the currently available experiment files. For each experiment, `explib` displays the name of the experiment and its subexperiments, whether an acquisition is active or its position in the acquisition queue, the current size of the experiments, the pulse sequence currently active in the experiments, and the first 50 characters of the text file in the experiment. `explib` also displays a message if the system is in automation mode.

See also: *NMR Spectroscopy User Guide*; *VnmrJ Walkup*

explist Display current experiment chain and approx. time for each (M)

See also: Displays approximate time for each experiment in a chained experiment.

Related: `autotime` Display approximate time for automation (M)

explog Display log file for experiment (M)

Description: Displays the log file for an experiment. This file includes when the experiment started, any acquisition errors that may have occurred, and when the experiment finished. Each acquisition generates this information, which is stored in the experiment's `acqfil` directory in a text file named `log`.

See also: *NMR Spectroscopy User Guide*

exptime Display experiment time (C)

Syntax: `exptime<(sequence)><:$seconds>`

Description: Estimates the acquisition time for an experiment, based on the parameters used in the current experiment, and displays the time in the format `hh:mm:ss`. The `time` macro uses `exptime` to determine the time of an experiment.

Arguments: `sequence` is a pulse sequence that exists in the `seqlib` directory. If this argument is used, `exptime` estimates the acquisition time for the specified sequence. The default is the current value of `seqlib`.

`$seconds` is a return argument with the number of seconds estimated for the experiment. If this argument is used, the time display is suppressed.

Examples: `exptime`
`exptime('apt')`
`exptime:$etime`
`exptime('noesy'):$est_time`

See also: *NMR Spectroscopy User Guide*

Related: `time` Display experiment time or recalculate number of transients (M)

F

f	Set display parameters to full spectrum (C)
f19	Automated fluorine acquisition (M)
f19p	Process 1D fluorine spectra (M)
f1coef	Coefficient to construct F1 interferogram (P)
f2coef	Coefficient to construct F2 interferogram (P)
f attn	Fine attenuator (P)
fb	Filter bandwidth (P)
fb c	Apply baseline correction for each spectrum in an array (M)
fdm1	Set, write 1D FDM parameters, run FDM (M)
fiddc3d	3D time-domain dc correction (P)
fiddle	Perform reference deconvolution (M)
fiddled	Perform reference deconvolution subtracting alternate FIDs (C)
fiddleu	Perform reference deconvolution subtracting successive FIDs (C)
fiddle2d	Perform 2D reference deconvolution (C)
fiddle2D	Perform 2D reference deconvolution (C)
fiddle2dd	2D reference deconvolution subtracting alternate FIDs (C)
fiddle2Dd	2D reference deconvolution subtracting alternate FIDs (C)
fidmax	Find the maximum point in an FID (C)
fidpar	Add parameters for FID display in current experiment (M)
fidsave	Save data (M)
fifolpsize	FIFO loop size (P)
file	File name of parameter set (P)
files	Interactively handle files (C)
filesinfo	Return file information for files display (C)
filtfile	File of FIR digital filter coefficients (P)
findxmlmenu	Find an xml menu (M)
fitspec	Perform spectrum deconvolution (C, U)
fixgrd	Convert gauss/cm value to DAC (M)
fixpar	Correct parameter characteristics in experiment (M)
fixpar3rf	Create parameters for third rf channel (M)
fixpar4rf	Create parameters for fourth rf channel (M)
fixpar5rf	Create parameters for fifth rf channel (M)
fixup	Adjust parameter values selected by setup macros (M)
fixpsg	Update psg libraries (M)
flashc	Convert compressed 2D data to standard 2D format (C)
flipflop	Set up parameters for FLIPFLOP pulse sequence (M)
Fluorine	Set up parameters for 19F experiment (M)
flush	Write out data in memory (C)
fn	Fourier number in directly detected dimension (P)
fn1	Fourier number in 1st indirectly detected dimension (P)
fn2	Fourier number in 2nd indirectly detected dimension (P)
fn2D	Fourier number to build up 2D DOSY display in freq. domain (P)
focus	Send keyboard focus to input window (C)

F

<code>foldcc</code>	Fold INADEQUATE data about two-quantum axis (C)
<code>foldj</code>	Fold J-resolved 2D spectrum about $f_1=0$ axis (C)
<code>foldt</code>	Fold COSY-like spectrum along diagonal axis (C)
<code>fontselect</code>	Open FontSelect window (C)
<code>format</code>	Format a real number or convert a string for output (C)
<code>fp</code>	Find peak heights or phases (C)
<code>fpmult</code>	First point multiplier for np FID data (P)
<code>fpmult1</code>	First point multiplier for ni interferogram data (P)
<code>fpmult2</code>	First point multiplier for ni2 interferogram data (P)
<code>fr</code>	Full recall of a display parameter set (M)
<code>fread</code>	Read parameters from file and load them into a tree (C)
<code>fsave</code>	Save parameters from a tree to a file (C)
<code>fsq</code>	Frequency-shifted quadrature detection (P)
<code>ft</code>	Fourier transform 1D data (C)
<code>ft1d</code>	Fourier transform along f_2 dimension (C)
<code>ft1da</code>	Fourier transform phase-sensitive data (M)
<code>ft1dac</code>	Combine arrayed 2D FID matrices (M)
<code>ft2d</code>	Fourier transform 2D data (C)
<code>ft2da</code>	Fourier transform phase-sensitive data (M)
<code>ft2dac</code>	Combine arrayed 2D FID matrices (M)
<code>ft3d</code>	Perform a 3D Fourier transform on a 3D FID data set (M,U)
<code>full</code>	Set display limits for a full screen (C)
<code>fullsq</code>	Display largest square 2D display (M)
<code>fullt</code>	Set display limits for a full screen with room for traces (C)

f

Set display parameters to full spectrum (C)

Description: Sets up the `sp` and `wp` display parameters for a full display of a 1D spectrum. If an FID is displayed, the parameters `sf` and `wf` are set for a full display. In multidimensional data sets, the parameters for both displayed dimensions are set up. For 2D data sets, the parameters `sp`, `wp`, `sp1`, and `wp1` would be set. For planes of higher dimensional data sets, the appropriate two groups of `sp-wp`, `sp1-wp1`, and `sp2-wp2`, parameter pairs are set.

See also: *NMR Spectroscopy User Guide*

Related:	<code>sf</code>	Start of FID (P)
	<code>sp</code>	Start of plot in directly detected dimension (P)
	<code>sp1</code>	Start of plot in 1st indirectly detected dimension (P)
	<code>sp2</code>	Start of plot in 2nd indirectly detected dimension (P)
	<code>wf</code>	Width of FID (P)
	<code>wp</code>	Width of plot in directly detected dimension (P)
	<code>wp1</code>	Width of plot in 1st indirectly detected dimension (P)
	<code>wp2</code>	Width of plot in 2nd indirectly detected dimension (P)

f19

Automated fluorine acquisition (M)

Syntax: `f19<(solvent)>`

Description: Prepares parameters for automatically acquiring a standard ^{19}F spectrum. The parameter `wexp` is set to 'procplot' for standard processing. If `f19` is used as the command for automation via the `enter` program, then the macro `au` is

supplied automatically and should not be entered on the MACRO line of the `enter` program. However, it is possible to customize the standard `f19` macro on the MACRO line by following it with additional commands and parameters. For example, `f19 nt=1` uses the standard `f19` setup but with only one transient.

Arguments: `solvent` is the name of the solvent. In automation mode, the solvent is supplied by the `enter` program. The default is 'CDC13'

Examples: `f19`
`f19 ( 'DMSO' )`

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (M)
	<code>enter</code>	Enter sample information for automation run (C)
	<code>f19p</code>	Process 1D fluorine spectra (M)
	<code>proc1d</code>	Processing macro for simple (non-arrayed) 1D spectra (M)
	<code>procplot</code>	Automatically process FIDs (M)
	<code>wexp</code>	When experiment completes (P)

f19p Process 1D fluorine spectra (M)

Description: Processes non-arrayed 1D fluorine spectra using a set of standard macros. `f19p` is called by `proc1d`, but can also be used directly. Fully automatic processing (up to a point where a spectrum could be plotted) is provided: Fourier transformation (using preset weighting functions), automatic phasing (`aphx` macro), select integral regions (`hregions` macro), adjust integral size (`integrate` macro), vertical scale adjustment (`vsadjc` macro), avoiding excessive noise (`noislm` macro), threshold adjustment (if required, `thadj` macro), and referencing to the TMS signal, if present (`tmsref` macro).

See also: *NMR Spectroscopy User Guide*

Related:	<code>aphx</code>	Perform optimized automatic phasing (M)
	<code>f19</code>	Automated fluorine acquisition (M)
	<code>hregions</code>	Select integral regions for proton spectra (M)
	<code>integrate</code>	Automatically integrate 1D spectrum (M)
	<code>noislm</code>	Avoids excessive noise (M)
	<code>proc1d</code>	Processing macro for simple (non-arrayed) 1D spectra (M)
	<code>thadj</code>	Adjust threshold (M)
	<code>tmsref</code>	Reference spectrum to TMS line (M)
	<code>vsadjh</code>	Adjust vertical scale for proton spectra (M)

f1coef Coefficient to construct F1 interferogram (P)

Description: Holds the coefficient to construct an F1 interferogram for 2D and 3D transformation. Coefficients are used by the `ft2da` and `ft3d` macros. If `f1coef` has a null value, `ft2da` uses the “standard” coefficients. `f1coef` is created by the `par2d` macro.

Values: Series of coefficients, separated by spaces (not a comma), and stored as a string variable. For example, the coefficient for standard States-Hypercomplex data set is `f1coef='1 0 0 0 0 0 -1 0'`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>f2coef</code>	Coefficient to construct F2 interferogram (P)
	<code>ft2da</code>	Fourier transform phase-sensitive data (M)
	<code>ft3d</code>	Perform a 3D Fourier transform on a 3D FID data set (M,U)

F

`make3dcoef` Make 3D coefficients file from 2D coefficients (M)
`par2d` Create 2D acquisition, processing, display parameters (M)

f2coef **Coefficient to construct F2 interferogram (P)**

Description: Holds the coefficient to construct an F2 interferogram for 2D and 3D transformation. Coefficients are used by the `ft2da('ni2')` and `ft3d` macros. If `f2coef` has a null value, `ft2da('ni2')` uses the “standard” coefficients. `f2coef` is created by the `par3d` macro.

Values: Series of coefficients, separated by spaces (not a comma), and stored as a string variable. For example, the coefficient for standard States-Hypercomplex data set is `f2coef='1 0 0 0 0 0 -1 0'`.

fatten **Fine attenuator (P)**

Description: Configuration parameter for whether the current rf channel has a fine attenuator. The value is set using the label Fine Attenuator in the Spectrometer Configuration window (opened from `config`).

Values: 0 specifies the fine attenuator is not present on the channel (Not Present choice in Spectrometer Configuration window).

4095 specifies the fine attenuator is present on the channel (Present choice in Spectrometer Configuration window).

See also: *VnmrJ Installation and Administration; User Guide: Solids; CP/MAS Installation*

Related: `config` Display current configuration and possibly change it (M)
`dpwrf` First decoupler fine power (P)
`tpwrf` Observe transmitter fine power (P)

fb **Filter bandwidth (P)**

Description: Sets the bandwidth of the audio filters, which prevents noise of higher frequency than the spectral limits from “folding in” to the spectrum. Because the transmitter is in the center of the spectrum, the range of audio frequencies that must be filtered out is half the spectral width `sw` (e.g., for a spectral width of 4000 Hz, frequencies higher than ± 2000 Hz should be filtered out). The audio filters have some attenuation at frequencies lower than their nominal cutoff frequency, which is the frequency at which signals have been attenuated by 3 dB (50%). This impacts on quantitative accuracy near the edges of the spectrum so that the standard value of `fb` is 10% more than half of `sw`.

`fb` is automatically changed whenever the spectral width `sw` is changed and thus is normally not a user-entered parameter. For example, typing `sw=4000` automatically sets `fb=2200`, which is 10% more than 2000 Hz. After changing the value of `sw`, `fb` can be changed.

Values: if `sw` is 500,000 or less: 1000 to 256000 Hz, 1000-Hz steps.
if `sw` is greater than 500,000: 256 kHz, 1 MHz.

See also: *NMR Spectroscopy User Guide*

Related: `sw` Spectral width in directly detected dimension (P)
`mrfb` Set the filter bandwidths for multiple receivers (P)

fbc Apply baseline correction for each spectrum in an array (M)

Description: Applies **bc** -type baseline correction to all the spectra in an array. The partial integral mode should be used to set integral regions to include all significant signals, while leaving blank as large an area of baseline as is possible.

See also: *NMR Spectroscopy User Guide*

Related: **dosy** Process DOSY experiments (M)

fdm1 Set, write 1D FDM parameters, run FDM (M)

Syntax: `fdm1<(filename<,n1, v1<, n2, v2<...>>>) >`
or
`fdm1 (i)` for the i-th trace

Description: Sets 1D Filter Diagonalization Method (FDM) parameters to the default values, writes the parameters to the `curexp/datadir/fdm1.inparm` file, and runs a stand-alone C++ program (`/vnmr/bin/fdm1d`).

Arguments: `filename` is the FID file; the default is `curexp+'acqfil/fid'`.
`n1, n2...` is one or more following variable names (the order is arbitrary):

<code>axis</code>	-1 (default) to reverse the spec.
<code>cheat</code>	No cheat if <code>cheat=1</code> , lines are narrower if <code>cheat<1</code> .
<code>cheatmore</code>	No cheatmore if <code>cheatmore=0</code> .
<code>error</code>	Error threshold for throwing away poles.
<code>fidfmt</code>	FID format: VnmrJ or ASCII.
<code>fdm</code>	1 for FDM; -1 for Digital or Discrete Fourier Transform.
<code>fn_Sp1D</code>	Spectrum file; default is <code>curexp/datadir/fdm1.parm</code> .
<code>Gamm</code>	Smoothing width (line broadening).
<code>Gcut</code>	Maximum width for a pole.
<code>idat</code>	Data type of ASCII FID file -4 for complex data, ignored if data is in VnmrJ format.
<code>i_fid</code>	The i-th trace of the FID.
<code>kcoef</code>	If <code>kcoef > 0</code> , use 'complicated' <code>dk(k)</code> . -1 is always preferred.
<code>Nb</code>	Number of basis functions in a single window.
<code>Nbc</code>	Number of coarse basis vectors.
<code>Npower</code>	Number of spectrum data points.
<code>Nsig</code>	Number of points to use.
<code>Nskip</code>	Number of points to skip.
<code>par</code>	Line list file; default is <code>curexp/datadir/fdm1.parm</code>
<code>rho</code>	<code>rho=1</code> is optimal.
<code>specfmt</code>	Spec format: VnmrJ or ASCII.
<code>spectyp</code>	Spectrum type: complex (default), real imag, or abs.
<code>ssw</code>	A test parameter.
<code>t0</code>	Delay of the first point.
<code>theta</code>	Overall phase of FID (rp in radians).
<code>wmax</code>	Maximum spectrum frequency in hertz.
<code>wmin</code>	Minimum spectrum frequency in hertz.

$v1, v2 \dots$ is the value for the variable(s).

Examples: `fdm1('cheat', 0.8)`
`fdm1('Nsig', 3000, 'Nb', 20, 1 'Gamm', 0.5)`

See also: *NMR Spectroscopy User Guide*

fiddc3d **3D time-domain dc correction (P)**

Description: Sets whether a 3D time-domain dc correction occurs. If `fiddc3d` does not exist, it is created by the macro `par3d`. The time-domain dc correction occurs immediately after any linear prediction operations and before all other operations on time-domain data.

Values: A three-character string. The default value is 'nnn'.

- The first character refers to the f_3 dimension (`sw`, `np`, `fn`), the second character refers to the f_1 dimension (`sw1`, `ni`, `fn1`), and the third character refers to the f_2 dimension (`sw2`, `ni2`, `fn2`).
- Each character may take one of two values: 'n' for no time-domain dc correction along the relevant dimension, and 'y' for time-domain dc correction along the relevant dimension.

See also: *NMR Spectroscopy User Guide*

Related:	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>fn1</code>	Fourier number in 1st indirectly detected dimension (P)
	<code>fn2</code>	Fourier number in 2nd indirectly detected dimension (P)
	<code>ft3d</code>	Perform a 3D Fourier transform (M)
	<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
	<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)
	<code>np</code>	Number of data points (P)
	<code>par3d</code>	Create 3D acquisition, processing, display parameters (C)
	<code>ptspec3d</code>	Region-selective 3D processing (P)
	<code>specdc3d</code>	3D spectral drift correction (P)
	<code>sw</code>	Spectral width in directly detected dimension (P)
	<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)
	<code>sw2</code>	Spectral width in 2nd indirectly detected dimension (P)

fiddle **Perform reference deconvolution (M)**

Syntax: `fiddle(option<, file><, option<, file>><, start>
<, finish><, increment>)`

Description: Performs reference deconvolution using a reference signal with known characteristics to correct instrumental errors in experimental 1D or 2D spectra.

Arguments: `option` can be any of the following:

- 'alternate' is a keyword specifying the alternate reference phase +/- (for phase sensitive gradient 2D data).
- 'autophase' is a keyword specifying to automatically adjust the phase of the reference signal.
- 'displaycf' is a keyword specifying to stop at the display of the correction function.
- 'fittedbaseline' is a keyword specifying to use cubic spline baseline correction defined by the choice of integral regions.
- 'invert' is a keyword specifying to invert the corrected difference spectrum/spectra.

- 'noaph' is a keyword specifying not to automatically adjust zero order phase of the reference region.
- 'nodc' is a keyword specifying not to use dc correction of reference region.
- 'noextrap' is a keyword specifying not to use extrapolated dispersion mode.
- 'nohilbert' is a keyword specifying not to use Hilbert transform algorithm and to use extrapolated dispersion mode reference signal unless 'noextrap' is also used as an option.
- 'normalise' is a keyword specifying to keep corrected spectrum integrals equal to that of the first spectrum.
- 'satellites' is a keyword specifying to use satellites defined in `file` in ideal reference region; `file` should be in `/vnmr/satellites`, and should immediately follow 'satellites' in the argument list.
- 'stop1' is a keyword specifying to stop at display of experimental reference FID.
- 'stop2' is a keyword specifying to stop at display of correction function.
- 'stop3' is a keyword specifying to stop at display of corrected FID.
- 'stop4' is a keyword specifying to stop at display of first corrected FID.
- 'verbose' is a specifying keyword to display information about processing in the main window.
- 'writecf' is a keyword specifying to write the correction function to file; the argument `file` must immediately follow 'writecf'.
- 'writefid' is a keyword specifying to write out corrected FID to file; if `file` does not begin with `/`, it is assumed to be in the current working directory. In the argument list, `file` should immediately follow 'writefid'.

`file` is the name of the file used with the 'satellites' and 'writefid' options.

`start` and `finish` are the indices of the first and last array elements to be processed. `increment` specifies the steps in which the index is to be incremented. The default is to process all the transformed spectra in an array.

See also: *NMR Spectroscopy User Guide*

Related:	<code>fiddled</code>	Perform reference deconvolution subtracting alternate FIDs
	<code>fiddleu</code>	Perform reference deconvolution subtracting successive FIDs
	<code>fiddle2d</code>	Perform 2D reference deconvolution
	<code>fiddle2D</code>	Perform 2D reference deconvolution
	<code>fiddle2dd</code>	Perform 2D reference deconvolution subtracting alternate FIDs
	<code>fiddle2Dd</code>	Perform 2D reference deconvolution subtracting alternate FIDs

fiddled **Perform reference deconvolution subtracting alternate FIDs (C)**

Description: Produces the corrected difference between successive spectra. Refer to the description of `fiddle` for details.

See also: *NMR Spectroscopy User Guide*

Related:	<code>fiddle</code>	Perform reference deconvolution

F

- fiddleu** **Perform reference deconvolution subtracting successive FIDs (C)**
 Description: Produces corrected differences between successive FIDs and the first FID. Refer to the description of [fiddle](#) for details.
 See also: *NMR Spectroscopy User Guide*
 Related: [fiddle](#) Perform reference deconvolution
- fiddle2d** **Perform 2D reference deconvolution (C)**
 Description: Functions the same as the [fiddle](#) program except `fiddle2d` performs 2D reference deconvolution. Refer to the description of [fiddle](#) for details.
 See also: *NMR Spectroscopy User Guide*
 Related: [fiddle](#) Perform reference deconvolution
- fiddle2D** **Perform 2D reference deconvolution (C)**
 Description: Functions the same as the [fiddle](#) program except `fiddle2D` performs 2D reference deconvolution. Refer to the description of [fiddle](#) for details.
 See also: *NMR Spectroscopy User Guide*
 Related: [fiddle](#) Perform reference deconvolution
- fiddle2dd** **2D reference deconvolution subtracting alternate FIDs (C)**
 Description: Functions the same as the [fiddle](#) program except `fiddle2dd` performs 2D reference deconvolution. Refer to the description of [fiddle](#) for details.
 See also: *NMR Spectroscopy User Guide*
 Related: [fiddle](#) Perform reference deconvolution
- fiddle2Dd** **2D reference deconvolution subtracting alternate FIDs (C)**
 Description: Functions the same as the [fiddle](#) program except `fiddle2Dd` performs 2D reference deconvolution. Refer to the description of [fiddle](#) for details.
 See also: *NMR Spectroscopy User Guide*
 Related: [fiddle](#) Perform reference deconvolution
- fidmax** **Find the maximum point in an FID (C)**
 Applicability: All
 Syntax: `fidmax<(trace)>:$max`
 `fidmax:$max`
 `fidmax(1):$max`
 `fidmax(arraydim):$max`
 Description: `fidmax` finds the absolute maximum value in an FID.
 Arguments: No arguments — `fidmax` uses the currently active FID
 FID selected by `df` or `select`.
 A FID index supplied as an argument.

- fidpar** **Add parameters for FID display in current experiment (M)**
- Description: Creates the FID display parameters `axisf`, `crf`, `deltaf`, `dotflag`, `vpf`, and `vpfi` in the current experiment. Use `fidpar` to define these parameters in old parameter sets (they are already defined in new parameter sets).
- See also: *NMR Spectroscopy User Guide*
- Related:
- | | |
|----------------------|---|
| <code>addpar</code> | Add selected parameters to current experiment (M) |
| <code>axisf</code> | Axis label for FID displays and plots (P) |
| <code>crf</code> | Current time domain cursor position (P) |
| <code>deltaf</code> | Difference of two time cursors (P) |
| <code>dotflag</code> | Display FID as connected dots (P) |
| <code>vpf</code> | Current vertical position of FID (P) |
| <code>vpfi</code> | Current vertical position of imaginary FID (P) |
-
- fidsave** **Save data (M)**
- Description: Macro to save data. It uses `svfdir` and `svfname` to construct the data filename.
-
- fifolpsize** **FIFO loop size (P)**
- Description: Configuration parameter for the size of the FIFO loop. The size depends on which controller board is present on the system—the Output board, the Acquisition Controller board, or the Pulse Sequence Controller board (refer to the description of the `acquire` statement in the manual *User Programming* for information on identifying the boards). The value is set using the label Fifo Loop Size in the Spectrometer Configuration window (opened by `config`).
- Values: 2048
- See also: *VnmrJ Installation and Administration*
- Related: `config` Display current configuration and possibly change it (M)
-
- file** **File name of parameter set (P)**
- Description: Contains the file name of the parameter set returned by a `rt` or `rtp` command. This parameter is reset when the `go` command is issued. If the system is not in automation mode (`auto='n'`), `file` is reset to the 'exp' value. If the system is in automation mode (`auto='y'`), `file` is set to the path of the directory where the data is stored.
- See also: *NMR Spectroscopy User Guide*
- Related:
- | | |
|-------------------|--------------------------------------|
| <code>auto</code> | Automation mode active (P) |
| <code>go</code> | Submit experiment to acquisition (C) |
| <code>rt</code> | Retrieve FID (C) |
| <code>rtp</code> | Retrieve parameters (C) |
-
- files** **Interactively handle files (C)**
- Syntax: `files<(files_menu)>`
- Description: Brings up the interactive file handling program. With this program, the mouse and keyboard are used to copy, delete, rename, change directories, and load and save experiment data. The `files` command uses the graphics window to display file names. A mouse clicked on a file name selects it and the file name is displayed in reverse video. Various operations can be conducted on one or more selected files. The menus used for the `files` program are placed in the

standard menulib directories. Refer to the manual *NMR Spectroscopy User Guide* for more information on using menus, and refer to the manual *User Programming* for information on programming menus.

Arguments: `files_menu` is the files menu to control the menu buttons; the default menu is 'files_main' or the last active files menu.

Examples: `files`
`files('files_dir')`

See also: *User Programming*

Related: `filesinfo` Return files display information (C)
`tape` Control tape options of files program (P)

filesinfo Return file information for files display (C)

Syntax: (1) `filesinfo('number'):$number_files`
 (2) `filesinfo('name'<,file_number>):$file`
 (3) `filesinfo('redisplay')`

Description: Allows access to the list of files selected from the `files` interactive display. `filesinfo` is normally used only by the macros that implement the menu functions of the file system and not entered from the keyboard. The command will not execute unless the `files` program is active.

Arguments: 'number' is a keyword to return the number of files selected in the `files` display, or 0 if no files have been selected.

`$number_files` is the return variable when 'number' is used.

'name' is a keyword to return a list of file names selected in the `files` display.

`file_number` is a number following the 'name' keyword to return only the file name in the list given by `file_number`.

`$file` is a string variable that returns the file name when 'name' is used.

'redisplay' is a keyword that causes the current contents of the directory to be displayed. This display is useful after making changes in the directory, such as deleting or creating a file.

See also: *User Programming*

Related: `files` Interactively handle files (C)

filtfile File of FIR digital filter coefficients (P)

Description: Specifies name of a file of FIR (finite impulse response) digital filter coefficients. This file is a text file with one real filter coefficient per line (complex filters are not supported). If the parameter `filtfile` does not exist in the current experiment, enter `addpar('downsamp')` or `addpar('oversamp')` to add it. Entering `addpar('downsamp')` creates the digital filtering and downsampling parameters `downsamp`, `dscoef`, `dsfb`, `dsfsfrq`, and `filtfile`. Similarly, entering `addpar('oversamp')` creates digital filtering and oversampling parameters `def_osfilt`, `filtfile`, `oscoef`, `osfb`, `osfilt`, `osfsfrq`, and `oversamp`.

Values: File name. The file must be in the user's `vnmr/sys/filtlib` directory.

Related: `addpar` Add selected parameters to current experiment (M)
`def_osfilt` Default value of `osfilt` (P)
`downsamp` Downsampling factor applied after digital filtering (P)

<code>dscoef</code>	Digital filter coefficients for downsampling (P)
<code>dsfb</code>	Digital filter bandwidth for downsampling (P)
<code>dslsfrq</code>	Bandpass filter offset for downsampling (P)
<code>oscoef</code>	Digital filter coefficients for oversampling (P)
<code>osfb</code>	Digital filter bandwidth for oversampling (P)
<code>osfilt</code>	Oversampling filter for real-time DSP (P)
<code>oslsfrq</code>	Bandpass filter offset for oversampling (P)
<code>oversamp</code>	Oversampling factor for acquisition (P)
<code>pards</code>	Create additional parameters used for downsampling (M)
<code>paros</code>	Create additional parameters used for oversampling (M)

findxmlmenu Find an xml menu (M)

Description: Find an xml menu. Used by the menu system to find and display VnmrJ menus.

fitspec Perform spectrum deconvolution (C, U)

Syntax: (From VnmrJ) `fitspec(<'usell'><,><'setsfreq'>)>`
 (From UNIX) `fitspec`

Description: Fits experimental data to Lorentzian and/or Gaussian lineshapes. `fitspec` uses as a starting point data in a file `fitspec.inpar`, which must be prepared prior to performing the calculation. This file contains the frequency, intensity, linewidth, and (optionally) the Gaussian fraction of the lineshape. Any number followed by an asterisk (*) is held fixed during the calculation; all other parameters are varied to obtain the best fit. `fitspec` creates a file `fitspec.data`, which is a text representation of the spectral data (that part of the spectrum between `sp` and `sp+wp`). After the calculation is finished, the results of the fit are contained in a file `fitspec.outpar`, with a format identical to `fitspec.inpar`.

It is often useful to use the output from a deconvolution as the input to a spin simulation to ensure the most accurate possible frequencies for the spin simulation calculation. For this reason, the frequencies and amplitudes of the calculated lines in a deconvolution are automatically stored in the parameters `slfreq`, respectively, from where they can serve as input to an iterative spin simulation. If the spin system is defined *after* a deconvolution is performed, this information is lost (`slfreq` is reset). In this case, `fitspec('setslfreq')` can be used to copy the information from `fitspec.outpar` back into `slfreq`. This is not necessary if you define the spin system before performing the deconvolution (you need not perform the entire spin simulation, only define the spin system).

Arguments: `'usell'` is a keyword to prepare the file `fitspec.inpar` from the last line listing (stored in `llfrq` and `llamp`). All lines are set to have a linewidth of `slw` and a fixed Gaussian fraction of 0. If another starting point is desired, this file can be edited with a text editor. Alternatively, the macro `usemark` may be used.

`'setslfreq'` is a keyword to copy the information from the file `fitspec.outpar` back into the parameters `slfreq`.

Examples: `fitspec`
`fitspec('usell')`
`fitspec('setslfreq')`

See also: *NMR Spectroscopy User Guide*

Related: `llamp` List of line amplitudes (P)
`llfrq` List of line frequencies (P)
`setgauss` Set a Gaussian fraction for lineshape (M)

F

<code>slfreq</code>	Measured line frequencies (P)
<code>sp</code>	Start of plot (P)
<code>usemark</code>	Use “mark” output as deconvolution starting point (M)
<code>wp</code>	Width of plot (P)

fixgrd Convert gauss/cm value to DAC (M)

Syntax: `fixgrd(gradient_value):parameter`

Description: Uses the `gcal` value in the probe table to return the DAC value for a specified gradient strength.

Arguments: `gradient_value` is the required gradient strength in gauss/cm.
`parameter` is any local variable or VnmrJ variable.

Examples: `fixgrd(20):gzlvl`

Related: `gcal` Gradient calibration constant (P)

fixpar Correct parameter characteristics in experiment (M)

Description: After bringing parameters into the current experiment with `convert`, `rt`, `rtf`, or `rtv`, `fixpar` is automatically executed. `fixpar` updates old parameter characteristics and reconciles parameter differences due to the hardware on the spectrometer. If a macro `userfixpar` exists, `fixpar` runs it also. This allows an easy mechanism to customize parameter sets.

Related:	<code>convert</code>	Convert data set from a VXR-style system (C)
	<code>fixpar3rf</code>	Create parameters for third rf channel (M)
	<code>fixpar4rf</code>	Create parameters for fourth rf channel (M)
	<code>parfix</code>	Update parameter set (M)
	<code>parversion</code>	Version of parameter set (P)
	<code>rt</code>	Retrieve FIDs (C)
	<code>rtf</code>	Retrieve parameters (C)
	<code>rtv</code>	Retrieve individual parameters (C)
	<code>updatepars</code>	Update all parameter sets saved in a directory (M)
	<code>userfixpar</code>	Macro called by <code>fixpar</code> (M)

fixpar3rf Create parameters for third rf channel (M)

Applicability: Systems with a second decoupler.

Description: Checks for the existence of all acquisition parameters related to the second decoupler. Any parameters found to be absent are created, characterized, and initialized by the macro. `fixpar3rf` is run as a part of the standard `fixpar` macro if the system configuration parameter `numrfch` is greater than 2 (i.e., the number of rf channels on the system is set at 3 or more).

fixpar4rf Create parameters for fourth rf channel (M)

Applicability: Systems with a third decoupler.

Description: Checks for the existence of all acquisition parameters related to the third decoupler. Any parameters found to be absent are created, characterized, and initialized. `fixpar4rf` is run as a part of the standard `fixpar` macro if the system configuration parameter `numrfch` is greater than 3 (i.e., the number of rf channels on the system is set at 4).

fixpar5rf Create parameters for fifth rf channel (M)

Applicability: Systems with a deuterium decoupler channel as the fourth decoupler.

Description: Checks for the existence of all acquisition parameters related to the fourth decoupler. Any parameters found to be absent are created, characterized, and initialized. `fixpar5rf` is run as a part of the standard `fixpar` macro if the system configuration parameter `numrfch` is greater than 4 (i.e., the number of rf channels on the system is set at 5).

fixup Adjust parameter values selected by setup macros (M)

Description: Called by the experiment setup macros `h1`, `c13`, `hc`, `hcapt`, `capt`, and `hcosy`. As provided, the text of `fixup` is all in quotes so that it does nothing. It is intended to provide each user with a mechanism to make adjustments to values selected by the setup macros.

fixpsg Update psg libraries (M)

Description: Used by `patchinstall` to recompile the psg files and create new psg libraries `libpsglib.so` in `/vnmr/lib`.

flashc Convert compressed 2D data to standard 2D format (C)

Syntax: `flashc (<'nf'>, 'ms' | 'mi' | 'rare', ns, traces, echoes)`

Description: Converts 2D FID data files from compressed formats (`seqcon='nncsn'`, `seqcon='nccnn'`, `seqcon='nnccn'`) to standard format (`seqcon='ncsnn'`) or from standard format to compressed format. Compressed data is taken by using the `nf` parameter; that is, compressed data is acquired as one large uninterrupted “multiFID” acquisition.

`flashc` reads the file `fid` in the `acqfil` subdirectory of the current experiment.

`flashc` can convert a compressed-compressed multislice, multiecho, or multi-image sequence. It can also convert a “rare” type sequence with a compressed phase-encode echo train.

`flashc` changes the values of the following parameters:

Compressed-compressed or standard format to compressed format

- `ni` is set to 1 if no argument is provided.
- `nf` is set to the value of `nf` divided by the multislice, `ms`, or multi-image, `mi`, value.
- `arraydim` is set to the product of its original value and the value of the `traces` argument.
- `arrayelems` is set to 1 if no parameters were arrayed during data acquisition or to 2 if any parameter was arrayed during data acquisition.

Compressed format to standard format

- `nf` is set to the value of the `traces` argument, or to 1 if no argument is provided.
- `ni` is set to the value of `nf` divided by the multislice, `ms`, or multi-image, `mi`, value.
- `arraydim` is set to the product of its original value and the original value of `nf`.
- `arrayelems` is set to 1 if no parameters were arrayed during data acquisition or to 2 if any parameter was arrayed during data acquisition.

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Arguments: **nf** is the number of FIDs in the second dimension of a 2D experiment. When converting data in the standard format to a compressed format, **nf** must always be the first argument.

When converting compressed-compressed or “rare” type sequences, the first argument must be a string defining the type of compression:

- 'mi' is a keyword for the multi-image type of compression.
- 'ms' is a keyword for the multislice type of compression.
- 'rare' is a keyword for the “rare” multiecho, rare type, fast-imaging data sets.

(Standard to compressed) **ns** is the number of images slices or array elements to be retained.

(Compressed-compressed or rare to standard) **traces** is the number of compressed traces to retain for each **ni**. The parameter **nf** is set to this number after **flashc** has run.

(Compressed-compressed or rare to standard) **echoes** is the number of compressed echoes, used with “rare” type formatting.

Examples: *Compressed-compressed or standard format to compressed format*
`flashc('nf')` (standard to compressed)
`flashc('nf','ms',ns)` (compressed phase-encode and multislice)
`flashc('nf','mi',ns)` (compressed multi-image and phase-encode)
Compressed-compressed format or rare format to standard format
`flashc` (simple compressed phase-encode)
`flashc('ms',ns)` (compressed phase-encode and multislice)
`flashc('mi',ns)` (compressed multi-image and phase-encode)
`flashc('rare',ns,etl)`

See also: *VnmrJ Imaging NMR*

Related:	arraydim	Dimension of experiment (P)
	ft2d	Fourier transform 2D data (C)
	ft3d	Fourier transform 3D data (C)
	nf	Number of FIDs (P)
	ni	Number of increments in 1st indirectly detected dimension (P)

flipflop **Set up parameters for FLIPFLOP pulse sequence (M)**

Applicability: Systems with solids module.

Description: Sets up a multipulse parameter set for tuning out “phase glitch” in the probe and pulse amplifier.

See also: *User Guide: Solid-State NMR*

Fluorine **Set up parameters for ¹⁹F experiment (M)**

Description: Set Up parameters for ¹⁹F experiment.

flush **Write out data in memory (C)**

Description: Writes out the current data and parameters in memory buffers. Normally, this information is not written to disk until exiting VnmrJ or joining another experiment. One reason to use **flush** is to be able to access experimental data from a program separate from the VnmrJ program.

See also: *User Programming*

- fn** **Fourier number in directly detected dimension (P)**
- Description: Selects the Fourier number for the Fourier transformation along the directly detected dimension. This dimension is often referred to as the f_2 dimension in 2D data sets, the f_3 dimension in 3D data sets, etc.
- Values: 'n' or a number equal to a power of 2 (minimum is 32). If **fn** is not *entered* exactly as a power of 2, it is automatically rounded to the nearest higher power of 2 (e.g., setting **fn**=32000 gives **fn**=32768). **fn** can be less than, equal to, or greater than **np**, the number of directly detected data points:
- If **fn** is less than **np**, only **fn** points are transformed.
 - If **fn** is greater than **np**, **fn** minus **np** zeros are added to the data table (“zero-filling”).
 - If **fn**= 'n', **fn** is automatically set to the power of 2 greater than or equal to **np**.
- fn1** **Fourier number in 1st indirectly detected dimension (P)**
- Description: Selects the Fourier number for the Fourier transformation along the first indirectly detected dimension. This dimension is often referred to as the f_1 dimension of a multi-dimensional data set. The number of increments along this dimension is controlled by the parameter **ni**.
- Values: **fn1** is set in a manner analogous to the parameter **fn**, with **np** being substituted by $2 * \mathbf{ni}$.
- See also: *NMR Spectroscopy User Guide*
- Related: **fn** Fourier number in directly detected dimension (P)
 fn2 Fourier number in 2nd indirectly detected dimension (P)
 ni Number of increments in 1st indirectly detected dimension (P)
 np Number of data points (P)
- fn2** **Fourier number in 2nd indirectly detected dimension (P)**
- Description: Selects the Fourier number for the Fourier transformation along the second indirectly detected dimension. This dimension is often referred to as the f_2 dimension of a multidimensional data set. The number of increments along this dimension is controlled by the parameter **ni2**. **fn2** is set in a manner analogous to the parameter **fn**, with **np** being substituted by $2 * \mathbf{ni2}$.
- See also: *NMR Spectroscopy User Guide*
- Related: **fn** Fourier number in directly detected dimension (P)
 fn1 Fourier number in 1st indirectly detected dimension (P)
 ni2 Number of increments in 2nd indirectly detected dimension (P)
 np Number of data points (P)
- fn2D** **Fourier number to build up 2D DOSY display in freq. domain (P)**
- Description: In 2D DOSY sequences (Dbppste, DgcsteSL, Doneshot, Dbppsteinept), replaces **fn** when setting up the 2D display.
- See also: *NMR Spectroscopy User Guide*
- Related: **ddif** Synthesize and display DOSY plot (C)
 dosy Process DOSY experiments (M)

F

focus **Send keyboard focus to input window (C)**

Description: Sends keyboard focus to the input window. This is only useful for macro programming.

See also: *User Programming*

foldcc **Fold INADEQUATE data about two-quantum axis (C)**

Syntax: `foldcc`

Description: Symmetrizes 2D INADEQUATE data along the P-type double-quantum axis and applies an automatic `dc` baseline correction. `foldcc` functions for both hypercomplex and complex 2D data.

See also: *NMR Spectroscopy User Guide*

Related: `dc` Calculate spectral drift correction (C)
`foldj` Fold J-resolved 2D spectrum about $f_1=0$ axis (C)
`foldt` Fold COSY-like spectrum along diagonal axis (C)
`rotate` Rotate 2D data (C)

foldj **Fold J-resolved 2D spectrum about $f_1=0$ axis (C)**

Description: Symmetrizes heteronuclear 2D-J, or rotated homonuclear 2D-J, experiments about the $f_1=0$ axis. The `foldj` command functions with both complex and hypercomplex 2D data.

Related: `foldcc` Fold INADEQUATE data about 2-quantum axis (C)
`foldt` Fold COSY-like spectrum along diagonal axis (C)
`rotate` Rotate 2D data (C)

foldt **Fold COSY-like spectrum along diagonal axis (C)**

Syntax: `foldt<('symm' | 'triang')>`

Description: Folds COSY-like correlation spectra about the diagonal. The 2D spectrum must exhibit a *P-type diagonal* for `foldt` to work properly (a P-type diagonal goes from the bottom left-hand side to the top right-hand side of the contour display.) `foldt` functions for both hypercomplex and complex 2D data but requires that `fn=fn1` and `sw=sw1`.

Arguments: `'symm'` is a keyword for the folding process to perform a symmetrization of the data by replacing every two symmetry-related points with the one point therein that has the least magnitude. This value is the default.
`'triang'` is a keyword for the folding process to perform a triangularization of the data by replacing every two symmetry-related points with their geometric mean.

Related: `fn` Fourier number in directly detected dimension (P)
`fn1` Fourier number in 1st indirectly detected dimension (P)
`foldcc` Fold INADEQUATE data about 2-quantum axis (C)
`foldj` Fold J-resolved 2D spectrum about $f_1=0$ axis (C)
`rotate` Rotate 2D data (C)
`sw` Spectral width in directly detected dimension (P)
`sw1` Spectral width in 1st indirectly detected dimension (P)

fontselect Open FontSelect window (C)

Description: Opens the FontSelect window for defining fonts in window panes created by `setgrid`. A different font can be selected for every window pane combination of rows and columns. Separate fonts can also be selected for a large or small overall graphic window.

See also: *NMR Spectroscopy User Guide*

Related: `curwin` Current window (P)
`jwin` Activate current window (M)
`mapwin` List of experiment numbers (P)
`setgrid` Activate selected window (M)
`setwin` Activate selected window (C)

format Format a real number or convert a string for output (C)

Applicability: All

Syntax: `format(realvar, 'length', 'precision'):$rval`
`format(stringvar, 'isreal'):$rval`
`format(stringvar, <'upper' or 'lower'>):$sval`

Description: Give the command these arguments to format the output as a real number. Accepts arguments specifying the real number length, precision, and output variable. The `realvar` input must be a real number, string holding a real number, or a string variable that satisfies the rules for a real number.

Give the command two arguments, `stringvar` and `isreal` to test the string. The command returns a 1 if the first argument can represent a real number and a 0 if it cannot. The output is written to the specified output variable.

Give the command two arguments, `stringvar` and either 'upper' or 'lower' to write the string to the output string variable (e.g., `$sval`) in either all upper case or all lower case. The temporary \$ parameter (e.g., `$sval`) must first be initialized as a string (e.g., `$sval=' '`).

Arguments: `realvar` a real variable
`stringvar` a string variable
length of the real number
precision of the real number
`$sval` a temporary string \$ parameter
`$rval` a temporary real \$ parameter

Examples: `format(a,5,2):sa`
If `a=24.1264` then string `sa='24.13'`

`format(solvent,'lower'):n1`
If `solvent='CDCl3'` then string `n1='cdcl3'`

`format($1,'isreal'):$a`
Sets `$a` to 1 if `$1` represents a number or Sets `$a` to 0 if `$1` represents a string.

`$sval=' '`
Initialize `$sval` to a string variable to return the value into a string

`$snum = '143.92'`
`$rnum = 32.75`

`format($rnum,3,1):$sval`
sets `$sval` to the string '32.8', `$sval` is a string return value.

`format($rnum,3,1):$rval`
sets `$rval` to the number 32.8. `$rval` is a real return value.

Format string value `$snum = '143.92'`

`format($snum,3,1):$sval` sets `$sval` to the string '143.9'

F

`format ($snum, 3, 1) : $rval` sets `$rval` to the number 143.9

See also: *User Programming*

Related: `n1, n2, n3` Name storage for macros (P)
`r1-r7` Real-value storage for macros (P)

fp Find peak heights or phases (C)

Syntax: `fp(<'phase', ><index1, index2, ...> >`

Description: Following a line listing (either `d11` or `n11`), `fp` measures the peak height of each peak in an array of spectra. The results of the analysis are written to a text file `fp.out` in the current experiment directory. If the `npoint` parameter is defined in the current parameter set and this parameter is “on,” it determines the range of data points over which a maximum is searched when determining peak heights. The possible values of `npoint` are 1 to `fn/4`. The default is 2.

Arguments: `'phase'` is a keyword to measure the phase of each peak instead of height.
`index1, index2, ...` restricts measuring peak heights or phases to the lines listed.

Examples: `fp`
`fp(1, 3)`
`fp('phase')`

See also: *NMR Spectroscopy User Guide*

Related: `d11` Display listed line frequencies and intensities (C)
`fn` Fourier number in directly detected dimension (P)
`get11` Get line frequency and intensity from line list (C)
`n1` Position cursor at the nearest line (C)
`n11` Find line frequencies and intensities (C)
`npoint` Number of points for `fp` peak search (P)

fpmult First point multiplier for np FID data (P)

Description: Allows error correction if the first point of an FID is misadjusted. In a 1D experiment, this adjustment influences the overall integral of the spectrum. For *n*-dimensional experiments, if the correction is not made, “ridges” can appear. In 2D experiments, the ridges appear as “*f*₂ ridges.” In 3D experiments, the ridges appear as “*f*₃ ridges.” These ridges can clearly be seen in the noise region on the top and bottom of a 2D spectrum (when `trace= 'f1'`) as a low-intensity profile of the diagonal. The sign and intensity of the ridges is controlled by the magnitude of `fpmult`.

It has been recognized that the first point of a FID that is sampled at exactly time equal to zero must be multiplied by 0.5 for the Fourier transform to function properly. The `fpmult` parameter gives you a method to fine-tune the actual correction factor.

Values: Default is 1.0, except that if the processing involves backward extension of the time-domain data with linear prediction, the default changes to 0.5. If `fpmult` is set to 'n', `fpmult` takes on its default value.

See also: *NMR Spectroscopy User Guide*

Related: `fpmult1` First point multiplier for *n*₁ interferogram data (P)
`fpmult2` First point multiplier for *n*₁₂ interferogram data (P)
`np` Number of data points (P)
`trace` Mode for *n*-dimensional data display (P)
`wft2da` Weight and Fourier transform phase-sensitive data (M)

fpmult1 First point multiplier for ni interferogram data (P)

Description: Operates on **ni** hypercomplex or complex interferogram data in a manner analogous to **fpmult**. In many 2D experiments, the t_1 values are adjusted so there is no first-order phasing in the f_1 and f_2 dimensions. In this case, **fpmult1** should be 0.5. If the t_1 value is adjusted so that there is a 180° first-order phase correction, **fpmult1** should be 1.0.

Values: Default value is 0.5. If **fpmult1** is set to 'n', it takes on its default value.

See also: *NMR Spectroscopy User Guide*

Related: **fpmult** First point multiplier for **np** FID data (P)
fpmult2 First point multiplier for **ni2** interferogram data (P)
ni Number of increments in 1st indirectly detected dimension (P)

fpmult2 First point multiplier for ni2 interferogram data (P)

Description: Operates on **ni2** hypercomplex or complex interferogram data in a manner analogous to **fpmult**. In many 3D experiments, the t_2 value is adjusted so that there is no first-order phasing in the f_1 and f_2 dimensions. In this case, **fpmult2** should be 0.5. If the t_2 value is adjusted so that there is a 180° first-order phase correction, **fpmult2** should be 1.0.

Values: Default value is 0.5. If **fpmult2** is set to 'n', it takes on its default value.

See also: *NMR Spectroscopy User Guide*

Related: **fpmult** First point multiplier for **np** FID data (P)
fpmult1 First point multiplier for **ni** interferogram data (P)
ni2 Number of increments in 2nd indirectly detected dimension (P)

fr Full recall of a display parameter set (M)

Applicability: All

Syntax: **fr** (n<, noupdate>)

Description: Recall all the parameters of the specified display parameter set and set the current display parameters to those values.

Arguments: n=1 to 9

noupdate as second argument prevents the automatic update of interactive programs.

Related: **r** Recall display parameter set (M)
s Save display parameters as a set (M)

fread Read parameters from file and load them into a tree (C)

Syntax: **fread**(file<, tree<, 'reset' | 'value'>>)

Description: Reads parameters from a file and loads the parameters into a tree. The tree can be global, current, processed, or system global. **fread** can read from any file that has parameters stored in the correct VnmrJ format.

Note that if parameters are read into the global tree, certain important system parameters are not loaded because these parameters should not be changed. The parameters that are not loaded are **userdir**, **systemdir**, **curexp**, **autodir**, **auto**, **vnmraddr**, and **acqaddr**.

Arguments: **file** is the name of the file containing parameters stored in VnmrJ format.

tree is one of the keywords 'global', 'current', 'processed', or 'systemglobal'. The default is 'current'. This argument specifies the

type of tree into which the parameters are loaded. Refer to the `create` command for more information on types of trees.

'reset' is a keyword that causes the parameter tree to be cleared before the new parameter file is read. Without this option, parameters read from a file are added to the existing preloaded parameters. To use this option, `tree` must also be specified.

'value' is a keyword that causes only the values of the parameters in the file to be loaded. If a preloaded variable does not already exist, a new one is not created. Parameter attributes are not changed, and enumerated values are not changed. To use this option, `tree` must also be specified.

Examples: `fread('/vnmr/stdpar/H1.par/procpar')`
`fread('sampvar','global')`
`fread('setvar','current','reset')`
`fread('var1','processed','value')`

See also: *User Programming*

Related:	<code>auto</code>	Automation mode active (P)
	<code>autodir</code>	Automation directory absolute path (P)
	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>curexp</code>	Current experiment directory (P)
	<code>destroy</code>	Destroy a parameter (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>fsave</code>	Save parameters from a tree to a file (C)
	<code>rtp</code>	Retrieve parameters (C)
	<code>systemdir</code>	System directory (P)
	<code>userdir</code>	User directory (P)

fsave Save parameters from a tree to a file (C)

Syntax: `fsave(file<,>,tree<,>)`

Description: Writes parameters from a parameter tree to a file.

Arguments: `file` is the name of the file, which can be any valid file for which the user has write permission. If the file already exists, it will be overwritten.

`tree` is one of the keywords 'global', 'current', 'processed', or 'systemglobal'. The default is 'current'. Refer to the `create` command for more information on types of trees.

Examples: `fsave('var1')`
`fsave('sampvar','global')`

See also: *User Programming*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>destroy</code>	Destroy a parameter (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>fread</code>	Read parameters from file and load them into a tree (C)
	<code>svp</code>	Save parameters from current experiment (C)

fsq Frequency-shifted quadrature detection (P)

Description: Selects whether to use frequency-shifted quadrature detection. When `fsq` is turned on, if `dsp` is on, the observe frequency is offset by `oslsfrq`, and the digital filter is also offset by `oslsfrq`. The default value of `oslsfrq` is $1.25 * sw$.

The effect of `fsq` is to offset only the digital filter by `oslsfrq`. The observe frequency must be offset by `oslsfrq` by modifying the pulse sequence as described in the manual *NMR Spectroscopy User Guide*.

Values: 'n' turns frequency-shifted quadrature detection off. 'y' turns it on.

See also: *NMR Spectroscopy User Guide*

Related: **dsp** Type of DSP for data acquisition (P)
oslsfrq Bandpass filter offset for oversampling (P)
oversamp Oversampling factor for acquisition (P)
sw Spectral width in directly detected dimension (P)

ft **Fourier transform 1D data (C)**

Syntax: (1) `ft(<options>,<'nf'><,start><,finish><,step>)>`
 (2) `ft('inverse',exp_number,expansion_factor)`

Description: In syntax 1, performs a Fourier transform on one or more 1D FIDs without weighting applied to the FID. `ft` executes a left-shift, zero-order phase rotation, and a frequency shift (first-order phase rotation) according to the parameters `lsfid`, `phfid`, and `lsfrq`, respectively, on the time-domain data, prior to Fourier transformation. The type of Fourier transform to be performed is determined by the parameter `proc`. Solvent suppression is turned on or off with the parameters `ssfilter` and `ssorder`. For arrayed data sets, `ft` Fourier transforms all of the array elements. To Fourier transform selected array elements, `ft` can be passed numeric arguments.

In syntax 2, `ft` performs an inverse Fourier transform of the entire spectrum. (VnmrJ does not currently support inverse Fourier transformation of arrayed 1D or 2D data sets.)

Arguments: `options` can be any of the following (all string arguments must precede the numeric arguments):

- 'acq' is a keyword to check if any elements of a multi-FID experiment have already been transformed. If so, these previously transformed elements will not be retransformed.
- 'dodc' is a keyword for all spectra to be dc corrected independently.
- 'nodc' is a keyword to not perform the usual dc drift correction.
- 'nods' is a keyword to prevent an automatic spectral display (`ds`) from occurring. This outcome is useful for various plotting macros.
- 'noft' is a keyword to skip the Fourier transform, thereby allowing use of all spectral manipulation and plotting commands on FIDs.
- 'zero' is a keyword to zero the imaginary channel of the FID prior to the Fourier transform. This zeroing occurs after any FID phasing. Its use is generally limited to wideline solids applications.

'nf' is a keyword that makes a single FID element containing `nf` traces to be transformed as if it were `nf` separate FID elements. If 'nf' precedes the list of numeric arguments, the rules for interpreting the numeric arguments change slightly. Passing no numeric arguments results in the transformation of all `nf` traces in the first FID element. Passing a single numeric argument results in the transformation of all `nf` traces in the requested FID element (e.g., `ft('nf',3)` transforms all `nf` traces for element 3). Regardless of the requested FID element, the resulting spectra are labeled as 1 to `nf` because multiple elements cannot be transformed using `ft('nf')`. Subsequent numeric arguments are interpreted as previously described.

`start` is the index of a particular element to be transformed. For an array, `start` is the index of the first element to be transformed.

`finish` is the index of the last element to be transformed for an array.

`step` specifies the increment between successive elements that are to be transformed for an array. The default is 1.

'inverse' is a keyword specifying an inverse Fourier transform.

exp_number is the number of the experiment, from 1 to 9, for storing the resulting FID from the inverse Fourier transform.

expansion_factor defines the expansion of the spectrum before the inverse Fourier transform is performed. This argument is equivalent to a multiplier for the fn parameter. The multiplier is restricted to between 1 and 32 and is rounded up internally to the nearest power of 2.

Examples: `ft`
`ft (1)`
`ft (3, 7)`
`ft (2, 10, 2)`
`ft ('nf', 3)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dcrmv</code>	Remove dc offsets from FIDs in special cases (P)
	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>lsfid</code>	Number of points to left-shift the np FID (P)
	<code>lsfrq</code>	Frequency shift of the fn spectrum in Hz (P)
	<code>nf</code>	Number of FIDs (P)
	<code>phfid</code>	Zero-order phasing constant for np FID (P)
	<code>proc</code>	Type of processing on the np FID (P)
	<code>ssfilter</code>	Full bandwidth of digital filter to yield a filtered FID (P)
	<code>ssorder</code>	Order of polynomial to fit digitally filtered FID (P)
	<code>wft</code>	Weight and Fourier transform 1D data (C)

ft1d **Fourier transform along f₂ dimension (C)**

Syntax: (1) `ft1d(element_number)`
 (2) `ft1d('nf', element_number)`
 (3) `ft1d(<options>, <coefficients>)`

Description: Performs the first Fourier transformation along the f₂ dimension, without weighting, and matrix transposition. `ft1d` allows the display of t₁ interferograms with the `dcon` and `dconi` commands. For arrayed 2D FID data, a single array element can be weighted and transformed using syntax 1 or 2. The keyword 'nf' is used in syntax 2 to specify that the 2D data is collected in the compressed form using 'nf'. Complex and hypercomplex interferograms can be constructed explicitly by supplying a series of options and coefficients using syntax 3.

For information on real as opposed to complex Fourier transforms, see the descriptions of the `proc`, `proc1`, and `proc2` parameters. For information about Hadamard transforms, see the description of the `proc1` parameter and the *VnmrJ NMR Liquids* user guide. For information on left-shifting, zero-order phase rotation, and frequency shifting of the FID and interferogram time-domain data during the 2D Fourier transformation, see the descriptions of the parameters `lsfid`, `lsfid1`, `lsfid2`, `phfid`, `phfid1`, `phfid2`, `lsfrq`, `lsfrq1`, and `lsfrq2`, as appropriate. For information on the lfs (low-frequency suppression) and zfs (zero-frequency suppression) solvent suppression options, see the description of the parameters `ssfilter` and `ssorder`, and the macro `parfidss`.

Arguments: `element_number` is a single array element to be weighted and transformed. `options` can be the keywords 'ptype' or 'ntype' but neither serve a useful function because the differential effect of these arguments is applied only during the course of the second Fourier transformation. The default is 'ntype'.

coefficients are a series of coefficients according to the following scheme: RR1 is the coefficient used to multiply the real part (first R) of spectra set 1 before it is added to the real part (second R) of the interferogram. IR2 would thus represent the contribution from the imaginary part of spectra set 2 to the real part of the interferogram, and so on. The scheme is depicted below.

```
ft1d(RR1, IR1, RR2, IR2, . . . , RI1, II1, RI2, II2, . . . )
```

where:

```
RR1*REAL(w2,element=1) -> REAL(t1)
IR1*IMAG(w2,element=1) -> + REAL(t1)
RR2*REAL(w2,element=2) -> + REAL(t1)
IR2*IMAG(w2,element=2) -> + REAL(t1)
. . .
RI1*REAL(w2,element=1) -> IMAG(t1)
II1*IMAG(w2,element=1) -> + IMAG(t1)
RI2*REAL(w2,element=2) -> + IMAG(t1)
II2*IMAG(w2,element=2) -> + IMAG(t1)
...
```

See also: *NMR Spectroscopy User Guide*

Related:	dconi	Interactive 2D data display (C)
	ft2d	Fourier transform 2D data (C)
	lsfid	Number of complex points to left-shift np FID (P)
	lsfid1	Number of complex points to left-shift ni interferogram (P)
	lsfid2	Number of complex points to left-shift ni2 interferogram (P)
	lsfrq	Frequency shift of the fn spectrum (P)
	lsfrq1	Frequency shift of the fn1 spectrum (P)
	lsfrq2	Frequency shift of the fn2 spectrum (P)
	parfidss	Create parameters for time-domain solvent subtraction (M)
	phfid	Zero-order phasing constant for np FID (P)
	phfid1	Zero-order phasing constant for ni interferogram (P)
	phfid2	Zero-order phasing constant for ni interferogram (P)
	proc	Type of processing on np FID (P)
	proc1	Type of processing on ni interferogram (P)
	proc2	Type of processing on ni2 interferogram (P)
	pmode	Processing mode for 2D data (P)
	ssorder	Order of polynomial to fit digitally filtered FID (P)
	ssfilter	Full bandwidth of digital filter to yield a filtered FID (P)
	wft2d	Weight and Fourier transform 2D data (C)

ft1da **Fourier transform phase-sensitive data (M)**

Syntax: `ft1da<(options)>`

Description: Performs the first (f_2) transform of a 2D transform or the first part of a 3D transform. Otherwise, `ft1da` has the same functionality as the [ft2da](#) command. See the description of [ft2da](#) for further information. For information about Hadamard transforms, see the description of the [proc1](#) parameter and the *VnmrJ NMR Liquids* user guide.

Arguments: `options` are the same as used with [ft2da](#). See [ft2da](#) for details.

See also: *NMR Spectroscopy User Guide*

Related:	ft2d	Fourier transform 2D data (C)
	ft2da	Fourier transform phase-sensitive data (M)
	wft1da	Weight and Fourier transform phase-sensitive data (M)
	wft2da	Weight and Fourier transform phase-sensitive data (M)

F

ft1dac Combine arrayed 2D FID matrices (M)

Syntax: `ft1dac(<mult1><,mult2>,...<,multn>)>`

Description: Allows ready combination of 2D FID matrices within the framework of the 2D Fourier transformation program. No weighting is performed. `ft1dac` requires that the data be acquired either without f_1 quadrature or with f_1 quadrature using the TPPI method. This macro is used for TOCSY (with multiple mixing times).

Arguments: `mult1`, `mult2`, ..., `multn` are multiplicative coefficients. The `nth` argument is a real number and specifies the multiplicative coefficient for the `nth` 2D FID matrix.

Related: `ft2dac` Combine arrayed 2D FID matrices (M)
`Tocsy` Set up parameters for TOCSY pulse sequence (M)
`wft1da` Weight and Fourier transform phase-sensitive data (M)
`wft1dac` Combine arrayed 2D FID matrices (M)

ft2d Fourier transform 2D data (C)

Syntax: (1) `ft2d(array_element)`
 (2) `ft2d('nf'<array_element>)`
 (3) `ft2d(<options>,<plane_number>,<coefficients>)>`
 (4) `ft2d('ni'|'ni2',element_number,increment)`
 (5) `ft2d('ni'|'ni2',increment,<coefficients>)`

Description: Performs the complete 2D Fourier transformation, without weighting, in both dimensions. If the first Fourier transformation has already been done using `ft1d`, `wft1d`, `ft1da`, or `wft1da`, the `ft2d` command performs only the second (t_1) transform.

For arrayed 2D FID data, a single array element can be weighted and transformed using syntax 1. If the data is collected in “compressed” form using ‘`nf`’, syntax 2 must be used. Complex and hypercomplex interferograms can be constructed explicitly by supplying a series of coefficients using syntax 3. If an arrayed 3D data set is to be selectively processed, the format of the arguments to `ft2d` changes to syntax 4. For example, `ft2d('ni',1,2)` performs a 2D transform along `np` and `ni` of the second `ni2` increment and the first element within the explicit array. This command yields a 2D `np-ni` frequency plane.

Arrayed 3D data sets can also be subjected to 2D processing to yield 2D absorptive spectra. If the States-Haberkorn method is used along both f_1 (`ni` dimension) and f_2 (`ni2` dimension), there are generally 4 spectra per (`ni,ni2`) 3D element. In this case, using syntax 5, entering `ft2d('ni2',2,<16 coefficients>)` performs a 2D transform along `np` and `ni2` of the second `ni` increment using the 16 coefficients to construct the 2D t_1 -interferogram from appropriate combinations of the 4 spectra per (`ni,ni2`) 3D element.

If there are `n` data sets to be transformed, as in typical phase-sensitive experiments, $4 * n$ coefficients must be supplied. The first $2 * n$ coefficients are the contributions to the real part of the interferogram, alternating between absorptive and dispersive parts of the successive data sets. The next $2 * n$ coefficients are the contributions to the imaginary part of the interferogram, in the same order. Thus, using the definition that the first letter refers to the source data set, the second letter refers to the interferogram, and the number identifies the source data set, we have the following cases:

<i>Data sets</i>	<i>Coefficient order</i>
1	RR1, IR1, RI1, II1
2	RR1, IR1, RR2, IR2, RI1, II1, RI2, II2
3	RR1, IR1, RR2, IR2, RR3, IR3, RI1, II1,

Data sets	Coefficient order

	RI2, II2, RI3, II3

...	...

The coefficients are often 1, 0, or -1, but this is not always the case. Any non-integral coefficient can be used, and as many coefficients can be nonzero as is desired. Up to 32 coefficients can be supplied, which at 4 per data set allows the addition, subtraction, etc., of eight 2D data sets (e.g., 8 different phase cycles).

For information on real as opposed to complex Fourier transforms, see the descriptions of the `proc`, `proc1`, and `proc2` parameters. For information about Hadamard transforms, see the description of the `proc1` parameter and the *VnmrJ NMR Liquids* user guide. For information on left-shifting, zero-order phase rotation, and frequency shifting of the FID and interferogram time-domain data during the 2D Fourier transformation, see the descriptions of the parameters `lsfid`, `lsfid1`, `lsfid2`, `phfid`, `phfid1`, `phfid2`, `lsfrq`, `lsfrq1`, and `lsfrq2`, as appropriate. For information on the lfs (low-frequency suppression) and zfs (zero-frequency suppression) solvent suppression options, see the description of parameters `ssfilter` and `ssorder`, and macro `parfidss`.

Arguments: `array_element` is a single array element to be transformed.

`options` can be any of the following (all string arguments must precede the numeric arguments):

- `'ptype'` is a keyword to transform P-type data to yield a P-type contour display.
- `'ntype'` is a keyword to transform N-type data to yield a P-type contour display. This is the default.
- `'t2dc'` is a keyword to apply a dc correction to each t_2 FID prior to the first Fourier transform. The last 1/16-th of the time domain data is used to calculate the dc level.
- `'t1dc'` is a keyword to apply a dc correction to each t_1 interferogram prior to the second Fourier transform. The last 1/16-th of the time domain data is used to calculate the dc level.
- `'f2sel'` is a keyword to allow only preselected f_2 regions to be transformed along t_1 . The t_1 interferograms in the non-selected f_2 regions are zeroed but *not* transformed. The same mechanism used to select baseline regions for baseline correction (`bc`) is used to select the f_2 regions to be transformed along t_1 . Set `intmod='partial'` and partition the integral of the spectrum into several regions. The even numbered f_2 regions (e.g., 2, 4, 6) are transformed along t_1 ; the odd numbered regions are not transformed along t_1 .
- `'nf'` is a keyword to transform arrayed or multi-slice 2D data that has been collected in the compressed form as single 2D FIDs with multiple (`nf`) traces.
- `'ni2'` is a keyword to transform non-arrayed 2D data that have been collected with `ni2` and `sw2` (instead of `ni` and `sw1`). `addpar('3d')` creates the necessary processing parameters for the `'ni2'` operation.
- `'noop'` is a keyword to not perform any operation on the FID data. This option is used mainly to allow macros, such as `wft2da`, to have the same flexibility as commands.

`coefficients` are a series of coefficients according to the following scheme: RR1 is the coefficient used to multiply the real part (first R) of spectra set 1 before it is added to the real part (second R) of the interferogram. IR2

would thus represent the contribution from the imaginary part of spectra set 2 to the real part of the interferogram, and so forth. The scheme is depicted below.

```
ft2d(RR1,IR1,RR2,IR2,...,RI1,II1,RI2,II2,...)
```

where:

```
RR1*REAL(w2,element=1) -> REAL(t1)
IR1*IMAG(w2,element=1) -> + REAL(t1)
RR2*REAL(w2,element=2) -> + REAL(t1)
IR2*IMAG(w2,element=2) -> + REAL(t1)
. . .
RI1*REAL(w2,element=1) -> IMAG(t1)
II1*IMAG(w2,element=1) -> + IMAG(t1)
RI2*REAL(w2,element=2) -> + IMAG(t1)
II2*IMAG(w2,element=2) -> + IMAG(t1)
```

'ni' is a keyword to selectively transform a particular **np-ni** 2D plane within a non-arrayed 3D data set. To identify the plane, 'ni' is followed by the `plane_number` argument, an integer from 1 through **ni2**.

'ni2' is a keyword to selectively transform a particular **np-ni2** 2D plane within a non-arrayed 3D data set. To identify the plane, 'ni2' is followed by the `plane_number` argument, an integer from 1 through **ni**.

`element_number` is the number of an element within the explicit array when selectively processing an arrayed 3D data set; it ranges from 1 to **ni2**

`increment` is the increment within the explicit array when selectively processing an arrayed 3D data set; it ranges 1 to `arraydim/(ni*ni2)`.

Examples: `ft2d(1,0,0,0,0,0,1,0)`

```
ft2d(1)
```

```
ft2d('nf',3)
```

```
ft2d('ptype',...)
```

See also: *NMR Spectroscopy User Guide*

Related:	dconi	Interactive 2D data display (C)
	dcrmv	Remove dc offsets from FIDs in special cases (P)
	fpmult	First point multiplier for np FID data (P)
	fpmult1	First point multiplier for ni interferogram data (P)
	ft1d	Fourier transform along f ₂ dimension (C)
	lsfid	Number of complex points to left-shift np FID (P)
	lsfid1	Number of complex points to left-shift ni interferogram (P)
	lsfid2	Number of complex points to left-shift ni2 interferogram (P)
	lsfrq	Frequency shift of the fn spectrum (P)
	lsfrq1	Frequency shift of the fn1 spectrum (P)
	lsfrq2	Frequency shift of the fn2 spectrum (P)
	parfidss	Create parameters for time-domain solvent subtraction (M)
	phfid	Zero-order phasing constant for np FID (P)
	phfid1	Zero-order phasing constant for ni interferogram (P)
	phfid2	Zero-order phasing constant for ni2 interferogram (P)
	proc	Type of processing on np FID (P)
	proc1	Type of processing on ni interferogram (P)
	proc2	Type of processing on ni2 interferogram (P)
	pmode	Processing mode for 2D data (P)
	ssorder	Order of polynomial to fit digitally filtered FID (P)
	ssfilter	Full bandwidth of digital filter to yield a filtered FID (P)
	wft1d	Weight and Fourier transform f ₂ for 2D data (C)
	wft2d	Weight and Fourier transform 2D data (C)

ft2da **Fourier transform phase-sensitive data (M)**

Syntax: `ft2da<(options)>`

Description: Processes 2D FID data and 2D planes at particular t_1 or t_2 times from a 3D data set for a pure absorptive display. `ft2da` differs from `wft2da` only in that, in the case of `wft1da`, weighting of the time-domain data is performed prior to the FT. `ft2da` functions analogously to `ft1da` and `wft1da`, except that `ft2da` and `wft2da` perform only the f_2 Fourier transform. For information about Hadamard transforms, see the description of the `proc1` parameter and the *VnmrJ NMR Liquids* user guide.

Macros `ft1da`, `wft1da`, `ft2da`, and `wft2da` function for hypercomplex 2D FID data (`phase=1, 2`) and for TPPI 2D FID data (`phase=3` or `phase=1, 4`) acquired either with `ni` or `ni2`. If the data were acquired with `ni`, no additional arguments need be used with the macros. If the data were acquired with `ni2`, the keyword '`ni2`' must be used.

For `phase=1, 2`:

```
wft2da=wft2d('ptype',1,0,0,0,0,0,1,0)
```

For `phase=3`: `wft2da=wft2d(1,0,0,0)`

For `phase=1, 4`:

```
wft2da=wft2d('ptype',1,0,0,0,0,0,1,0)
```

Macros `ft1da`, `wft1da`, `ft2da`, and `wft2da` support selective 2D processing within a 3D FID data set. All permutations of hypercomplex and TPPI modes of data acquisition in t_1 and t_2 can be handled. For selective f_2f_3 processing, the numeric argument immediately following the '`ni2`' keyword is interpreted to be the t_1 increment number, which specifies the particular f_2f_3 plane (`plane_number`, see below) to be processed. For selective f_1f_3 processing, the t_2 increment number either follows the keyword '`ni`', which is optional, or is associated with the first numeric argument that does not immediately follow a '`bc`' keyword.

For information on real as compared to complex Fourier transformation, see the description of `proc` or `proc1`. For information on the lfs (low-frequency suppression) and zfs (zero-frequency suppression) solvent suppression options, see the description of parameters `ssfilter` and `ssorder`, and the macro `parfidss`.

Arguments: `options` can be any of the following (the order is not important):

- '`ntype`', '`t2dc`', '`t1dc`', and '`f2sel`' are keywords that function the same as when supplied to the `ft2d` and `wft2d` commands. Refer to the `ft2d` command for a description of these options.
- '`bc`' is a keyword for a baseline correction of the phase-corrected f_2 spectra prior to the f_1 Fourier transform. The baseline regions must have been previously determined. The default polynomial order is 1, which leads to a spline fit. A different polynomial order can be specified by inserting a numerical argument following '`bc`'.
- '`dc`' is a keyword for a drift correction (`dc`) of the f_2 spectra prior to the f_1 Fourier transformation.
- '`ni`' is a keyword to selectively transform a particular `np-ni` 2D plane within a non-arrayed 3D data set. To identify the plane, '`ni`' is followed by `plane_number`, an integer from 1 through `ni2`.
- '`ni2`' is a keyword to selectively transform a particular `np-ni2` 2D plane within a non-arrayed 3D data set. To identify the plane, '`ni2`' is followed by `plane_number`, an integer from 1 through `ni`.
- '`old`' is a keyword to allow data acquired before the February 25, 1988, software release to be processed correctly. '`old`' does not function for

selective 2D processing within 3D data sets. If no **ni2** or **ni** **plane_number** is given, it is assumed that the data set is only 2D in either **ni2** or **ni**, respectively.

See also: *NMR Spectroscopy User Guide*

Related:	f1coef	Coefficient to construct F1 interferogram (P)
	f2coef	Coefficient to construct F2 interferogram (P)
	ft1da	Fourier transform phase-sensitive data (M)
	parfidss	Create parameters for time-domain solvent subtraction (M)
	phase	Phase selection (P)
	proc	Type of processing on the np FID (P)
	proc1	Type of processing on the ni interferogram (P)
	ssorder	Order of polynomial to fit digitally filtered FID (P)
	ssfilter	Full bandwidth of digital filter to yield a filtered FID (P)
	wft1da	Weight and Fourier transform phase-sensitive data (M)
	wft2da	Weight and Fourier transform phase-sensitive data (M)

ft2dac **Combine arrayed 2D FID matrices (M)**

Syntax: **ft2dac**<(<mult1><,mult2>,...<,multn>)>

Description: Allows ready combination of 2D FID matrices within the framework of the 2D FT program. No weighting is performed. Data must be acquired either without f_1 quadrature or with f_1 quadrature using the TPPI method. **ft2dac** is used with TOCSY (with multiple mixing times).

Arguments: **mult1**, **mult2**,...,**multn** are multiplicative coefficients. The **n**th argument is a real number and specifies the coefficient for the **n**th 2D FID matrix.

Related:	ft1dac	Combine arrayed 2D FID matrices (M)
	Tocsy	Set up parameters for a TOCSY pulse sequence (M)
	wft1dac	Combine arrayed 2D FID matrices (M)
	wft2dac	Combine arrayed 2D FID matrices (M)

ft3d **Perform a 3D Fourier transform on a 3D FID data set (M,U)**

Syntax: (From VnmrJ) **ft3d**<(<data_directory><,number_files>
<,'noccoef'><,'t1t2'|'t2t1'><,'fdf'><,'nofdf'>
<,'plane_type'>)>

Description: Transforms 3D FID data into 3D spectral data. **ft3d** can be entered from a macro or directly from UNIX. Each type of entry is described below. A final section explains the **ft3d** coefficient file.

Additional parameter control for the operation of **ft3d** is available. This allows drift corrections and partial Fourier transformation. See the descriptions of **specdc3d**, **fiddc3d**, and **ptspec3d** for information.

The 3D FID data must be loaded into the experiment in which the **ft3d** macro is to be run. **ft3d** is started up in background mode by this macro so that VnmrJ remains free for interactive processing. You can start a 3D transform from within **exp4** and, at the same time, continue with any 1D or 2D processing of the 3D FID data within the same experiment using VnmrJ.

Distributed f_1f_2 processing has the following system and network requirements:

- The system on which the macro **ft3d** is executed from within VnmrJ must define the names of the networked computers that are to participate in the

distributed processing. The file `/etc/hosts.3D` must contain these names in the following format:

```
unity1
unity2
datastation1
datastation2
```

- Each participating computer must recognize the name of the user that started up the master `ft3d` program as a valid user name on its system. For example, if user `steve` issues the `ft3d` command within `VnmrJ` running on computer `unity0`, `steve` must be a valid user on all other computer systems that are to be used in the distributed f_1f_2 processing.
- Each computer system must have NFS access to the 3D data directory.

Arguments: The order of the arguments is not important.

`data_directory` (without the `/data` subdirectory appended) specifies the output directory for the 3D spectral data file(s). The default directory for the 3D spectral data is `curexp/datadir3d`.

`number_files` sets the number of 3D data files (`data1`, `data2`, ..., `data $n$` , where n is `number_files`) used to store the transformed 3D data. `number_files` must be an integer and be 32 or less. When `number_files` is entered, distributed f_1f_2 processing is performed by `ft3d` if possible.

'`nocoeff`' is a keyword for the `set3dproc` command within the `ft3d` macro to not create a 3D coefficient file prior to invoking the `ft3d` program. This option is useful if you have modified an existing 3D coefficient file and do not want it to be overwritten prior to the 3D transform. See below for information on coefficient files. By default, `ft3d` calls the `make3dcoef` macro to create a coefficient file using the `f1coef` and `f2coef` string parameter values.

'`t1t2`' and '`t2t1`' are keywords to explicitly define the order of the `t1` and `t2` arrays (other than `ni` and `ni2`). By default, `ft3d` looks at the `array` parameter and if any parameter other than `phase` and `phase2` are arrayed, the macro aborts.

'`fdf`' indicates that the output of `ft3d` is to be an FDF (Flexible Data Format) file named `data.fdf`. This is the default if the parameter `appmode` is set to '`imaging`'. Distributed processing can still be performed if `number_files` is set appropriately. 3D FDF files can be viewed with the `ImageBrowser`.

'`nofdf`' indicates that the final output is the group of `data1`, `data2`, ... files, and that no FDF format file should be produced. This is the default if the parameter `appmode` is *not* set to '`imaging`'.

`plane_type` sets plane extraction following the complete 3D FT with the following keywords:

- '`xall`' indicates that all three 2D plane types, f_1f_3 , f_2f_3 , and f_1f_2 , are to be automatically extracted at the end of the 3D Fourier transform.
- '`f1f3`', '`f2f3`', and '`f1f2`' can be used to select any combination of plane types to be extracted.

Any of these options can be submitted more than once to the `ft3d` program, but the `getplane` program will display an error and abort if any one plane type is defined for extraction more than once.

Examples: `ft3d`
`ft3d('nocoeff','f1f3','f2f3')`
 ft3d Entered from UNIX
 (From UNIX) `ft3d -e exp_number -f -r <options>`

The `ft3d` program can also be run directly from the UNIX environment on the host computer. An information file must be present before `ft3d` can execute successfully but it need contain only valid processing information for the t_3 dimension and valid Fourier numbers for the t_1 and t_2 transforms. Valid weighting and phasing parameters for the f_1 and f_2 dimension do not need to be set while `wftt3` executes. After several FIDs have been collected, you can determine acceptable f_3 weighting and phasing parameters. After setting `fn1` and `fn2` to the desired values, the 3D processing information file can be created by typing `set3dproc` in the VnmrJ command line. At that point, the next invocation of `ft3d` by the macro `wftt3` causes all (t_1, t_2) increment sets up to and including the current increment in t_3 to be processed.

To start `ft3d` on a remote computer running as a data station for the system, log in as `root` and enter one of the following commands so that the master `ft3d` program can properly communicate with the computer:

- Enter `/vnmr/acqbin/Infoprc &`

With the `Infoprc` or `acqinfo_svc` program running, enter `ft3d` with the `-h` option and the necessary arguments. The `ft3d` program invoked with the `-h` option is considered to be the master program and is responsible for spawning additional remote `ft3d` processes.

Each remote computer must be able to access the 3D data directory as if it were stored on a local disk, must recognize the user name under which the master `ft3d` program is being run, and must also have permission to read from and write to that directory. If the 3D data directory contains four f_3 transformed data files (`data1`–`data4`), the master `ft3d` program uses the first three remote computer systems listed in file `hosts.3D` that respond.

If the multihost processing option is selected, the number of computers involved will be no more than the number of sets the f_3 spectral data is partitioned into. This number is selected with the `-m` option (see below).

If you are unsure of whether to use `Infoprc` or `acqinfo_svc` on the remote computer, change directories to `/vnmr/acqbin`, enter `lf`, and check which program is present.

Note that if the host computer is rebooted, the background command (`Infoprc` or `acqinfo_svc`) has to be entered again.

Arguments: Note that entering `ft3d` with an ampersand (&) after the arguments makes the command execute in the background. As a result, the UNIX prompt reappears after the command is entered and further commands can be entered and executed while the `ft3d` command is processing.

- `-e exp_number` is the experiment number where 3D processing is to occur. This argument is required. It must be written as a minus sign, the letter e, a space, and a valid experiment number from 1 to 9 (e.g., `-e 3` sets experiment 3). The experiment must already exist.

The following two options should always be set for reliable operation:

- `-f` specifies that any existing 3D data sets in the experiment should be deleted. This option requires no additional value.
- `-r` calls for explicit data reduction after the 3D Fourier transform. Data reduction consists of retaining only the “real-real-real” part of the completely transformed 3D data set. The `-r` option is mandatory and is enforced within `ft3d` regardless of the user command line input.

options can be any of the following:

- `-F header_file` indicates that an FDF (Flexible Data Format) output file should be produced, using the FDF header found in `header_file`. The output file will be named `data.fdf`, and the `data1`, `data2`, ... files will not be produced.

- `-h` selects the multihost processing option. The `/etc/hosts.3D` file must exist and contain the names of the remote hosts, one host name per line. Each remote host must also have either the program `Infopr` or the program `acqinfo_svc` running in the background (one of these programs is already running on any computer being used as a spectrometer host).
- `-l` specifies that a log file be generated in the data subdirectory of the `datadir3d` directory.
- `-m` partitions the f_3 transformed spectral data over more than one data file. This partitioning is necessary if the distributed processing capability of `ft3d` is to be used in performing the remaining f_1 and f_2 transforms. The syntax `-mnfiles` is used to specify `nfiles`, the number of data files into which the 3D spectral data is to be divided (e.g., `-m4` specifies 4 data files). Each such data file contains an f_3 subset of the f_1f_2 spectral planes. If `nfiles` is not specified, `ft3d` reports an error and aborts. If `nfiles` is less than an internally calculated value (based on `memsize` and the maximum size for a single 2D transform), the number of data files is set to the internally calculated value; otherwise, `nfiles` determines the number of data files to be used. The maximum number of such files is currently defined to be 32. These 3D data files are labeled `data1, data2, ..., datan`.
- `-o` specifies an alternative output directory for the processed 3D data. The default directory is `datadir3d` within the current experiment. A full UNIX path must follow the `-o` option.
- `-p` specifies the time-domain dimensions to be processed. If `-p` is used, the processed dimensions can be specified as `f3f2f1`, `f3f2`, `f2f3`, `f2f1`, `f1f2`, `f3`, `f2`, and `f1`. The values `f3f1` and `f1f3` are not allowed because processing must be done sequentially in the order f_3 , then f_2 , and then f_1 . If the `-p` option is not invoked, `ft3d` defaults to `f3f2f1`, resulting in a completely transformed 3D data set.
- `-s` specifies processing of the f_3 dimension of the 3D FID data concurrently with data acquisition. In practice, concurrent f_3 processing is realized by setting `wnt = 'wftt3'` in the VnmrJ parameter set and starting the 3D acquisition by entering `au`. The macro `wftt3` handles the call to `ft3d` at the appropriate times during data collection.
- `-x` specifies that plane extractions be performed at the end of 3D processing. The available planes are defined as `f1f2`, `f1f3`, and `f2f3`. If more than one plane extraction is desired, the planes are separated by a colon. For example, `-x f1f2:f1f3:f2f3` would extract all three planes. The planes are placed in the `extr` subdirectory of `datadir3d`.

Examples: (From UNIX) `ft3d -r -f -l -e 2 &`
 (From UNIX) `ft3d -r -f -l -e 2 -x f1f2:f1f3:f2f3 &`

See also: *NMR Spectroscopy User Guide*

Related:	<code>appmode</code>	Application mode (P)
	<code>dconl</code>	Interactive 2D data display (C)
	<code>fiddc3d</code>	3D time-domain dc correction (P)
	<code>f1coef</code>	Coefficient to construct F1 interferogram (P)
	<code>f2coef</code>	Coefficient to construct F2 interferogram (P)
	<code>getplane</code>	Extract planes from a 3D spectral data set (M)
	<code>killft3d</code>	Terminate any <code>ft3d</code> process started in an experiment (M,U)
	<code>make3dcoef</code>	Make 3D coefficients file from 2D coefficients (M)
	<code>ptspec3d</code>	Region-selective 3D processing (P)

F

<code>set3dproc</code>	Set 3D processing (C)
<code>specdc3d</code>	3D spectral drift correction (P)
<code>wftt3</code>	Process f_3 dimension during 3D acquisition (M)

full **Set display limits for a full screen (C)**

Description: Sets the horizontal control parameters (`sc` and `wc`) and the vertical control parameters (`sc2` and `wc2`) to produce a display (and subsequent plot) on the entire screen (and page). For 2D data, space is left for the scales.

Related:	<code>center</code>	Set display limits for center of screen (C)
	<code>fullt</code>	Set display limits for full screen with room for traces (C)
	<code>left</code>	Set display limits for left half of screen (C)
	<code>right</code>	Set display limits for right half of screen (C)
	<code>sc</code>	Start of chart (P)
	<code>sc2</code>	Start of chart in second direction (P)
	<code>wc</code>	Width of chart (P)
	<code>wc2</code>	Width of chart in second direction (P)

fullsq **Display largest square 2D display (M)**

Description: Adjusts `sc`, `sc2`, `wc`, and `wc2` parameters to show the largest possible square 2D display.

Related:	<code>full</code>	Set display limits for a full screen (C)
	<code>fullt</code>	Set display limits for a full screen with room for traces (C)
	<code>sc</code>	Start of chart (P)
	<code>sc2</code>	Start of chart in second direction (P)
	<code>wc</code>	Width of chart (P)
	<code>wc2</code>	Width of chart in second direction (P)

fullt **Set display limits for a full screen with room for traces (C)**

Description: Sets the horizontal control parameters (`sc` and `wc`) and the vertical control parameters (`sc2` and `wc2`) to produce a display (and subsequent plot) in the entire screen (and page) with room for traces (`dconi`). For 2D data, space is left for the scales.

Related:	<code>center</code>	Set display limits for center of screen (C)
	<code>full</code>	Set display limits for a full screen (C)
	<code>left</code>	Set display limits for left half of screen (C)
	<code>right</code>	Set display limits for right half of screen (C)

D

d0	Overhead delay between FIDs (P)
d1	First delay (P)
d2	Incremented delay in 1st indirectly detected dimension (P)
d2pul	Set up parameters for D2PUL pulse sequence (M)
d3	Incremented delay for 2nd indirectly detected dimension (P)
d4	Incremented delay for 3rd indirectly detected dimension (P)
DAC_to_G	Store gradient calibration value in DOSY sequences (P)
da	Display acquisition parameter arrays (C)
daslp	Increment for t1 dependent first-order phase correction (P)
date	Date (P)
daxis	Display horizontal LC axis (M)
Dbppste	Set up parameters for Dbppste pulse sequence (M)
Dbppsteinept	Set up parameters for Dbppsteinept pulse sequence (M)
dbsetup	Set up VnmrJ database (U)
dbupdate	Update the VnmrJ database (U)
dc	Calculate spectral drift correction (C)
dc2d	Apply drift correction to 2D spectra (C)
dcg	Drift correction group (P)
dcon	Display non interactive color intensity map (C)
dconi	Interactive 2D data display (C)
dconi	Control display selection for the dconi program (P)
dconn	Display color intensity map without screen erase (C)
dcrmv	Remove dc offsets from FIDs in special cases (P)
ddf	Display data file in current experiment (C)
ddff	Display FID file in current experiment (C)
ddfp	Display phase file in current experiment (C)
ddif	Synthesize and show DOSY plot (C)
ddrcr	Direct digital receiver coefficient ratio (P)
ddrpm	Set ddr precession mode (P)
ddrtc	Set ddr time constant (P)
dds	Default display (M)
dds_seqfil	Sequence-specific default display (M)
debug	Trace order of macro and command execution (C)
decasynctype	Select the type of decoupler asynchronous mode (P)
deccwarnings	Control reporting of DECC warnings from PSG (P)
decomp	Decompose a VXR-style directory (M)
def_osfilt	Default value of osfilt parameter (P)
defaultdir	Default directory for Files menu system (P)
delcom	Delete a user macro (M)
delete	Delete a file, parameter directory, or FID directory (C)
delexp	Delete an experiment (M)
deletenucleus	Removes nucleus entry to probe file (M)
dels	Delete spectra from T_1 or T_2 analysis (C)

D

<code>delta</code>	Cursor difference in directly detected dimension (P)
<code>delta1</code>	Cursor difference in 1st indirectly detected dimension (P)
<code>delta2</code>	Cursor difference in 2nd indirectly detected dimension (P)
<code>deltaf</code>	Difference of two time-domain cursors (P)
<code>Dept</code>	Set up parameters for DEPT experiment (M)
<code>deptgl</code>	Set up parameters for DEPTGL pulse sequence (M)
<code>deptproc</code>	Process array of DEPT spectra (M)
<code>destroy</code>	Destroy a parameter (C)
<code>destroygroup</code>	Destroy parameters of a group in a tree (C)
<code>df</code>	Display a single FID (C)
<code>df2d</code>	Display FIDs of 2D experiment (C)
<code>dfid</code>	Display a single FID (C)
<code>dfmode</code>	Current state of display of imaginary part of a FID (P)
<code>dfrq</code>	Transmitter frequency of first decoupler (P)
<code>dfrq2</code>	Transmitter frequency of second decoupler (P)
<code>dfrq3</code>	Transmitter frequency of third decoupler (P)
<code>dfrq4</code>	Transmitter frequency of fourth decoupler (P)
<code>dfs</code>	Display stacked FIDs (C)
<code>dfsa</code>	Display stacked FIDs automatically (C)
<code>dfsan</code>	Display stacked FIDs automatically without screen erase (C)
<code>dfsh</code>	Display stacked FIDs horizontally (C)
<code>dfshn</code>	Display stacked FIDs horizontally without screen erase (C)
<code>dfsn</code>	Display stacked FIDs without screen erase (C)
<code>dfww</code>	Display FIDs in whitewash mode (C)
<code>dg</code>	Display group of acquisition/processing parameters (C)
<code>dg</code>	Control dg parameter group display (P)
<code>dg1</code>	Display group of display parameters (M)
<code>dg1</code>	Control dg1 parameter group display (P)
<code>dg2</code>	Display group of 3rd and 4th rf channel/3D parameters (M)
<code>dg2</code>	Control dg2 parameter group display (P)
<code>dga</code>	Display group of spin simulation parameters (M)
<code>DgcsteSL</code>	Set up parameters for DgcsteSL pulse sequence (M)
<code>Dgcstecosy</code>	Set up parameters for Dgcstecosy pulse sequence (M)
<code>Dgcstehmqc</code>	Set up parameters for Dgcstehmqc pulse sequence (M)
<code>dglc</code>	Display group of LC-NMR parameters (M)
<code>dglc</code>	Control dglc parameter group display (P)
<code>dglp</code>	Control dglp parameter group of linear prediction parameters (P)
<code>dgs</code>	Display group of shims and automation parameters (M)
<code>dgs</code>	Control dgs parameter group display (P)
<code>dhp</code>	Decoupler high-power control with class C amplifier (P)
<code>dialog</code>	Display a dialog box from a macro (C)
<code>diffparams</code>	Report differences between two parameter sets (U)
<code>diffshims</code>	Compare two sets of shims (M,U)
<code>digfilt</code>	Write digitally filtered FIDs to another experiment (M)
<code>dir</code>	List files in directory (C)
<code>display</code>	Display parameters and their attributes (C)
<code>dla</code>	Display spin simulation parameter arrays (M)

<code>dlalong</code>	Long display of spin simulation parameter arrays (C)
<code>dli</code>	Display list of integrals (C)
<code>dlivast</code>	Produce text file and process wells (M)
<code>dll</code>	Display listed line frequencies and intensities (C)
<code>dlni</code>	Display list of normalized integrals (M)
<code>dlp</code>	Decoupler low-power control with class C amplifier (P)
<code>dm</code>	Decoupler mode for first decoupler (P)
<code>dm2</code>	Decoupler mode for second decoupler (P)
<code>dm3</code>	Decoupler mode for third decoupler (P)
<code>dm4</code>	Decoupler mode for fourth decoupler (P)
<code>dmf</code>	Decoupler modulation frequency for first decoupler (P)
<code>dmf2</code>	Decoupler modulation frequency for second decoupler (P)
<code>dmf3</code>	Decoupler modulation frequency for third decoupler (P)
<code>dmf4</code>	Decoupler modulation frequency for fourth decoupler (P)
<code>dmfadj</code>	Adjust tip-angle resolution time for first decoupler (M)
<code>dmf2adj</code>	Adjust tip-angle resolution time for second decoupler (M)
<code>dmf3adj</code>	Adjust tip-angle resolution time for third decoupler (M)
<code>dmf4adj</code>	Adjust tip-angle resolution time for fourth decoupler (M)
<code>dmg</code>	Data display mode in directly detected dimension (P)
<code>dmg1</code>	Data display mode in 1st indirectly detected dimension (P)
<code>dmg2</code>	Data display mode in 2nd indirectly detected dimension (P)
<code>dmgf</code>	Absolute-value display of FID data or spectrum in acqi (P)
<code>dmm</code>	Decoupler modulation mode for first decoupler (P)
<code>dmm2</code>	Decoupler modulation mode for second decoupler (P)
<code>dmm3</code>	Decoupler modulation mode for third decoupler (P)
<code>dmm4</code>	Decoupler modulation mode for fourth decoupler (P)
<code>dn</code>	Nucleus for first decoupler (P)
<code>dn2</code>	Nucleus for second decoupler (P)
<code>dn3</code>	Nucleus for third decoupler (P)
<code>dn4</code>	Nucleus for fourth decoupler (P)
<code>dndfid</code>	Retrieve and process fid data from the locator (M)
<code>dndjoin</code>	Join a work space from the locator (M)
<code>dndpar</code>	Retrieve a parameter set from the locator (M)
<code>dndshims</code>	Retrieve a shimset set from the locator (M)
<code>dnode</code>	Display list of valid limNET nodes (M,U)
<code>doautodialog</code>	Start a dialog window using <code>def</code> file (M)
<code>dodialog</code>	Start a dialog window with <code>dialoglib</code> file (M)
<code>dof</code>	Frequency offset for first decoupler (P)
<code>dof2</code>	Frequency offset for second decoupler (P)
<code>dof3</code>	Frequency offset for third decoupler (P)
<code>dof4</code>	Frequency offset for fourth decoupler (P)
<code>Doneshot</code>	Set up parameters for Doneshot pulse sequence (M)
<code>dopardialog</code>	Start a dialog with <code>dialoglib/experiment def</code> file (M)
<code>do_pcsh</code>	Calculate proton chemical shifts spectrum (C)
<code>dosy</code>	Process DOSY experiments (M)
<code>dosy2d</code>	Apptype macro for dosy 2D experiments (M)
<code>dosyfrq</code>	Larmor frequency of phase encoded nucleus in DOSY (P)

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<code>dosygamma</code>	Gyromagnetic constant of phase encoded nucleus in DOSY (P)
<code>dosytimecubed</code>	Gyromagnetic constant of phase encoded nucleus in DOSY (P)
<code>dot1</code>	Set up a T_1 experiment (M)
<code>dotflag</code>	Display FID as connected dots (P)
<code>downsamp</code>	Downsampling factor applied after digital filtering (P)
<code>dp</code>	Double precision (P)
<code>dpcon</code>	Display plotted contours (C)
<code>dpconn</code>	Display plotted contours without screen erase (C)
<code>dpf</code>	Display peak frequencies over spectrum (C)
<code>dpir</code>	Display integral amplitudes below spectrum (C)
<code>dpirn</code>	Display normalized integral amplitudes below spectrum (M)
<code>dpiv</code>	Display integral amplitudes below spectrum (M)
<code>dpirn</code>	Display normalized integral amplitudes below spectrum (C)
<code>dpl</code>	Default plot (M)
<code>dpl_seqfil</code>	Sequence-specific default plot (M)
<code>dplane</code>	Display a 3D plane (M)
<code>dpr</code>	Default process (M)
<code>dpr_seqfil</code>	Sequence-specific default process (M)
<code>dprofile</code>	Display pulse excitation profile (M)
<code>dproj</code>	Display a 3D plane projection (M)
<code>dps</code>	Display pulse sequence (C)
<code>dpwr</code>	Power level for first decoupler with linear amplifier (P)
<code>dpwr2</code>	Power level for second decoupler with linear amplifier (P)
<code>dpwr3</code>	Power level for third decoupler with linear amplifier (P)
<code>dpwr4</code>	Power level for fourth decoupler amplifier (P)
<code>dpwrf</code>	First decoupler fine power (P)
<code>dpwrf2</code>	Second decoupler fine power (P)
<code>dpwrf3</code>	Third decoupler fine power (P)
<code>dpwrm</code>	First decoupler linear modulator power (P)
<code>dpwrm2</code>	Second decoupler linear modulator power (P)
<code>dpwrm3</code>	Third decoupler linear modulator power (P)
<code>Dqcosy</code>	Convert the parameter to a DQCOSY experiment (M)
<code>draw</code>	Draw line from current location to another location (C)
<code>dres</code>	Measure linewidth and digital resolution (C)
<code>dres</code>	Tip-angle resolution for first decoupler (P)
<code>dres2</code>	Tip-angle resolution for second decoupler (P)
<code>dres3</code>	Tip-angle resolution for third decoupler (P)
<code>dres4</code>	Tip-angle resolution for fourth decoupler (P)
<code>ds</code>	Display a spectrum (C)
<code>ds2d</code>	Display 2D spectra in whitewash mode (C)
<code>ds2dn</code>	Display 2D spectra in whitewash mode without screen erase (C)
<code>dsnarray</code>	Report statistical signal-to-noise for Cold Probes (M)
<code>dscale</code>	Display scale below spectrum or FID (C)
<code>dscoef</code>	Digital filter coefficients for downsampling (P)
<code>dseq</code>	Decoupler sequence for first decoupler (P)
<code>dseq2</code>	Decoupler sequence for second decoupler (P)
<code>dseq3</code>	Decoupler sequence for third decoupler (P)

dseq4	Decoupler sequence for fourth decoupler (P)
dsfb	Digital filter bandwidth for downsampling (P)
dshape	Display pulse shape or modulation pattern (M)
dshapef	Display last generated pulse shape (M)
dshapei	Display pulse shape or modulation pattern interactively (M)
dshim	Display a shim “method” string (M)
dsfsfrq	Bandpass filter offset for downsampling (P)
dsn	Measure signal-to-noise (C)
dsnmax	Calculate maximum signal-to-noise (M)
dsp	Display calculated spectrum (C)
dsp	Type of DSP for data acquisition (P)
dsplanes	Display a series of 3D planes (M)
dsptype	Type of DSP (P)
dss	Display stacked spectra (C)
dssa	Display stacked spectra automatically (C)
dssan	Display stacked spectra automatically without erasing (C)
dssh	Display stacked spectra horizontally (C)
dsshn	Display stacked spectra horizontally without erasing (C)
dssl	Label a display of stacked spectra (M)
dssn	Display stacked spectra without screen erase (C)
dsvast	Display VAST data in a stacked 1D-NMR matrix format (M)
dsvast2d	Display VAST data in a pseudo-2D format (M)
dsww	Display spectra in whitewash mode (C)
dtext	Display a text file in graphics window (M)
dtrig	Delay to wait for another trigger or acquire a spectrum (P)
dutyc	Duty cycle for homodecoupling (optional) (P)

d0 Overhead delay between FIDs (P)

Description: Defines the extra overhead delay at the start of each FID or array element. Overhead times between increments and transients are deterministic, i.e., both known and constant. However, the time between increments (typically x) is longer than the time between transients (y , not including times that are actually part of the pulse sequence, such as **d1**). Some experiments may benefit if it is ensured that these two times are not only constant but equal. To ensure that the times are constant and equal, insert the time **d0** at the start of each transient (before the pulse sequence actually starts); the actual delay is then $y+d0$. However, the overhead time may differ with different system configurations. To keep the **d0** delay consistent across systems, set **d0** greater than the overhead delay. The inter-FID delay x is then padded so that $y+d0=x+(d0-(x-y))$. Currently, **d0** only takes into account the extra delay at the start of each array element. It does not take into account the overhead delays at the start and end of each scan. It also does not take into account delays when arraying status statements, shims, or spinner speeds.

The **d0** parameter does not exist in any parameter set and must be created by the user. To create **d0**, enter `create('d0','delay')`. If **d0** is nonexistent, do not insert a delay between transients.

Values: 'n', 'y', or 0 to the maximum delay time (in seconds).

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If `d0= 'n'`, the software calculates the overhead time for an array element and then delays that length of time at the beginning of subsequent transients for every array element. The calculated value of `d0` can be viewed by entering `d0= 'y'` in the input window.

If `d0` is set to a value, that value is the length of delay time at the beginning of subsequent transients for every array element. If the value is greater than the array overhead time, the array overhead time is padded to `d0`.

See also: *User Programming*

Related: [create](#) Create new parameter in parameter tree (C)

d1 First delay (P)

Description: Length of the first delay in the standard two-pulse sequence and most other pulse sequences. This delay is used to allow recovery of magnetization back to equilibrium, if such a delay is desired.

Values: 0.1 μ s to 8190 sec, smallest value possible is 0.1 μ s, finest increment possible is 12.5 ns.

See also: *NMR Spectroscopy User Guide*

Related: [alfa](#) Set `alfa` delay before acquisition (P)
[d2](#) Incremented delay in 1st indirectly detected dimension (P)
[d3](#) Incremented delay in 2nd indirectly detected dimension (P)
[d4](#) Incremented delay in 3rd indirectly detected dimension (P)
[pad](#) Preacquisition delay (P)

d2 Incremented delay in 1st indirectly detected dimension (P)

Description: Length of the second delay in the standard two-pulse sequence. The delay is controlled by the parameters `ni` and `sw1` in a 2D experiment.

Values: 0.1 μ s to 8190 sec, smallest value possible is 0.1 μ s, finest increment possible is 12.5 ns.

See also: *NMR Spectroscopy User Guide*

Related: [d1](#) First delay (P)
[ni](#) Number of increments in 1st indirectly detected dimension (P)
[sw1](#) Spectral width in 1st indirectly detected dimension (P)

d2pul Set up parameters for D2PUL pulse sequence (M)

Description: Sets up a standard two-pulse sequence using the decoupler as transmitter.

See also: *NMR Spectroscopy User Guide*

Related: [dhp](#) Decoupler high power with class C amplifier (P)
[dn](#) Nucleus for the first decoupler (P)
[dof](#) Frequency offset for first decoupler (P)
[dpwr](#) Power level for first decoupler with linear amplifiers (P)
[s2pul](#) Set up parameters for standard two-pulse sequence (M)
[tn](#) Nucleus for the observe transmitter (P)
[tof](#) Frequency offset for observe transmitter (P)
[tpwr](#) Power level of observe transmitter with linear amplifiers (P)

d3 Incremented delay for 2nd indirectly detected dimension (P)

Description: Length of a delay controlled by the parameters `ni2` and `sw2` in a 3D experiment. The `d2` delay, which is controlled by `ni` and `sw1`, is incremented

through its entire implicit array first before d3 is incremented. To create parameters d3, **ni2**, **phase2**, and **sw2** to acquire a 3D data set in the current experiment, enter **addpar** (' 3d ') .

Values: 0.1 μ s to 8190 sec, smallest value possible is 0.1 μ s, finest increment possible is 12.5 ns.

See also: *NMR Spectroscopy User Guide*

Related:	addpar	Add selected parameters to the current experiment (M)
	d1	First delay (P)
	ni2	Number of increments in 2nd indirectly detected dimension (P)
	par3d	Create 3D acquisition, processing, display parameters (C)
	phase2	Phase selection for 3D acquisition (P)
	sw2	Spectral width in 2nd indirectly detected dimension (P)

d4 **Incremented delay for 3rd indirectly detected dimension (P)**

Description: Length of a delay controlled by the parameters **ni3** and **sw3** in a 4D experiment. The **d3** delay, which is controlled by **ni2** and **sw2**, is incremented through its entire implicit array first before d4 is incremented. To create parameters d4, **ni3**, **phase3**, and **sw3** to acquire a 4D data set in the current experiment, enter **addpar** (' 4d ') .

Values: 0.1 μ s to 8190 sec, smallest value possible is 0.1 μ s, finest increment possible is 12.5 ns.

See also: *NMR Spectroscopy User Guide*

Related:	addpar	Add selected parameters to the current experiment (M)
	d1	First delay (P)
	ni3	Number of increments in 3rd indirectly detected dimension (P)
	par4d	Create 4D acquisition parameters (C)
	phase3	Phase selection for 4D acquisition (P)
	sw3	Spectral width in 3rd indirectly detected dimension (P)

DAC_to_G **Store gradient calibration value in DOSY sequences (P)**

Description: **DAG_to_G** is automatically set by the **setup_dosy** macro by retrieving the gradient strength from the probe calibration file if **probe**<>' ' and storing it in **DAC_to_G**. If **probe**= ' ' (i.e., the probe is not defined), then **DAC_to_G** is set to the current value of the global parameter **gcal**

See also: *NMR Spectroscopy User Guide*.

Related:	dosy	Process DOSY experiments (M)
	setup_dosy	Set up gradient levels for DOSY experiments (M)
	setgcal	Set the gradient calibration constant (M)

da **Display acquisition parameter arrays (C)**

Syntax: **da**<(par1<,par2><,par3...>)>

Description: Displays arrayed acquisition parameters.

Arguments: **par1**, **par2**, **par3**, ... are names of parameters to be displayed. The default is to display all such parameters.

Examples: **da**
da (' d2 ')

See also: *NMR Spectroscopy User Guide*

Related:	dg	Display parameters of acquisition/processing group (C)

D

daslp Increment for t1 dependent first-order phase correction (P)

Description: Causes “shearing” of f_1 traces of a 2D dataset and is used to rotate the narrow projection of some solids correlations into the f_1 dimension. Several solids experiments for Dynamic Angle Spinning (DAS) and a triple-quantum filtered 2D MAS experiment require the use of `daslp`. (Note that the command `rotate` shears two traces and is inapplicable for these experiments.)

When created, the value of `lp` for each increment of a 2D experiment is incremented by the value of `daslp` after the first Fourier transformation. The incremented phase correction is applied to the interferogram created from the coefficient table by `ft1d`, `ft2d`, `wft1d` and `wft2d`, when coefficients are present. `daslp` is also used with `ft1da`, `ft2da`, `wft1da` and `wft2da`.

Values: Real values, typically similar in size to the value of parameter `lp`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>ft1da</code>	Fourier transform phase-sensitive data (M)
	<code>ft2d</code>	Fourier transform 2D data (C)
	<code>ft2da</code>	Fourier transform phase-sensitive data (M)
	<code>lp</code>	First-order phase in directly detected dimension (P)
	<code>rotate</code>	Rotate 2D data (C)
	<code>wft1d</code>	Weight and Fourier transform f_2 for 2D data (C)
	<code>wft1da</code>	Weight and Fourier transform phase-sensitive data (M)
	<code>wft2d</code>	Weight and Fourier transform 2D data (C)
	<code>wft2da</code>	Weight and Fourier transform phase-sensitive data (M)

date Date (P)

Description: An informational parameter taken from the UNIX-level calendar (which is set by the UNIX system operator only and cannot be entered by the user). Whenever data are acquired, the date is copied from UNIX and written into the acquisition parameters, thus maintaining a record of the date of acquisition.

See also: *NMR Spectroscopy User Guide*

daxis Display horizontal LC axis (M)

Applicability: Systems with LC-NMR accessory.

Syntax: `daxis (time, major_tic, minor_tic)`

Description: Displays a horizontal LC axis. Horizontal axes are assumed to be used with “LC plots” of an entire LC run and are labeled accordingly.

Arguments: `time` is the time scale, in minutes (decimal values are fine), of the axis.
`major_tic` is spacing, in minutes (decimal values are fine), of major tics.
`minor_tic` is spacing, in minutes (decimal values are fine), of minor tics.

See also: *NMR Spectroscopy User Guide*

Related: `paxis` Display horizontal LC axis (M)

Dbppste Set up parameters for Dbppste pulse sequence (M)

Description: Converts a parameter set to Dbppste experiment; replaces the macro `bppste`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dosy</code>	Process DOSY experiments (M)
	<code>fiddle</code>	Perform reference deconvolution (M)
	<code>setup_dosy</code>	Set up gradient levels for DOSY experiments (M)

Dbppsteinept Set up parameters for Dbppsteinept pulse sequence (M)

Description: Converts a parameter set to Dbppsteinept experiment.

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)
`fiddle` Perform reference deconvolution (M)
`setup_dosy` Set up gradient levels for DOSY experiments (M)

dbsetup Set up VnmrJ database (U)

Syntax: `dbsetup <vnmr_adm|remove|standard|imaging>`
`dbsetup vnmr_adm <remove|standard|imaging>`

As Root:

`dbsetup vnmr_adm VnmrJ_Home_dir <standard|imaging>`

Arguments: `vnmr_adm` is the login ID of the VnmrJ system administrator.
`remove` only removes the data-database; does not recreate a database.
`standard` creates the database for standard use.
`imaging` creates the database for imaging spectroscopy.

Description: The UNIX script `dbsetup` is used during the installation of VnmrJ software and can only be run by the VnmrJ administrator (`vnmr_adm`) or the UNIX administrator (`root`). Normally it is never used again. `dbsetup` creates and deletes the data-database in `/vnmr/pgsql/data` and the user information in `/vnmr/adm/users`.

When run as `root` at least two arguments must be supplied, the login ID of the VnmrJ administrator and the VnmrJ home directory. When run as `root` `dbsetup` will delete and recreate the data-database in `/vnmr/pgsql/data` for all users in `/vnmr/adm/users`. If no user list exists yet, the list is created with the VnmrJ administrator as the only user. The mode can be specified with the third argument as '`standard`' or '`imaging`'; if neither is specified the mode is taken from the `global` file of the VnmrJ administrator. It defaults to `standard`. The VnmrJ administrator does not need to supply any of the arguments.

Note that additional users are created using `vnmrj adm`.

Examples: `dbsetup`
`dbsetup vnmr1`

See also: *NMR Spectroscopy User Guide*
VnmrJ Imaging NMR
VnmrJ Installation and Administration

dbupdate Update the VnmrJ database (U)

Applicability: Systems with the VnmrJ software.

Syntax: `dbupdate stop|once [slow_ms]|forever [slow_ms]`

Arguments: `slow_ms` is an optional argument used to slow down the database update so as not to use all of the available CPU time. `slow_ms=0` is full speed.
`slow_ms=1000` uses about 2-5% of the CPU.
The `dbupdate` command is runs under `nice` so that any other process will be able to take the CPU away from this update anyway. The default `slow_ms` for `forever` is 1000. The default `slow_ms` for `once` is 0.

Description: A UNIX command to start and stop a program to update the VnmrJ database used by the Locator. This command might be needed at a data station to view newly acquired data. The database at the spectrometer will automatically be updated.

D

dc Calculate spectral drift correction (C)

Description: Turns on a linear baseline correction. The beginning and end of the straight line to be used for baseline correction are determined from the display parameters **sp** and **wp**. **dc** applies this correction to the spectrum and stores the definition of the straight line in the parameters **lvl** (level) and **tlt** (tilt). The correction is turned off by the command **cdc**.

Care must be taken to ensure that a resonance does not appear too close to either end of the spectrum, or **dc** can produce the opposite effect from that intended; namely, it induces a sloping baseline where none was present!

See also: *NMR Spectroscopy User Guide*

Related:

bc	1D and 2D baseline correction (C)
cdc	Cancel drift correction (C)
dc	Drift correction group (P)
lvl	Zero-order baseline correction (P)
sp	Start of plot (P)
tlt	First-order baseline correction (P)
wp	Width of plot (P)

dc2d Apply drift correction to 2D spectra (C)

Syntax: `dc2d('f1' | 'f2')`

Description: Computes a drift correction and applies it to each individual trace.

Arguments: 'f1' is a keyword to apply drift correction in the f_1 axis direction.
'f2' is a keyword to apply drift correction in the f_2 axis direction.

Examples: `dc2d('f1')`
`dc2d('f2')`

See also: *NMR Spectroscopy User Guide*

Related:

axis	Axis label for displays and plots (P)
bc	1D and 2D baseline correction (C)

dgc Drift correction group (P)

Description: Contains the results of the **dc** or **cdc** command. This parameter cannot be set in the usual way but it can be queried by entering **dgc?** to determine whether drift correction is active.

Values: 'dc' indicates drift correction is active.
'cdc' indicates drift correction is inactive.

See also: *NMR Spectroscopy User Guide*

Related:

cdc	Cancel drift correction (C)
dc	Calculate spectral drift correction (C)

dcon Display noninteractive color intensity map (C)

Syntax: `dcon<(options)>`

Description: Produces a "contour plot," actually a color intensity map, in the graphics window. The parameters **sp** and **wp**, **sp1** and **wp1**, and **sp2** and **wp2** control which portion of the spectrum is displayed. The parameters **sf** and **wf**, **sf1** and **wf1**, and **sf2** and **wf2** control which portion of time-domain data (FIDs and interferograms) is displayed. The parameter **trace** selects which dimension is displayed along the horizontal axis. The parameters **sc**, **wc**, **sc2**, and **wc2** control where on the screen the display occurs. The parameter **th** is

active as a threshold to black out all contours whose intensity is below **th**. That is, if **th**=7, the colors 1 to 6 are not used for the display. The parameter **vs** controls the vertical scale of the spectrum.

dcon displays either absolute-value mode or phase-sensitive 2D data. In **av** mode, data are shown in 15 different colors (starting with black), with each color representing a factor of two in intensity (a single color is used on monochrome screens). In the **ph** mode, the normal display of colors ranges from -6 to +6, each representing a factor of two in intensity, with the color black representing intensity 0 in the center.

Arguments: options can be any of the following:

- 'linear' is a keyword to use linear instead of logarithmic increments.
- 'phcolor' is a keyword to use a phased color set with positive and negative peaks.
- 'avcolor' is a keyword to use an absolute-value color set with positive peaks. Negative contours only *cannot* be displayed, but if the data can be rephased, 180° added to **rp1**, and **dcon** ('avcolor') entered again, the same thing is accomplished by inverting the phase of all peaks. Alternatively, **dpcon** can display negative peaks only.
- 'gray' is a keyword to use a gray scale color set.
- 'noaxis' is a keyword to omit the display outline and any horizontal or vertical axis.
- 'plot' causes the **dcon** display to be sent to the plotter instead of being drawn on the graphics window.

Examples: **dcon**
dcon ('gray')
dcon ('linear', 'phcolor', 'plot')

See also: *NMR Spectroscopy User Guide*

Related:	dconi	Interactive 2D data display (C)
	dconi	Control display selection for the dconi program (P)
	dconn	Display color intensity map without screen erase (C)
	dpcon	Display plotted contours (C)
	imageprint	Plot noninteractive gray scale image (M)
	sc	Start of chart (P)
	sc2	Start of chart in second direction (P)
	sf	Start of FID (P)
	sp	Start of plot (P)
	sp1	Start of plot in 1st indirectly detected dimension (P)
	sp2	Start of plot in 2nd indirectly detected dimension (P)
	th	Threshold (P)
	trace	Mode for <i>n</i> -dimensional data display (P)
	wc	Width of chart (P)
	wc2	Width of chart in second direction (P)
	wf	Width of FID (P)
	wp	Width of plot (P)
	wp1	Width of plot in 1st indirectly detected dimension (P)
	wp2	Width of plot in 2nd indirectly detected dimension (P)

dconi Interactive 2D data display (C)

Syntax: **dconi**<(options)>

Description: Opens a 2D data display that can be interactively adjusted. The **dconi** program can accommodate any data set that can be displayed by **dcon**, **dpcon**, and

ds2d, including 2D FIDs, interferograms, 2D spectra, planes from 3D data sets, and images. These data sets are generated by the commands **df2d**, **ft1d**, **ft2d**, and **ft3d**.

Arguments: options can be any of the following (note that the **dcon**i parameter is also available to control the **dcon**i program display):

- '**dcon**' is a keyword to display a color intensity map; this is the default mode, but '**dcon**' is provided for compatibility with certain macros. If '**dcon**' is the first argument, it can be followed by any of the keywords '**linear**', '**phcolor**', '**avcolor**', '**gray**', and '**noaxis**'; all of these keywords have the same meaning as when used with **dcon**.
- '**dpcon**' is a keyword to display a true contour plot. If '**dpcon**' is the first argument, it can be followed by any of the keywords '**pos**', '**neg**', and '**noaxis**', and then followed by values for **levels** and **spacing**. All of these options have the same meaning as when used with **dpcon**.
- '**ds2d**' is a keyword to display a stacked plot in whitewash mode (after the first spectra, each spectra is blanked out in regions in which it is behind an earlier spectra). If '**ds2d**' is the first argument, it can be followed by any of the keywords '**nobase**', '**fill**', '**fillnb**', and '**noaxis**'. All of these keywords have the same meaning as used with **ds2d**.
- '**again**' is a keyword to make **dcon**i identify which display mode is currently being used and redraw the screen in that mode.
- '**restart**' is a keyword to activate **dcon**i without redrawing the 2D data set. This action causes **dcon**i to make sure that 2D data is already displayed.
- '**toggle**' is a keyword to toggle between the cursor and box modes.
- '**trace**' is a keyword to draw a trace above the spectrum.
- '**expand**' is a keyword to toggle between the expand and full views of the spectrum.
- '**plot**' is a keyword to plot a projection or a trace.
- '**hproj_max**' is a keyword to do a horizontal projection of the maximum trace.
- '**hproj_sum**' is a keyword to do a horizontal projection of the sum of all traces.
- '**vproj_max**' is a keyword to do a vertical projection of the maximum trace.
- '**vproj_sum**' is a keyword to do a vertical projection of the sum of all traces.

Examples: **dcon**i
dconi('dcon','gray','linear')
dconi('dpcon')

See also: *NMR Spectroscopy User Guide*

Related:	boxes	Draw boxes selected by the mark command (C)
	crmode	Current state of cursors in dfid , ds , or dcon i (P)
	dcon	Display noninteractive color intensity map (C)
	dcon i	Control display selection for the dcon i program (P)
	dconn	Display color intensity map without screen erase (C)
	delta1	Cursor difference in 1st indirectly detected dimension (P)
	df2d	Display FIDs of 2D experiment (C)
	dpcon	Display plotted contours (C)
	ds2d	Display 2D spectra in whitewash mode (C)

<code>ft1d</code>	Fourier transform along f_2 dimension (C)
<code>ft2d</code>	Fourier transform 2D data (C)
<code>ft3d</code>	Perform a 3D Fourier transform on a 3D FID data set (M,U)
<code>imconi</code>	Display 2D data in interactive gray-scale mode (M)
<code>is</code>	Integral scale (P)
<code>ll2d</code>	Automatic and interactive 2D peak picking (C)
<code>proj</code>	Project 2D data (C)
<code>sf</code>	Start of FID (P)
<code>sp</code>	Start of plot (P)
<code>sp1</code>	Start of plot in 1st indirectly detected dimension (P)
<code>th</code>	Threshold (P)
<code>vs2d</code>	Vertical scale for 2D displays (P)
<code>vsadj</code>	Automatic vertical scale adjustment (M)
<code>wf</code>	Width of FID (P)
<code>wp</code>	Width of plot (P)
<code>wp1</code>	Width of plot in 1st indirectly detected dimension (P)

dconi **Control display selection for the dconi program (P)**

Description: Controls the selection of the 2D display that follows entering the `dconi` command. Because `dconi` is implicitly executed by `ft2d`, the `dconi` parameter also controls the display that follows the `ft2d` or `wft2d` command.

`dconi` can be a string parameter in the “current” parameter set. Its syntax is similar to an argument string passed to the `dconi` program. For example, if `dconi = 'dpcon, pos, 12, 1.2 '`, the `dconi` command displays twelve positive contours with `dpcon`, using a spacing of 1.2. The first component of the `dconi` string must be the name of the display program, such as `dcon`, `dconn`, `dpcon`, `dpconn`, `ds2d`, or `ds2dn`. Subsequent components of the string are arguments appropriate for that display program. Because the entire `dconi` parameter is a string, single quotes around words are not necessary and mixing words and numbers is not a problem, as the example above shows.

If the `dconi` parameter does not exist or is set to the null string (' '), the `dconi` program uses its normal default. If the `dconi` parameter is set to a string (e.g., `dconi = 'dcon, gray, linear'` for image display), and arguments are supplied to the `dconi` program, (e.g., `dconi ( 'dpcon' )`), the supplied arguments to the command take precedence. In the case of the examples above, a contour map, not an image, is displayed.

If the `dconi` parameter does not exist in the current experiment, it can be created by the commands `create ( 'dconi', 'string' )` and `setgroup ( 'dconi', 'display' )`.

Values: ' ' (two single quotes) indicates that this parameter is ignored.

String `'display_program'` selects the named program for 2D displays.

String `'display_program, option1, option2'` selects the named program for 2D displays with options appropriate to the program.

Examples: `dconi = 'dpcon'` selects contour drawing rather than default color map
`dconi = 'dcon, gray, linear'` selects image display mode.

See also: *NMR Spectroscopy User Guide; VnmrJ Imaging NMR*

Related:	<code>dcon</code>	Display noninteractive color intensity map (C)
	<code>dconi</code>	Interactive 2D data display (C)
	<code>dconn</code>	Display color intensity map without screen erase (C)
	<code>dpcon</code>	Display plotted contours (C)
	<code>dpconn</code>	Display plotted contours without screen erase (C)
	<code>ds2d</code>	Display 2D spectra in whitewash mode (C)
	<code>ds2dn</code>	Display 2D spectra in whitewash mode without screen erase (C)

D

<code>ft2d</code>	Fourier transform 2D data (C)
<code>imconi</code>	Display 2D data in interactive gray-scale mode (M)
<code>wft2d</code>	Weight and Fourier transform 2D data (C)

dconn Display color intensity map without screen erase (C)

Syntax: `dconn<(options)>`

Description: Produces a “contour plot,” actually a color intensity map, on the screen the same as the `dcon` command, but without erasing the screen before starting the plot. The options available are the same as the `dcon` command.

See also: *NMR Spectroscopy User Guide*

Related: `dcon` Display noninteractive color intensity map (C)
`dconi` Control display selection for the dcon program (P)

dcrmv Remove dc offsets from FIDs in special cases (P)

Description: If `dcrmv` exists and is set to 'y', hardware information is used to remove the dc offset from the FID providing `ct=1`. This only works on systems with `sw` less than 100 kHz. If this feature is desired for a particular experiment, create `dcrmv` in that experiment by entering `create('dcrmv','string')` `setgroup('dcrmv','processing')` `dcrmv='y'`
 To create image parameters `dcrmv`, `grayctr` and `graysl` in the current experiment, enter `addpar('image')`.

See also: *NMR Spectroscopy User Guide; VnmrJ Imaging NMR*

Related: `addpar` Add selected parameters to the current experiment (M)
`create` Create new parameter in a parameter tree (C)
`ct` Completed transients (P)
`dc` Calculate spectral drift correction (C)
`setgroup` Set group of a variable in a tree (C)

ddf Display data file in current experiment (C)

Syntax: `ddf<(block_number,trace_number,first_number)>`

Description: Displays the file header of the data file in the current experiment. If entered with arguments, it also displays a block header and part of the data file of that block.

Arguments: `block_number` is the block number. Default is 1.
`trace_number` is the trace number within the block. Default is 1.
`first_number` is the first data element number within the trace. Default is 1.

See also: *User Programming*

Related: `ddff` Display FID file in current experiment (C)
`ddfp` Display phase file in current experiment (C)

ddff Display FID file in current experiment (C)

Syntax: `ddff<(block_number,trace_number,first_number)>`

Description: Displays the file header of the FID file in the current experiment. If entered with arguments, it also displays a block header and part of the FID data of the block.

Arguments: `block_number` is the block number. Default is 1.
`trace_number` is the trace number within the block. Default is 1.
`first_number` is the first data element number within the trace. Default is 1.

See also: *User Programming*

Related: **ddf** Display data file in current experiment (C)
ddfp Display phase file in current experiment (C)

ddfp Display phase file in current experiment (C)

Syntax: `ddfp<(block_number,trace_number,first_number)>`

Description: Displays the file header of the phase file in the current experiment. With arguments, it also display a block header and part of the phase file data of that block.

Arguments: `block_number` is the block number. Default is 1.
`trace_number` is the trace number within the block. Default is 1.
`first_number` is the first data element number within the trace. Default is 1.

See also: *User Programming*

Related: **ddf** Display data file in current experiment (C)
ddff Display FID file in current experiment (C)

ddif Synthesize and show DOSY plot (C)

Syntax: `ddif(<option>,lowerlimit,upperlimit)`

Description: Synthesizes a 2D spectrum from 1D spectra using the information produced by the **dosy** macro. **ddif** takes the 1D spectrum and a table of diffusion data stored in the file `diffusion_display.inp` in the current experiment and synthesizes a 2D DOSY spectrum. It is normally run by **dosy**, but can be directly run, for example, to recalculate a 2D DOSY spectrum with different digitization.

Arguments: `option` is either 'i' or 'c'.
 'i' is for a display in which the 2D peak volume is proportional to 1D peak height.
 'c' is for a display in which the 2D peak height equals the 1D.
`lowerlimit` is the lower diffusion limit (in units of $10^{-10} \text{ m}^2/\text{s}$).
`upperlimit` is the upper diffusion limit (in units of $10^{-10} \text{ m}^2/\text{s}$).
 If arguments are not supplied, **ddif** defaults to showing the full range of diffusion coefficients in the file `diffusion_display.inp` in the current experiment. Make sure that the first increment of the DOSY data set has been transformed with the desired `fn2D` before using **ddif**. Digitization of the resultant spectrum is determined by `fn2D` in the spectral (F2) domain and `fn1` in the diffusion (F1) domain. Make sure that the product `fn2D*fn1` is not too large, or memory and processing time problems might result. Typical values are `fn2D=16384` (max: 64k) and `fn1=512`. After **dosy** or **ddif**, 1D data is overwritten by the 2D (the **dosy** macro keeps a copy of the 1D data, which can be retrieved with the command **undosy**). Similarly, after a DOSY spectrum has been calculated, it can be retrieved with the command **redosy**.

See also: *NMR Spectroscopy User Guide*

Related: **dosy** Process DOSY experiments (M)
fn2D Fourier number to build up 2D DOSY display in frequency domain (P)
redosy Restore the previous 2D DOSY display from the subexperiment (M)
undosy Restore original 1D NMR data from the subexperiment (M)

ddrcr Direct digital receiver coefficient ratio (P)

Applicability: VNMRs systems and 400 - MR systems

D

Syntax: `ddrcr=<value>`

Description: Sets the filter sharpness or filter coefficient ratio. The default value of 75 is used if the parameter does not exist.

Examples:

```
create('ddrce','integer')
setlimit('ddrcr',1000,2,1)
ddrcr=300
```

Values: Integer values between 2 and 1000

See also: *NMR Spectroscopy User Guide* and *VnmrJ User Programming*.

Related: `sw` Spectral width in directly detected dimension (P)

ddrpm Set ddr precession mode (P)

Applicability: VNMRS systems

Syntax: `ddrpm=<'mode'>`

Values: mode can be either of following:

Mode	Description

p	Pulse — default if no argument is supplied. The value is calculated as follows if <code>ddrpm</code> does not exist or <code>ddrpm='p'</code> : $\text{ddrtc} = \text{alfa} + \text{rof2} + 2 * \text{pw}[1] / \pi$
e	Echo — The value is calculated as follows: $\text{ddrtc} = \text{alfa}$.

See also: *VnmrJ User Programming*

Related: `setrc` Set frequency referencing based upon lock signal shift (M)
`ddrtc` Set ddr precession mode (P)

ddrtc Set ddr time constant (P)

Applicability: VNMRS systems

Syntax: `ddrtc=<'value'>`

Description: The value of `ddrtc` is set in the `setrc` macro and is determined by the `ddrpm` parameter.

A value of `ddrtc = alfa` is used by `psg` if the `ddrtc` parameter does not exist.

Values: value 0 to 1000 μsec .

See also: *VnmrJ User Programming*

Related: `setrc` Set frequency referencing based upon lock signal shift (M)
`setlp0` Set parameters for zero linear phase (M)
`ddrpm` Set ddr precession mode (P)

dds Default display (M)

Description: Looks for sequence-specific default display macro (`dds_seqfil`) and executes if one is found. If not, the `dds` macro displays 1D, 2D, or array spectrum as the case may be.

Related: `dds_seqfil` Sequence-specific default display (M)
`dpl` Default plot (M)
`dpr` Default process (M)

dds_seqfil Sequence-specific default display (M)

Description: Sequence-specific default display. These macros are called by the dds macro.

Examples: dds_NOESY1D
dds_TOCSY1D

Related: dds Default display (M)
dpl Default plot (M)
dpr Default process (M)

debug Trace order of macro and command execution (C)

Syntax: debug ('c' | 'C')

Description: Controls VnmrJ command and macro tracing. When turned on, debug displays a list of each command and macro in the shell tool from which VnmrJ was started. If VnmrJ is started when the user logs in, or if it was started from a drop-down menu or the CDE tool, the output goes to a Console window. If no Console window is present, the output goes into a file in the /var/tmp directory. This last option is not recommended. Nesting of the calls is indicated by indentation of the output. This feature is primarily a debugging tool for MAGICAL programming.

To associate the debug('c') output with a particular terminal, enter tty. The system responds with /dev/pts/yyy, where yyy is a numerical value. On the VnmrJ command line, enter jFunc (55, ' /dev/pts/yyy'), substituting the numerical value for the yyy.

Arguments: 'c' is a keyword to turn on command and macro tracing.
'C' is a keyword to turn off command and macro tracing.

Examples: debug ('c')
debug ('C')

See also: *User Programming*

decasynctype Select the type of decoupler asynchronous mode (P)

Applicability: VNMR systems, 400 MR

Syntax: decasynctype=<value>

Description: Optional parameter to select the type of decoupler asynchronous mode. The default type is p (progressive mode), which simulates a free running decoupler with respect to the pulse sequence timing. The other available options are b (bit reversed mode) and r (random mode). The b mode (bit-reversed mode) may be especially appropriate for reducing unwanted decoupling side-band intensity, when the number of transients is small. In the r mode (random mode) the starting decoupling stage is randomized. The decasynctype setting affects the decoupling on all the rf channels (dm, dm2, dm3 etc.). This parameter is optional and if it does not exist the decoupler asynchronous mode is set to p (progressive mode).

Values: 'p' — progressive mode, mode used by Inova systems
'b' — bit-reversed mode
'r' — random mode

Examples: decasynctype='p' for progressive mode.

Related: dm Decoupler mode for first decoupler (P)

`dm2` Decoupler mode for second decoupler (P)
`dm3` Decoupler mode for third decoupler (P)

deccwarnings Control reporting of DECC warnings from PSG (P)

Applicability: Systems with DECC (Digital Eddy Current Compensation) boards for gradient compensation.

Description: A global parameter that controls whether PSG will warn the user when the ECC corrections are large enough that they could exceed the capabilities of the DECC board. By default, this parameter does not exist, and a warning is printed whenever an experiment is started if the ECC amplitudes are possibly too large. The warning does indicate a definite be a problem, only that not enough ECC drive capability is available to compensate for an instantaneous gradient swing from minus the maximum gradient strength to the maximum positive gradient. To disable the warnings, create this global string parameter and set it to 'n'.

Values: 'n' or 'N' to suppress warnings. If the value starts with any other character, the normal warnings are printed.

decomp Decompose a VXR-style directory (M)

Syntax: `decomp< (VXR_file) >`

Description: Takes a library, as loaded from a VXR-style system (VXR, XL, or Gemini), and extracts each entry into a separate UNIX file. The file can be obtained from a magnetic tape or over limNET. `decomp` creates a UNIX subdirectory in the current working directory and uses that to write each entry as a UNIX file. The name of the UNIX subdirectory is derived from the library name.

Arguments: `VXR_file` is the name of the original file. It must have an extension in the form .NNN, where NNN is the number of entries in the original library. A limit of 432 entries is imposed.

See also: *NMR Spectroscopy User Guide*

Related: `convert` Convert data set from a VXR-style system (C,U)

def_osfilt Default value of osfilt parameter (P)

Description: A global parameter that establishes the default type of digital filter, AnalogPlus™ or brickwall, when DSP is configured. The *actual* filter used in any experiment is set by the local parameter `osfilt`. Usually, `def_osfilt` is set to the value for normal use, and then `osfilt` is changed within a given experiment if different filter characteristics are desired.

Values: 'a' or 'A' for the AnalogPlus digital filter. This filter is flatter in the passband and drops off somewhat more sharply than analog filters.

'b' or 'B' for the brickwall digital filter. This filter is extremely flat across the passband and drops off sharply on the edge; however, the enhanced filtering comes at the expense of somewhat reduced baseline performance.

See also: *NMR Spectroscopy User Guide*

Related: `dsp` Type of DSP for data acquisition (P)
`osfilt` Oversampling filter for real-time DSP (P)

defaultdir Default directory for Files menu system (P)

Description: Stores the name to the default directory for use with the Directory Menu in the Files menu system. Initial value for `defaultdir` is the home or login

directory of the user. Selecting the Default button in the Directory Menu sets the current directory to the value of `defaultdir`. The opposite action, setting the value of `defaultdir` to the current directory, occurs when the Set Default button in the Directory Menu is selected. If the entry for a directory is marked and the Set Default button is selected, the directory marked becomes the new value of `defaultdir`.

See also: *NMR Spectroscopy User Guide*

delcom Delete a user macro (M)

Syntax: `delcom (file)`

Description: Deletes a macro file in a user's macro library (`maclib`). Note that `delcom` will not delete a macro in the VnmrJ system macro library.

Arguments: `file` is the file name of the user's macro to be deleted.

Examples: `delcom ('lds')`

See also: *User Programming*

Related: `crcom` Create user macro without using a text editor (C)
`macrorm` Remove a user macro (C)

delete Delete a file, parameter directory, or FID directory (C)

Syntax: `delete (file1<, file2, ...>)`

Description: Delete files and directories in a somewhat safer manner than the `rm` command. Using `rm` is not recommended in VnmrJ because `rm` allows wildcard characters (`*` and `?`) in the file description and recursive file deletion with the `-r` option. The `delete` command does not allow wildcard characters or the `-r` option, but you can still use the `delete` command to delete a file as well as remove `.fid` and `.par` directories, normally the only directories that need to be removed (experiment directories are deleted with the `delexp` macro).

Arguments: `file1`, `file2`, ... are the names of one or more files or directories to be deleted. When the `delete` command is entered, it first searches for `file1`. If it finds that file and it is not a directory, `file1` is deleted. If `file1` is not found, `.fid` is appended to the file name and `delete` searches for the file in that `.fid` directory. If the file is found, it is removed; otherwise, `.par` is appended to the file name and `delete` searches for the file in that `.par` directory. If the file is found, it is removed; otherwise, the command takes no action and continues to the next file name. The process is repeated for each file name given as an argument.

Examples: `delete ('/home/vnmr1/memo')`
`delete ('/vnmr/fidlib/fid1d')`

See also: *NMR Spectroscopy User Guide*

Related: `delexp` Delete an experiment (M)
`rm` Delete file (C)
`rmdir` Remove directory (C)

delexp Delete an experiment (M)

Syntax: `delexp (experiment_number)`

Description: Deletes an experiment.

D

Arguments: `experiment_number` is the number (from 2 through 9999) of the experiment to be deleted (experiment 1 cannot be deleted). `delexp` also deletes the corresponding `jexpXXX` macro if necessary.

Examples: `delexp(321)`

See also: *NMR Spectroscopy User Guide*

Related: `cexp` Create an experiment (M)
`jexp` Join existing experiment (C)

deletenucleus Removes nucleus entry from current probe file (M)

Applicability: ALL

Description: All lines for the specified nucleus are removed from the current probe file. The argument should correspond to an entry in the probe file.

Syntax: `deletenucleus('nucleus')`

Arguments: `nucleus` — name followed by atomic number, e.g. C13 not 13C.

Examples: `deletenucleus('Si29')`

Related: `addnucleus` Adds nucleus entry to probe file (M)
`addprobe` Create new probe directory and probe file (M)

dels Delete spectra from T_1 or T_2 analysis (C)

Syntax: `dels(index1<,index2,...>)`

Description: Deletes the spectra selected from the file `fp.out` (the output file of `fp`) used by the `t1` or `t2` analysis. Spectra may be restored by rerunning `fp`.

Arguments: `index1, index2, ...` are the indexes of the spectra to be deleted.

Examples: `dels(7)`
`dels(2,5)`

See also: *NMR Spectroscopy User Guide*

Related: `dll` Display listed line frequencies and intensities (C)
`fp` Find peak heights or phases (C)
`getll` Get frequency and intensity of a line (C)
`t1` T_1 exponential analysis (M)
`t2` T_2 exponential analysis (M)

delta Cursor difference in directly detected dimension (P)

Description: Difference between two frequency cursors along the directly detected dimension. The value is changed by moving the right cursor, relative to the left, in the `ds` or `dconi` display.

Values: Positive number, in Hz.

See also: *NMR Spectroscopy User Guide*

Related: `dconi` Interactive 2D data display (C)
`delta1` Cursor difference in 1st indirectly detected dimension (P)
`delta2` Cursor difference in 2nd indirectly detected dimension (P)
`ds` Display a spectrum (C)
`split` Split difference between two cursors (M)

- delta1** **Cursor difference in 1st indirectly detected dimension (P)**
- Description: Difference of two frequency cursors along the first indirectly detected dimension. Analogous to the [delta](#) parameter except that `delta1` applies to the first indirectly detected dimension of a multidimensional data set.
- Values: Positive number, in Hz.
- See also: *NMR Spectroscopy User Guide*
- Related: [delta](#) Cursor difference in directly detected dimension (P)
-
- delta2** **Cursor difference in 2nd indirectly detected dimension (P)**
- Description: Difference of two frequency cursors along the second indirectly detected dimension. Analogous to the [delta](#) parameter except that `delta2` applies to the second indirectly detected dimension of a multidimensional data set.
- Values: Positive number, in Hz.
- See also: *NMR Spectroscopy User Guide*
- Related: [delta](#) Cursor difference in directly detected dimension (P)
-
- deltaf** **Difference of two time-domain cursors (P)**
- Description: Difference between the two time-domain cursors of the [df](#) (or [dfid](#)) display. To create this parameter and the other FID display parameters [axisf](#), [dotflag](#), [vpf](#), [vpfi](#), and [crf](#) (if the parameter set is older and lacks these parameters), enter `addpar('fid')`.
- Values: Number, in seconds.
- See also: *NMR Spectroscopy User Guide*
- Related: [addpar](#) Add selected parameters to the current experiment (M)
[crf](#) Current time-domain cursor position (P)
[df](#) Display a single FID (C)
[dfid](#) Display a single FID (C)
-
- Dept** **Set up parameters for DEPT experiment (M)**
- Description: Set up parameters for DEPT experiment
- See also: *NMR Spectroscopy User Guide*
- Related: [adept](#) Automatic DEPT analysis and spectrum editing (C)
[autodept](#) Automated complete analysis of DEPT data (M)
[deptgl](#) Set up parameters for DEPTGL pulse sequence (M)
[deptproc](#) Process array of DEPT spectra (M)
[padept](#) Plot automatic DEPT analysis (C)
[ppcal](#) Proton decoupler pulse calibration (M)
-
- deptgl** **Set up parameters for DEPTGL pulse sequence (M)**
- Description: Macro for the DEPTGL pulse sequence for spectral editing and polarization transfer experiments.
- See also: *NMR Spectroscopy User Guide*
- Related: [Dept](#) Set up parameters for DEPT pulse sequence (M)

D

deptproc **Process array of DEPT spectra (M)**

Description: Automatically processes arrays of DEPT-type spectra. The FIDs are transformed (using `lb=2.5`), phased, and scaled. In foreground operation, a stacked display is produced. By default, an automatic DEPT analysis (`adept`) is performed.

See also: *NMR Spectroscopy User Guide*

Related: `adept` Automatically edit DEPT spectra (C)
 `Dept` Set up parameters for DEPT experiment
 `lb` Line broadening along the directly detected dimension (P)
 `pldept` Plot DEPT type spectra (M)
 `procplot` Automatically process FIDs (M)

destroy **Destroy a parameter (C)**

Syntax: `destroy(parameter<, tree>)`

Description: Removes a parameter from one of the parameter trees. If the destroyed parameter was an array, the `array` parameter is automatically updated.

If `destroy` is called for a non-existent parameter, the command will abort with a message. If an optional return value is given, it will indicate success (1) or failure (0) and the command will not abort.

Arguments: `parameter` is the name of the parameter to be destroyed.

`tree` is a keyword for the type of parameter tree: 'global', 'current', 'processed', or 'systemglobal'. The default is 'current'. Refer to the `create` command for more information on types of trees.

Examples: `destroy('a')`
`destroy('c', 'global')`

See also: *User Programming*

Related: `array` Parameter order and precedence (P)
 `create` Create new parameter in a parameter tree (C)
 `display` Display parameters and their attributes (C)
 `paramvi` Edit a variable and its attributes using `vi` text editor (C)
 `prune` Prune extra parameters from current tree (C)

destroygroup **Destroy parameters of a group in a tree (C)**

Syntax: `destroygroup(group<, tree>)`

Description: Removes parameters of a group from one of the parameters trees.

Arguments: `group` is a keyword for the type of parameter group: 'all', 'sample', 'acquisition', 'processing', 'display', or 'spin'.

`tree` is a keyword for the type of parameter tree: 'global', 'current', or 'processed'. The default is 'current'. Refer to the `create` command for more information on trees.

Examples: `destroygroup('sample')`
`destroygroup('all', 'global')`

See also: *User Programming*

Related: `create` Create new parameter in a parameter tree (C)
 `destroy` Destroy a parameter (C)
 `display` Display parameters and their attributes (C)
 `groupcopy` Copy parameters of group from one tree to another (C)
 `setgroup` Set group of a variable in a tree (C)

df Display a single FID (C)

Syntax: (1) `df<(index)>`
 (2) `df(options)`

Description: Displays a single FID. Parameter entry after an FID has been displayed causes the display to be updated. The FID is left-shifted by the number of complex data points specified by the parameter `lsfid`. The FID is also phase-rotated (zero-order only) by the number of degrees specified by the parameter `phfid`. Left shifting and phasing can be avoided by setting `lsfid` and `phfid` to 'n'. `df` is identical in function to the `dfid` command.

Arguments: `index` (used with syntax 1) is the number of a particular FID for arrayed 1D experiments or for 2D experiments. Default is 1.

`options` (used with syntax 2) is any of the following:

- 'toggle' is a keyword to switch between box and cursor modes.
- 'restart' is a keyword to redraw the cursor if it has been turned off.
- 'expand' is a keyword to switch between expanded and full views of the FID.
- 'imaginary' is a keyword to switch on and off the display of the imaginary FID.
- 'sfwf' is a keyword to interactively adjust the start and width of the FID display.
- 'phase' is a keyword to enter an interactive phasing mode.
- 'dscale' is a keyword to toggle the scale below the FID on and off.

Examples: `df`
`df(4)`
`df('restart')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>crmode</code>	Current state of cursors in <code>dfid</code> , <code>ds</code> , or <code>dconi</code> (P)
	<code>dfid</code>	Display a single FID (C)
	<code>df2d</code>	Display FIDs of 2D experiment (C)
	<code>dfmode</code>	Current state of display of imaginary part of a FID (P)
	<code>lsfid</code>	Number of complex points to left-shift the <code>np</code> FID (P)
	<code>phfid</code>	Zero-order phasing constant for the <code>np</code> FID (P)

df2d Display FIDs of 2D experiment (C)

Syntax: `df2d(<'nf',><array_index>)>`

Description: Produces a color intensity map of the raw 2D FIDs as a function of t_1 and t_2 . The display can be modified by subsequent display commands, for example, `df2d dconn` will display the 2D FIDs without clearing the graphics screen.

Arguments: 'nf' is a keyword specifying that the data has been collected in the compressed form using `nf`. In other words, each array element is collected as one 2D FID or image comprised of `nf` FIDs or traces.

`array_index` is the index of the array to be displayed.

Examples: `df2d`
`df2d(1)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dconi</code>	Interactive 2D data display (C)
	<code>df</code>	Display a single FID (C)

D

dfid **Display a single FID (C)**

Syntax: (1) `dfid<(index)>`
(2) `dfid<(options)>`

Description: Functions the same as the `df` command. See `df` for information.

See also: *NMR Spectroscopy User Guide*

Related: `df` Display a single FID (C)

dfmode **Current state of display of imaginary part of a FID (P)**

Description: Holds a string variable that reflects the state of display of the imaginary part of a FID. `dfmode` is primarily used by the programmable menu `dfid` to determine the status of the display of the imaginary part of a FID.

Values: 'r' indicates the current display is real only.
'i' indicates the current display is imaginary.
'z' indicates the display is zero imaginary.

See also: *User Programming*

dfreq **Transmitter frequency of first decoupler (P)**

Description: Contains the transmitter frequency for the first decoupler. `dfreq` is automatically set when the parameter `dn` is changed and should not be necessary for the user to manually set.

Values: Frequency, in MHz. The value is limited by synthesizer used with the channel.

See also: *NMR Spectroscopy User Guide*

Related: `dfreq2` Transmitter frequency of second decoupler (P)
`dfreq3` Transmitter frequency of third decoupler (P)
`dfreq4` Transmitter frequency of fourth decoupler (P)
`dn` Nucleus for first decoupler (P)
`dof` Frequency offset for first decoupler (P)
`sfrq` Transmitter frequency of observe nucleus (P)
`spcfrq` Display frequencies of rf channels (M)

dfreq2 **Transmitter frequency of second decoupler (P)**

Applicability: Systems with a second decoupler.

Description: Contains the transmitter frequency for the second decoupler. `dfreq2` is automatically set when parameter `dn2` is changed and should not be necessary for the user to manually set.

Values: Frequency, in MHz. Value is limited by synthesizer used with the channel. If `dn2=' '` (two single quotes with no space in between) and a second decoupler is present in the console, `dfreq2` is internally set to 1 MHz.

See also: *NMR Spectroscopy User Guide*

Related: `dn2` Nucleus for second decoupler (P)
`dof2` Frequency offset for second decoupler (P)

dfreq3 **Transmitter frequency of third decoupler (P)**

Applicability: Systems with a third decoupler.

Description: Contains the transmitter frequency for the third decoupler. `dfreq3` is automatically set when the parameter `dn3` is changed and should not be necessary for the user to manually set.

Values: Frequency, in MHz. Value is limited by synthesizer used with the channel. If `dn3=' '` (two single quotes with no space in between) and a third decoupler is present in the console, `dfreq3` is internally set to 1 MHz.

See also: *NMR Spectroscopy User Guide*

Related: `dn3` Nucleus for third decoupler (P)
`dof3` Frequency offset for third decoupler (P)

dfreq4 Transmitter frequency of fourth decoupler (P)

Applicability: Systems with a deuterium decoupler channel as the fourth decoupler.

Description: Contains the transmitter frequency for the fourth decoupler. `dfreq4` is automatically set when the parameter `dn4` is changed and should not be necessary for the user to manually set.

Values: Frequency, in MHz. Value is limited by a synthesizer used with the channel. If `dn4=' '` (two single quotes with no space in between) and a fourth decoupler is present in the console, `dfreq4` is internally set to 1 MHz.

See also: *NMR Spectroscopy User Guide*

Related: `dn4` Nucleus for fourth decoupler (P)
`dof4` Frequency offset for fourth decoupler (P)
`spcfrq` Display frequencies of rf channels (M)
`rftype` type of rf generation

dfs Display stacked FIDs (C)

Syntax: `dfs(<start><, finish><, step><, 'all' | 'imag'><, color>)>`

Description: Displays one or more FIDs. The position of the first FIDs is governed by the parameters `wc`, `sc`, and `vpf`. A subsequent FID is positioned relative to the preceding FID by the parameters `vo` and `ho`.

Arguments: `start` is the index number of the first FID for multiple FIDs. It can also be the index number of a particular FID for arrayed 1D or 2D data sets.

`finish` is the index number of the last FID for multiple FIDs. To include all FIDs, set `start` to 1 and `finish` to `arraydim` (see example below).

`step` is the increment for the FID index. The default is 1.

`'all'` is a keyword to display all of the FIDs. This is the default.

`'imag'` is a keyword to display only the imaginary FID channel.

`color` is the color of the display: `'red'`, `'green'`, `'blue'`, `'cyan'`, `'magenta'`, `'yellow'`, `'black'`, or `'white'`.

Examples: `dfs(1,arraydim,3)`
`dfs('imag')`

See also: *NMR Spectroscopy User Guide*

Related: `arraydim` Dimension of experiment (P)
`dfsa` Display stacked FIDs automatically (C)
`dfsan` Display stacked FIDs automatically without screen erase (C)
`dfsh` Display stacked FIDs horizontally (C)
`dfshn` Display stacked FIDs horizontally without screen erase (C)
`dfsn` Display stacked FIDs without screen erase (C)
`dfww` Display FIDs in whitewash mode (C)

<code>ho</code>	Horizontal offset (P)
<code>plfid</code>	Plot FID (C)
<code>pfww</code>	Plot FIDs in whitewash mode (C)
<code>sc</code>	Start of chart (P)
<code>vo</code>	Vertical offset (P)
<code>vpf</code>	Current vertical position of FID (P)
<code>wc</code>	Width of chart (P)

dfsa Display stacked FIDs automatically (C)

Syntax: `dfsa(<start><,finish><,step><,'all' | 'imag'><,color>)>`

Description: Displays one or more FIDs automatically by adjusting the parameters `vo` and `ho` to fill the screen in a lower left to upper right presentation (`wc` must be set to less than full screen width for this to work). The position of the first FID is governed by parameters `wc`, `sc`, and `vpf`.

Arguments: `start` is the index number of the first FID for multiple FIDs. It can also be the index number of a particular FID for arrayed 1D or 2D data sets.

`finish` is the index number of the last FID for multiple FIDs.

`step` is the increment for the FID index. The default is 1.

`'all'` is a keyword to display all of the FIDs. This is the default.

`'imag'` is a keyword to display only the imaginary FID channel.

`color` is the color of the display: `'red'`, `'green'`, `'blue'`, `'cyan'`, `'magenta'`, `'yellow'`, `'black'`, or `'white'`.

See also: *NMR Spectroscopy User Guide*

Related: `dfs` Display stacked FIDs (C)
`dfsan` Display stacked FIDs automatically without screen erase (C)

dfsan Display stacked FIDs automatically without screen erase (C)

Syntax: `dfsan(<start><,finish><,step><,'all' | 'imag'><,color>)>`

Description: Functions the same as the command `dfsa` except the graphics window is not erased before starting the display. This allows composite displays of many FIDs to be created. The arguments are the same as `dfsa`.

See also: *NMR Spectroscopy User Guide*

Related: `dfsa` Display stacked FIDs automatically (C)

dfsh Display stacked FIDs horizontally (C)

Syntax: `dfsh(<start><,finish><,step><,'all' | 'imag'><,color>)>`

Description: Displays one or more FIDs horizontally by setting `vo` to zero and adjusting `ho`, `sc`, and `wc` to fill the screen from left to right with the entire array. The position of the first FID is governed by parameters `wc`, `sc`, and `vpf`.

Arguments: `start` is the index number of the first FID for multiple FIDs. It can also be the index number of a particular FID for arrayed 1D or 2D data sets.

`finish` is the index number of the last FID for multiple FIDs. To display all FIDs, set `finish` to the parameter `arraydim`.

`step` is the increment for the FID index. The default is 1.

`'all'` is a keyword to display all of the FIDs. This is the default.

`'imag'` is a keyword to display only the imaginary FID channel.

color is the color of the display: 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'black', or 'white'.

See also: *NMR Spectroscopy User Guide*

Related: **dfs** Display stacked FIDs (C)
dfshn Display stacked FIDs horizontally without screen erase (C)

dfshn Display stacked FIDs horizontally without screen erase (C)

Syntax: `dfshn(<start><,finish><,step><,'all' | 'imag'><,color>)>`

Description: Functions the same as the command **dfsh** except the graphics window is not erased before starting the display. This allows composite displays of many FIDs to be created. The arguments are the same as **dfsh**.

See also: *NMR Spectroscopy User Guide*

Related: **dfsh** Display stacked FIDs horizontally (C)

dfsn Display stacked FIDs without screen erase (C)

Syntax: `dfsn(<start><,finish><,step><,'all' | 'imag'><,color>)>`

Description: Functions the same as the command **dfs** except the graphics window is not erased before starting the display. This allows composite displays of many FIDs to be created. The arguments are the same as **dfs**.

See also: *NMR Spectroscopy User Guide*

Related: **dfs** Display stacked FIDs (C)

dfww Display FIDs in whitewash mode (C)

Syntax: `dfww(<start><,finish><,step><,'all' | 'imag'><,color>)>`

Description: Displays FIDs in whitewash mode (after the first FID, each FID is blanked out in regions in which it is behind an earlier FID). The position of the first FIDs is governed by parameters **wc**, **sc**, and **vpf**.

Arguments: **start** is the index number of the first FID for multiple FIDs. It can also be the index number of a particular FID for arrayed 1D or 2D data sets.

finish is the index number of the last FID for multiple FIDs.

step is the increment for the FID index. The default is 1.

'all' is a keyword to display all of the FIDs. This is the default.

'imag' is a keyword to display only the imaginary FID channel.

color is the color of the display: 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'black', or 'white'.

See also: *NMR Spectroscopy User Guide*

Related: **dfs** Display stacked FIDs (C)
pfww Plot FIDs in whitewash mode (C)

dg Display group of acquisition/processing parameters (C)

Syntax: `dg('template',<'file_name'>)`

Description: Displays the group of acquisition and 1D/2D processing parameters. To display an individual parameter, enter the name of the parameter followed by a question mark (e.g., **sw?**). Parameters do not have to be displayed in order to be entered or changed. The **dg** display is controlled by the string parameter **dg**.

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Arguments: `template` is the name of the template parameter. The default is `'dg'`. See the manual *User Programming* for rules on constructing a template. The macros `dg dg1, dg2, dg1p, and dgs` activate `dg` with a `template` argument such as `'dg', 'dg1', 'dg2', 'dg1p', 'dgs'`, etc. or a user defined template.

`file_name` is the name of the file to which the `dg` command will write the parameters specified by `template`.

Examples: `dg`
`dg ('dgexp')`
`dg ('dg', 'dgout')`

See also: *NMR Spectroscopy User Guide; User Programming*

Related:

<code>?</code>	Display the value of an individual parameter (C)
<code>da</code>	Display acquisition parameter arrays (C)
<code>dg1p</code>	Display group of linear prediction parameters (C)
<code>da</code>	Display acquisition parameter arrays (P)
<code>dg</code>	Control <code>dg</code> parameter group display (P)
<code>dg1p</code>	Control <code>dg1p</code> parameter group of linear prediction parameters (P)
<code>dg1</code>	Display group of display parameters (M)
<code>dg2</code>	Display group of 3rd and 4th rf channel/3D parameters (M)
<code>dgs</code>	Display group of special/automation parameters (M)

dg Control dg parameter group display (P)

Description: Controls the display of the `dg` command for the group of acquisition and 1D/2D processing parameters. `dg`, a string parameter, can be modified with the command `paramvi ('dg')`.

See also: *NMR Spectroscopy User Guide*

Related:

<code>dg</code>	Display group of acquisition/processing parameters (C)
<code>paramvi</code>	Edit a parameter and its attributes with <code>vi</code> text editor (C)

dg1 Display group of display parameters (M)

Description: Displays the group of display parameters. To display an individual parameter, enter the name of the parameter followed by a question mark (e.g., `sp?`). Parameters do not have to be displayed in order to be entered or changed. The `dg1` display is controlled by the string parameter `dg1`.

See also: *NMR Spectroscopy User Guide*

Related:

<code>?</code>	Display individual parameter value (C)
<code>dg1</code>	Control <code>dg1</code> parameter group display (P)
<code>dg</code>	Display group of acquisition/processing parameters (C)

dg1 Control dg1 parameter group display (P)

Description: Controls the display of the `dg1` command for the group of display parameters. `dg1`, a string parameter, can be modified with `paramvi ('dg1')`.

See also: *NMR Spectroscopy User Guide*

Related:

<code>dg1</code>	Display group of display parameters (M)
<code>paramvi</code>	Edit a parameter and its attributes with <code>vi</code> text editor (C)

dg2 Display group of 3rd and 4th rf channel/3D parameters (M)

Description: Displays the group of acquisition parameters associated with a second decoupler channel on a system with a third rf channel. It also displays the group

of parameters associated with selective 2D processing of 3D data sets. To display an individual parameter, enter the name of the parameter followed by a question mark (e.g., `sw?`). Parameters do not have to be displayed in order to be entered or changed. The `dg2` display is controlled by the string parameter `dg2`.

See also: *NMR Spectroscopy User Guide*

Related: `dg` Display group of acquisition/processing parameters (C)
`dg2` Control `dg2` parameter group display (P)

dg2 Control dg2 parameter group display (P)

Description: Controls the display of the `dg2` command for the group of 3rd and 4th rf channel/3D parameters. `dg2`, a string parameter, can be modified with the command `paramvi('dg2')`. To retrieve the `dg2` and `ap` display templates for the current experiment, enter `addpar('3rf')`.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to the current experiment (M)
`dg2` Display group of 3rd and 4th rf channel/3D parameters (M)
`paramvi` Edit a parameter and its attributes with `vi` text editor (M)

dga Display group of spin simulation parameters (M)

Description: Displays the file of spin simulation parameters (Group A). There is one such group of parameters in the data system, not one per experiment as with normal NMR parameters.

See also: *NMR Spectroscopy User Guide*

Related: `dg` Display group of acquisition/processing parameters (C)
`dla` Display spin simulation parameter arrays (C)

DgcsteSL Set up parameters for DgcsteSL pulse sequence (M)

Description: Converts a parameter set to DgcsteSL experiment.

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)
`fiddle` Perform reference deconvolution (M)
`setup_dosy` Set up gradient levels for DOSY experiments (M)

Dgcstecosy Set up parameters for Dgcstecosy pulse sequence (M)

Description: Converts a parameter set to Dgcstecosy experiment

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)
`makeslice` Synthesize 2D projection of a 3D DOSY spectrum (C)
`setup_dosy` Set up gradient levels for DOSY experiments (M)
`showoriginal` Restore first 2D spectrum in 3D DOSY spectrum (M)

Dgcstehmqc Set up parameters for Dgcstehmqc pulse sequence (M)

Description: Converts a parameter set to Dgcstehmqc experiment

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See also: *NMR Spectroscopy User Guide*

Related: **dosy** Process DOSY experiments (M)
makeslice Synthesize 2D projection of 3D DOSY spectrum (C)
setup_dosy Set up gradient levels for DOSY experiments (M)
showoriginal Restore first 2D spectrum in 3D DOSY spectrum (M)

dglc Display group of LC-NMR parameters (M)

Applicability: Systems with LC-NMR accessory.

Description: Displays parameters related to LC-NMR on a separate screen. This macro is equivalent to the command `dg ( ' dglc ' )`.

See also: *NMR Spectroscopy User Guide*

Related: **dglc** Control LC-NMR parameter display (P)

dglc Control dglc parameter group display (P)

Applicability: Systems with LC-NMR accessory.

Description: Controls the display of the LC-NMR parameters by the macro **dglc** and the equivalent command `dg ( ' dglc ' )`. If this parameter does not exist, the **parlc** macro can create it.

See also: *NMR Spectroscopy User Guide*

Related: **dglc** Display LC-NMR parameters (M)
parlc Create LC-NMR parameters (M)

dglp Display group of linear prediction parameters (C)

Syntax: `dglp`

Description: Displays the linear prediction parameters group. Parameters do not have to be displayed in order to be entered or changed. The `dglp` display is controlled by the string parameter **dglp**.

Examples: `dglp`

See also: *NMR Spectroscopy User Guide; User Programming*

Related: **dglp** Control dg parameter group display (P)

dgs Display group of shims and automation parameters (M)

Description: Displays the group of shims and automation parameters. To display an individual parameter, enter name of the parameter followed by a question mark (e.g., `sw?`). Parameters do not have to be displayed in order to be entered or changed. The `dgs` display is controlled by the parameter **dgs**.

See also: *NMR Spectroscopy User Guide*

Related: **dg** Display group of acquisition/processing parameters (C)
dgs Control dgs parameter group display (P)

dgs Control dgs parameter group display (P)

Description: Controls display of the **dgs** command for the group of shims and automation parameters. `dgs`, a string parameter, can be modified by `paramvi ( ' dgs ' )`.

See also: *NMR Spectroscopy User Guide*

Related: [dgs](#) Display group of special/automation parameters (M)
[paramvi](#) Edit a parameter and its attributes with vi text editor (C)

dhp Decoupler high-power control with class C amplifier (P)

Applicability: System with a class C amplifier.

Description: dhp selects a decoupler high-power level for systems with class C amplifiers on the decoupler channel. Specific values of dhp should be calibrated periodically for any particular instrument and probe combination. As a rough guide, dhp=75 corresponds to approximately 2 watts at 200 MHz.

CAUTION: Decoupler power greater than 2 watts in a switchable probe will damage the probe. Always carefully calibrate high-power decoupling to avoid exceeding 2 watts of power.

For systems equipped with a linear amplifier on the decoupler channel, dhp is nonfunctional and is replaced by the parameter [dpwr](#).

Note that dhp runs in the opposite direction from [dlp](#) (i.e., for dhp a higher number means more power, for [dlp](#) a higher number means less power).

Values: 0 to 255 (where 255 is maximum power) in uncalibrated, non-linear units.

'n' selects low-power decoupling under the control of the parameter [dlp](#).

See also: *NMR Spectroscopy User Guide*

Related: [dlp](#) Decoupler low power with class C amplifier (P)
[dpwr](#) Power level for first decoupler with linear amplifier (P)
[tn](#) Nucleus for observe transmitter (P)

dialog Display a dialog box from a macro (C)

Syntax: `dialog(definition_file,output_file<,'nowait'>)`

Description: Opens a dialog box from a macro. The output is written to a file that can be read by the macro using the [lookup](#) command.

Arguments: `definition_file` is the name of the file (specified by an absolute path) that defines the layout of the dialog box.

`output_file` is the name of the file (specified by an absolute path) where the results of the dialog box are written.

'nowait' is a keyword to return immediately, without waiting for input into the dialog box.

Examples: `dialog(userdir+'/dialoglib/array','/tmp/array')`

See also: *User Programming*

Related: [lookup](#) Look up words and lines from a text file (C)

diffparams Report differences between two parameter sets (U)

Syntax: `diffparams <-list> file1 file2 <macroname>`

Description: Reports differences between parameter sets. A macro can optionally be created that will convert `file1` into `file2`.

Arguments: `file1` and `file2` are parameter files, like `$HOME/vnmrsys/exp1/procpar` `$HOME/vnmrsys/exp1/curpar` `$HOME/vnmrsys/global/vnmr/conpar xyz.fid` or `xyz.par`, or a local experiment like `~/vnmrsys/exp1`; in this case `diffparams` will look for a subfile `procpar`

in these directories. The optional `-list` argument will cause a list of the parameters which are different to be printed. If the `-list` option is used, the macro feature is turned off. If a parameter exists in `file1` but not `file2`, it is not listed. If a parameter exists in `file2` but not `file1`, it is listed. If the parameter exists in both files, it is listed if the values are different. It is not listed if other information associated with the parameter is different. This other information is things like protection bits, maximum values, group, type, etc.

An optional third argument specifies the pathname of a macro to output. This macro will contain the MAGICAL commands necessary to convert `file1` into `file2`.

Examples: `diffparams abc.fid xyz.fid`
`diffparams -list abc.fid xyz.fid`
`diffparams ~/vnmrsys/exp1 ~/vnmrsys/exp3`
`diffparams ~/vnmrsys/exp1 ~/vnmrsys/exp3 ~/vnmrsys/maclib/change1to3`

diffshims **Compare two sets of shims (M,U)**

Syntax: `diffshims (shimfile1,shimfile2)`
 (From UNIX) `diffshims shimfile1 shimfile2`

Description: Compares values for room-temperature shims stored in two separate files.

Arguments: `shimfile1` and `shimfile2` are names of separate files containing shim values. Both files must have been written using the `svs` command.

See also: *NMR Spectroscopy User Guide*

Related: `svs` Save shim coil settings (C)

digfilt **Write digitally filtered FIDs to another experiment (M)**

Syntax: `digfilt (exp_number<,option>)`

Description: Saves digitally filtered FIDs to another experiment.

Arguments: `exp_number` specifies the number of the experiment, from 1 to 9, for saving the FIDs.

`option` is one of the keywords 'nodc', 'zero', 'lfs', 'zfs', or 't2dc'. Use a keyword for an option if the same option was used when processing the data with `ft`, `wft`, `ft2d`, or `wft2d`.

See also: *NMR Spectroscopy User Guide*

Related: `downsamp` Sampling factor applied after digital filtering (P)
`ft` Fourier transform 1D data (C)
`ft2d` Fourier transform 2D data (C)
`wft` Weight and Fourier transform 1D data (C)
`wft2d` Weight and Fourier transform 2D data (C)

dir **List files in directory (C)**

Syntax: `dir<(string)>`

Description: Displays files in a directory on the text window. The `dir` command is identical to the `ls` and `lf` commands.

Arguments: `string` is a string argument containing the options and/or directory names used if this were the UNIX `ls` command (e.g., `dir ('-l *.fid')` requests a long listing (-l) of all files ending with `.fid` (`*.fid`)). If no argument is entered, `dir` lists all files in the current working directory.

Examples: `dir`
`dir('data')`
`dir('-l *.fid')`

See also: *NMR Spectroscopy User Guide*

Related: `lf` List files in directory (C)
`ls` List files in directory (C)

display Display parameters and their attributes (C)

Syntax: `display(parameter| '*' | '**' <, tree>)`

Description: Displays one or more parameters and their attributes from a parameter tree.

Arguments: Three levels of display are available: `parameter`, `'*'`, and `'**'`.

- `parameter` is the name of a single parameter and the display is of its attributes (e.g., `display('a')` displays the attributes of parameter `a` in the (default) current tree).
- `'*'` is a keyword to display the name and values of all parameters in a tree (e.g., `display('*', 'global')` displays all parameter names and values in the global tree).
- `'**'` is a keyword to display the attributes of all parameters in a tree (e.g., `display '**', 'processed'`) displays the attributes of all parameters in the processed tree).

`tree` is the type of parameter tree and can be `'global'`, `'current'`, `'processed'`, or `'systemglobal'`. The default is `'current'`. Refer to the `create` command for more information on types of trees.

Examples: `display('a')`
`display('*', 'global')`
`display '**', 'processed')`

See also: *User Programming*

Related: `create` Create new parameter in a parameter tree (C)
`destroy` Destroy a parameter (C)
`paramvi` Edit a parameter and its attributes with the `vi` text editor (C)
`prune` Prune extra parameters from current tree (C)

dla Display spin simulation parameter arrays (M)

Syntax: `dla<('long')>`

Description: Displays the parameters containing the line assignments for spin simulation iteration (matching simulated spectra to actual data). A `clindex` value of a calculated transition gives the index of the assigned measured line. The value is zero for unassigned transitions.

Arguments: `'long'` is a keyword to display the parameters containing the line assignments for spin simulation iteration (matching simulated spectra to actual data) and put the line assignments into the file `spini.la`. This option is most useful when the `dla` display is too large to display all the calculated transitions in the text window. The `dlaalong` command operates the same as the `dla('long')` command.

Examples: `dla`
`dla('long')`

D

See also: *NMR Spectroscopy User Guide*

Related:	<code>assign</code>	Assign transitions to experimental lines (M)
	<code>clindex</code>	Index of experimental frequency of a transition (P)
	<code>dga</code>	Display parameters of spin simulation group (C)
	<code>dlalong</code>	Long display of spin simulation parameter arrays (C)

dlalong Long display of spin simulation parameter arrays (C)

Syntax: `dlalong`

Description: Puts line assignments into the file `spini.la` in a more complete form, then displays this file in the text window. It is most useful when the `dla` display is too large to display all the calculated transitions in the text window. The `dla('long')` command operates the same as `dlalong`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dla</code>	Display spin simulation parameter arrays (M)

dli Display list of integrals (C)

Description: Displays a list of integrals at the integral reset points. The frequency units of the displayed list of integrals is controlled by the parameter `axis`. The reset points may be defined with the `z` command and these frequencies are stored in `lifrq`. The calculated amplitudes of the integral region are stored in `liamp`. The reset points are stored as hertz and are not referenced to `rfl` and `rfp`. The amplitudes are stored as the actual value; they are not scaled by `ins` or by `insref`. When the integral blanking mode is used (i.e., `intmod='partial'`), only the integrals corresponding to the displayed integral regions are listed.

The displayed integral value can be scaled with the `setint` macro. The integral is scaled by the parameters `ins` and `insref`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>axis</code>	Axis label for displays and plots (P)
	<code>cz</code>	Clear integral reset points (C)
	<code>dlni</code>	Display list of normalized integrals (M)
	<code>ins</code>	Integral normalization scale (P)
	<code>insref</code>	Fourier number scaled value of an integral (P)
	<code>liamp</code>	Amplitudes of integral reset points (P)
	<code>lifrq</code>	Frequencies of integral reset points (P)
	<code>nli</code>	Find integral values (C)
	<code>rfl</code>	Reference peak position in directly detected dimension (P)
	<code>rfp</code>	Reference peak frequency in directly detected dimension (P)
	<code>setint</code>	Set value of an integral (M)
	<code>z</code>	Add integral reset point at cursor position (C)

dlivast Produce text file and process wells (M)

Applicability: VAST accessory.

Syntax: `dlivast<(last)>`

Description: Produces a text file containing the integral of the partial regions and processes the wells.

Arguments: `last` is the number of the last well. The default is 96.

See also: *NMR Spectroscopy User Guide*

Related: **combiplate** View a color map for visual analysis of VAST microtiter plate (U)
combi-show Display regions as red, green, and blue in CombiPlate window (M)

d11 Display listed line frequencies and intensities (C)

Syntax: `d11<('pos'<,noise_mult>)><:number_lines,scale>`

Description: Displays a list of line frequencies and amplitudes that are above a threshold defined by **th**. Frequency units are defined by the parameter **axis**. The results of this calculation are stored in **llfrq** and **llamp**. The frequencies are stored as Hz and are not referenced to **rfl** and **rfp**. Amplitudes are stored as the actual data point value; they are not scaled by **vs**.

Arguments: 'pos' is a keyword to list only positive lines.

noise_mult is a numerical value that determines the number of noise peaks listed for broad, noisy peaks. The default value is 3. A smaller value results in more peaks, a larger value results in fewer peaks, and a value of 0.0 results in a line listing containing all peaks above the threshold **th**. Negative values of **noise_mult** are changed to 3.

number_lines is a return argument with the number of lines above the threshold.

scale is a return argument with a scaling factor for line amplitudes. This scaling factor accounts for **vs** and whether the lines are listed in absolute intensity mode or normalized mode.

Examples: `d11`
`d11('pos')`
`d11(2.5)`
`d11:r1,sc`

See also: *NMR Spectroscopy User Guide*

Related: **axis** Axis label for displays and plots (P)
dels Delete spectra from T_1 or T_2 analysis (C)
fp Find peak heights (C)
getll Get frequency and intensity of a line (C)
llamp List of line amplitudes (P)
llfrq List of line frequencies (P)
nl Position the cursor at the nearest line (C)
nll Find line frequencies and intensities (C)
rfl Reference peak position in directly detected dimension (P)
rfp Reference peak frequency in directly detected dimension (P)
th Threshold (P)
vs Vertical scale (P)

d1ni Display list of normalized integrals (M)

Description: Displays integrals in a normalized format. The parameter **ins** represents the value of the sum of all the integrals. When the integral blanking mode is used (i.e., **intmod**= 'partial'), only the integrals corresponding to the displayed integral regions are listed and are used in the summation.

See also: *NMR Spectroscopy User Guide*

cz Clear integral reset points (C)
dli Display list of integrals (C)
ins Integral normalization scale (P)

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<code>nli</code>	Find integral values (C)
<code>z</code>	Add integral reset point at cursor position (C)

d1p Decoupler low-power control with class C amplifier (P)

Applicability: Systems with a class C amplifier.

Description: `d1p` controls the decoupler power level for systems with a class C decoupler amplifier in the low-power mode, generally used for homonuclear decoupling. `d1p` specifies dB of attenuation of the decoupler, below a nominal 1 watt value. `d1p` is active only if `dhp` = 'n'.

On systems with a decoupler linear amplifier, `d1p` is nonfunctional and `dpwr` controls decoupler power.

Values: 0 to 39 (in dB of attenuation, 0 is maximum power).

See also: *NMR Spectroscopy User Guide*

Related:	<code>dhp</code>	Decoupler high-power control with class C amplifier (P)
	<code>dm</code>	Decoupler mode for first decoupler (P)
	<code>dmf</code>	Decoupler modulation frequency for first decoupler (P)
	<code>dpwr</code>	Power level for first decoupler with linear amplifier (P)

dm Decoupler mode for first decoupler (P)

Description: Determines the state of first decoupler during different status periods within a pulse sequence (refer to the manual *User Programming* for a discussion of status periods). Pulse sequences may require one, two, three, or more different decoupler states. The number of letters that make up the `dm` parameter vary appropriately, with each letter representing a status period (e.g., `dm` = 'yny' or `dm` = 'ns'). If the decoupler status is constant for the entire pulse sequence, it can be entered as a single letter (e.g., `dm` = 'n').

Values: 'n', 'y', 'a', or 's' (or a combination of these values), where:

'n' specifies no decoupler rf.

'y' specifies the asynchronous mode. In this mode, the decoupler rf is gated on and modulation is started at a random places in the modulation sequence.

'a' specifies the asynchronous mode, the same as 'y'.

's' specifies the synchronous mode in which the decoupler rf is gated on and modulation is started at the beginning of the modulation sequence.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dm2</code>	Decoupler mode for second decoupler (P)
	<code>dm3</code>	Decoupler mode for third decoupler (P)
	<code>dm4</code>	Decoupler mode for fourth decoupler (P)
	<code>dmf</code>	Decoupler modulation frequency for first decoupler (P)
	<code>dmm</code>	Decoupler modulation mode for first decoupler (P)
	<code>dn</code>	Nucleus for first decoupler (P)
	<code>decasynctype</code>	Select the type of decoupler asynchronous mode (P)

dm2 Decoupler mode for second decoupler (P)

Applicability: Systems with a second decoupler.

Description: Determines the state of second decoupler during different status periods within a pulse sequence. It functions analogously to `dm`.

Values: Same as `dm`, except that if `dn2 = ' '` (two single quotes with no space in between) and a second decoupler is present in the console, `dm2` assumes a default value of `'n'` when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related: `dm` Decoupler mode of first decoupler (P)
`dmf2` Decoupler modulation frequency for second decoupler (P)
`dmm2` Decoupler modulation mode for second decoupler (P)
`dn2` Nucleus for second decoupler (P)

dm3 Decoupler mode for third decoupler (P)

Applicability: Systems with a third decoupler.

Description: Determines the state of third decoupler during different status periods within a pulse sequence. It functions analogously to `dm`.

Values: Same as `dm`, except that if `dn3 = ' '` (two single quotes with no space in between) and a third decoupler is present in the console, `dm3` assumes a default value of `'n'` when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related: `dm` Decoupler mode of first decoupler (P)
`dmf3` Decoupler modulation frequency for third decoupler (P)
`dmm3` Decoupler modulation mode for third decoupler (P)
`dn3` Nucleus for third decoupler (P)
`decasyntype` Select the type of decoupler asynchronous mode (P)

dm4 Decoupler mode for fourth decoupler (P)

Applicability: Systems with a deuterium decoupler channel as the fourth decoupler.

Description: Determines the state of fourth decoupler during different status periods within a pulse sequence. It functions analogously to `dm`.

Values: Same as `dm`, except that if `dn4 = ' '` (two single quotes with no space in between) and a fourth decoupler is present in the console, `dm4` assumes a default value of `'n'` when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related: `dm` Decoupler mode of first decoupler (P)
`dmf4` Decoupler modulation frequency for fourth decoupler (P)
`dmm4` Decoupler modulation mode for fourth decoupler (P)
`dn4` Nucleus for fourth decoupler (P)
`decasyntype` Select the type of decoupler asynchronous mode (P)

dmf Decoupler modulation frequency for first decoupler (P)

Description: Controls modulation frequency of the first decoupler. It specifies $1/\text{pw90}$ at the particular power level used. After calibrating the decoupler field strength γH_2 (expressed in units of Hz), `dmf` should be set equal to $4 \cdot \gamma\text{H}_2$ for WALTZ, MLEV16, GARP, and XY32 (when available).

`dmf` is inactive for CW mode decoupling (`dmm = 'c'`).

`dmf` is also active for square wave mode decoupling (`dmm = 'r'`) and fm-fm mode (`dmm = 'f'`) decoupling. For `dmm = 'f'`, the modulation frequency is swept back and forth between about 0.5% and 5% of the `dmf` frequency (e.g., if `dmf` is 100 kHz, the modulation is swept between approximately 500 Hz and 5 kHz). A reasonable optimum value for `dmf` when `dmm = 'f'` is the decoupler frequency divided by 4000.

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Values: 5 Hz to 2 MHz in steps of 5 Hz (steps are actually approximately 4.768 Hz).
For GARP modulation, the `dmf` value is internally multiplied by 45, making the limit of possible `dmf` values to 5 Hz to 44.4 kHz when `dmm` = 'g'.

See also: *NMR Spectroscopy User Guide*

Related: `dmf2` Decoupler modulation frequency for second decoupler (P)
`dmf3` Decoupler modulation frequency for third decoupler (P)
`dmf4` Decoupler modulation frequency for fourth decoupler (P)
`dmm` Decoupler modulation mode for first decoupler (P)
`pw90` 90° pulse width (P)

`dmf2` Decoupler modulation frequency for second decoupler (P)

Applicability: Systems with a second decoupler.

Description: Controls the modulation frequency of the second decoupler. It functions analogously to the parameter `dmf`.

Values: Same as `dmf` except that if `dn2` = ' ' (two single quotes with no space in between) and a second decoupler is present in the console (`numrfch` greater than 2), `dmf2` assumes a default value of 1000 Hz when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related: `dm2` Decoupler mode for second channel (P)
`dmf` Decoupler modulation frequency for first decoupler (P)
`dmm2` Decoupler modulation mode for second decoupler (P)
`dn2` Nucleus for second decoupler (P)
`numrfch` Number of rf channels (P)

`dmf3` Decoupler modulation frequency for third decoupler (P)

Applicability: Systems with a third decoupler.

Description: Controls the modulation frequency of the third decoupler. It functions analogously to the parameter `dmf`.

Values: Same as `dmf` except that if `dn3` = ' ' (two single quotes with no space in between) and a third decoupler is present in the console (`numrfch` equals 4), `dmf3` assumes a default value of 1000 Hz when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related: `dm3` Decoupler mode for third channel (P)
`dmf` Decoupler modulation frequency for first decoupler (P)
`dmm3` Decoupler modulation mode for third decoupler (P)
`dn3` Nucleus for third decoupler (P)
`numrfch` Number of rf channels (P)

`dmf4` Decoupler modulation frequency for fourth decoupler (P)

Applicability: Systems with a deuterium decoupler channel as the fourth decoupler.

Description: Controls the modulation frequency of the fourth decoupler. It functions analogously to the parameter `dmf`.

Values: Same as `dmf` except that if `dn4` = ' ' (two single quotes with no space in between) and a fourth decoupler is present in the console (`numrfch` equals 5), `dmf4` assumes a default value of 1000 Hz when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related:	dm4	Decoupler mode for fourth channel (P)
	dmf	Decoupler modulation frequency for first decoupler (P)
	dmm4	Decoupler modulation mode for fourth decoupler (P)
	dn4	Nucleus for fourth decoupler (P)
	numrfch	Number of rf channels (P)

dmfadj **Adjust tip-angle resolution time for first decoupler (M)**

Syntax: `dmfadj<(tipangle_resolution)>`

Description: Adjusts the parameter **dmf** so that time associated with the first decoupler tip-angle resolution is an integral multiple of 50 ns. This eliminates time truncation error in execution of programmable decoupling or spin-locking sequence by the waveform generator. For example, the tip-angle resolution for an MLEV-16 decoupling sequence should be 90.0° since every pulse in that sequence can be represented as an integral multiple of 90.0°; however, the tip-angle resolution for a GARP decoupling sequence should be 1.0°.

Arguments: `tipangle_resolution` specifies the necessary tip-angle resolution for the programmable decoupling or spin-locking sequence to be executed. The default value is the current value of the parameter **dres**.

Examples: `dmfadj`
`dmfadj(90.0)`

See also: *NMR Spectroscopy User Guide*

Related:	dmf	Decoupler modulation frequency for first decoupler (P)
	dmf2adj	Adjust tip-angle resolution time for second decoupler (M)
	dmf3adj	Adjust tip-angle resolution time third decoupler (M)
	dmf4adj	Adjust tip-angle resolution time fourth decoupler (M)
	dres	Tip angle resolution for programmable decoupling (P)

dmf2adj **Adjust tip-angle resolution time for second decoupler (M)**

Applicability: Systems with a second decoupler.

Syntax: `dmf2adj<(tipangle_resolution)>`

Description: Adjusts the parameter **dmf2** to make time associated with the second decoupler tip-angle resolution an integral multiple of 50 ns. `dmf2adj` functions analogously to the macro `dmfadj`.

Arguments: `tipangle_resolution` specifies the necessary tip-angle resolution for the programmable decoupling or spin-locking sequence to be executed. The default value is the current value of the parameter **dres2**.

Examples: `dmf2adj`
`dmf2adj(90.0)`

See also: *NMR Spectroscopy User Guide*

Related:	dmf2	Decoupler modulation frequency for second decoupler (P)
	dmfadj	Adjust decoupler tip-angle resolution time (M)
	dres2	Tip angle resolution for second decoupler (P)

dmf3adj **Adjust tip-angle resolution time for third decoupler (M)**

Applicability: Systems with a third decoupler.

Syntax: `dmf3adj<(tipangle_resolution)>`

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Description: Adjusts the parameter `dmf3` to make time associated with the third decoupler tip-angle resolution an integral multiple of 50 ns. `dmf3adj` functions analogously to the macro `dmfadj`.

Arguments: `tipangle_resolution` specifies the necessary tip-angle resolution for the programmable decoupling or spin-locking sequence to be executed. The default value is the current value of the parameter `dres3`.

Examples: `dmf3adj`
`dmf3adj (90.0)`

See also: *NMR Spectroscopy User Guide*

Related: `dmf3` Decoupler modulation frequency for third decoupler (P)
`dres3` Tip-angle resolution for third decoupler (P)

dmf4adj Adjust tip-angle resolution time for fourth decoupler (M)

Applicability: Systems with a deuterium decoupler as the fourth decoupler.

Syntax: `dmf4adj <(tipangle_resolution)>`

Description: Adjusts the parameter `dmf4` to make time associated with the fourth decoupler tip-angle resolution an integral multiple of 50 ns. `dmf4adj` functions analogously to the macro `dmfadj`.

Arguments: `tipangle_resolution` specifies the necessary tip-angle resolution for the programmable decoupling or spin-locking sequence to be executed. The default value is the current value of the parameter `dres4`.

Examples: `dmf4adj`

See also: *NMR Spectroscopy User Guide*

Related: `dmf4` Decoupler modulation frequency for fourth decoupler (P)
`dres4` Tip-angle resolution for fourth decoupler (P)

dmg Data display mode in directly detected dimension (P)

Description: Controls the mode of data display along the directly detected dimension. `dmg` is in the display group and can be set manually or by executing the commands `ph`, `av`, `pwr`, or `pa` for the values 'ph', 'av', 'pwr', or 'pa', respectively.

Values: 'ph' sets the *phased mode* in which each real point in the displayed spectrum is calculated from a linear combination of real and imaginary points comprising each respective complex data point.

'av' sets the *absolute-value mode* in which each real point in the displayed spectrum is calculated as the square root of the sum of squares of the real and imaginary points comprising each respective complex data point.

'pwr' sets the *power mode* in which each real point in the displayed spectrum is calculated as the sum of squares of the real and imaginary points comprising each respective complex data point.

'pa' sets the *phase angle mode* in which each real point in the displayed spectrum is calculated as the phase angle from the arc tangent of the real and imaginary points comprising each respective complex data point.

See also: *NMR Spectroscopy User Guide*

Related: `aig` Absolute intensity group (P)
`av` Set absolute-value mode in directly detected dimension (C)
`dccg` Drift correction group (P)
`dmg1` Data display mode in 1st indirectly detected dimension (P)
`dmg2` Data display mode in 2nd indirectly detected dimension (P)
`ft` Fourier transform 1D data (C)

<code>ft1d</code>	Fourier transform along f_2 dimension (C)
<code>ft2d</code>	Fourier transform 2D data (C)
<code>pa</code>	Set phase angle mode in directly detected dimension (C)
<code>ph</code>	Set phased mode in directly detected dimension (C)
<code>pmode</code>	Processing mode for 2D data (P)
<code>pwr</code>	Set power mode in directly detected dimension (C)
<code>wft</code>	Weigh and Fourier transform 1D data (C)
<code>wft1d</code>	Weigh and Fourier transform of 2D data (C)
<code>wft2d</code>	Weigh and Fourier transform 2D data (C)

dmg1 Data display mode in 1st indirectly detected dimension (P)

Description: Controls the mode of data display along the first indirectly detected dimension of a multidimensional data set. `dmg1` is in the display group and can be set manually or by executing the commands `ph1`, `av1`, `pwr1`, or `pa1` for the values 'ph1', 'av1', 'pwr1', or 'pa1', respectively. If `dmg1` does not exist or if it is set to the empty string (`dmg1= ''`), VnmrJ uses the value of `dmg` to decide the display mode along the first indirectly detected dimension.

Values: 'ph1' sets phased mode.
' av1 ' sets absolute-value mode.
' pwr1 ' sets power mode.
' pa1 ' sets phase angle mode.

See also: *NMR Spectroscopy User Guide*

Related:	<code>av1</code>	Set absolute-value mode in 1st indirectly det. dim. (C)
	<code>dmg</code>	Data display mode in directly detected dimension (P)
	<code>pa1</code>	Set phase angle mode in 1st indirectly detected dimension (C)
	<code>ph1</code>	Set phased mode in 1st indirectly detected dimension (C)
	<code>pwr1</code>	Set power mode in 1st indirectly detected dimension (C)

dmg2 Data display mode in 2nd indirectly detected dimension (P)

Description: Controls the mode of data display along the second indirectly detected dimension of a multidimensional data set. `dmg2` is in the display group and can be set manually or by executing the commands `ph2`, `av2`, or `pwr2` for the values 'ph2', 'av2', or 'pwr2', respectively. If `dmg2` does not exist or if it is set to the empty string (`dmg2= ''`), VnmrJ uses the value of the parameter `dmg` instead of `dmg2` to decide the display mode along the second indirectly detected dimension.

Values: 'ph2' sets phased mode.
' av2 ' sets absolute-value mode.
' pwr2 ' sets power mode.

See also: *NMR Spectroscopy User Guide*

Related:	<code>av2</code>	Set absolute-value mode in 2nd indirectly det. dim. (C)
	<code>dmg</code>	Data display mode in directly detected dimension (P)
	<code>ph2</code>	Set phased mode in 2nd indirectly det. dim. (C)
	<code>pwr2</code>	Set power mode in 2nd indirectly det. dim. (C)

dmgf Absolute-value display of FID data or spectrum in acqi (P)

Description: If the parameter `dmgf` exists and is set to 'av', the FID display in the `acqi` program is set to the absolute-value mode, which displays the square root of the sum of the squares of the real and imaginary channels. `dmgf` has no function

outside of the `acqi` program. This display mode may cause the displayed FID to exceed the displayed ADC limits in `acqi` by as much as a factor of the square root of 2.

See also: *NMR Spectroscopy User Guide*

Related: `acqi` Interactive acquisition display process (C)
`av` Set absolute-value mode in directly detected dimension (C)
`gf` Prepare parameters for FID/spectrum display in `acqi` (M)

dmm Decoupler modulation mode for first decoupler (P)

Description: Sets the modulation modes for the first decoupler. In the standard two-pulse sequence, `dmm` typically has a single state because the decoupler modulation is normally not changed during the pulse sequence, but this is not fixed. For example, `dmm= 'c cw'` gives single-frequency CW decoupling during the first part of the sequence and WALTZ-16 decoupling during acquisition.

In pulse sequences using the decoupler for pulsing (INEPT, DEPT, HETCOR, etc.), decoupler modulation must be set to 'c' during periods of the pulse sequence when the decoupler is to be pulsed.

Values: 'c', 'f', 'g', 'm', 'p', 'r', 'u', 'w', and 'x' are available,;

- 'c' sets continuous wave (CW) modulation.
- 'f' sets fm-fm modulation (swept-square wave).
- 'g' sets GARP modulation.
- 'm' sets MLEV-16 modulation.
- 'n' sets noise modulation.
- 'p' sets programmable pulse modulation using the `dseq` parameter to specify the decoupling sequence.
- 'r' sets square-wave modulation.
- 'u' sets user-supplied modulation using external hardware.
- 'w' sets WALTZ-16 modulation.
- 'x' sets XY32 modulation.

See also: *NMR Spectroscopy User Guide*

Related: `dm` Decoupler mode for first decoupler (P)
`dmf` Decoupler modulation frequency for first decoupler (P)
`dmm2` Decoupler modulation mode for second decoupler (P)
`dmm3` Decoupler modulation mode for third decoupler (P)
`dmm4` Decoupler modulation mode for fourth decoupler (P)
`dseq` Decoupler sequence for the first decoupler (P)

dmm2 Decoupler modulation mode for second decoupler (P)

Applicability: Systems with a second decoupler.

Description: Sets the type of decoupler modulation for the second decoupler during different status periods within a pulse sequence. It functions analogously to `dmm`.

Values: 'c', 'f', 'g', 'm', 'p', 'r', 'u', 'w', and 'x' are available. Refer to `dmm` for the definition of these values (note that if the mode 'p' is selected, `dseq2` specifies the decoupling sequence). If `dn2= ' '` (two single quotes) and a second decoupler is present in the console (`numrfch` greater than 2), `dmm2` is internally set to 'c' when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dm2</code>	Decoupler modulation for the second decoupler (P)
	<code>dmf2</code>	Decoupler modulation frequency for the second decoupler (P)
	<code>dmm</code>	Decoupler modulation mode for first decoupler (P)
	<code>dn2</code>	Nucleus for the second decoupler (P)
	<code>dseq2</code>	Decoupler sequence for the second decoupler (P)
	<code>numrfch</code>	Number of rf channels (P)

dmm3 Decoupler modulation mode for third decoupler (P)

Applicability: Systems with a third decoupler.

Description: Sets type of decoupler modulation for the third decoupler during different status periods within a pulse sequence. It functions analogously to `dmm`.

Values: 'c', 'f', 'g', 'm', 'p', 'r', 'u', 'w', and 'x' are available. Refer to `dmm` for the definition of these values (note that if the mode 'p' is selected, `dseq3` specifies the decoupling sequence). If `dn3` = ' ' (two single quotes) and a third decoupler is present in the console (`numrfch` equal to 4), `dmm3` is internally set to 'c' when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dm3</code>	Decoupler modulation for third decoupler (P)
	<code>dmf3</code>	Decoupler modulation frequency for third decoupler (P)
	<code>dmm</code>	Decoupler modulation mode for first decoupler (P)
	<code>dn3</code>	Nucleus for the third decoupler (P)
	<code>dseq3</code>	Decoupler sequence for the third decoupler (P)
	<code>numrfch</code>	Number of rf channels (P)

dmm4 Decoupler modulation mode for fourth decoupler (P)

Applicability: Systems with a deuterium decoupler channel as the fourth decoupler.

Description: Sets type of decoupler modulation for the fourth decoupler during different status periods within a pulse sequence. It functions analogously to `dmm`.

Values: 'c', 'f', 'g', 'm', 'r', 'u', 'w', and 'x' are available. Refer to `dmm` for the definition of these values. If `dn4` = ' ' (two single quotes) and a fourth decoupler is present in the console (`numrfch` greater than 4), `dmm4` is internally set to 'c' when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dm4</code>	Decoupler modulation for the fourth decoupler (P)
	<code>dmf4</code>	Decoupler modulation frequency for the fourth decoupler (P)
	<code>dmm</code>	Decoupler modulation mode for first decoupler (P)
	<code>dn4</code>	Nucleus for the fourth decoupler (P)
	<code>dseq4</code>	Decoupler sequence for the fourth decoupler (P)
	<code>numrfch</code>	Number of rf channels (P)

dn Nucleus for first decoupler (P)

Description: Changing the value of `dn` causes a macro (named `_dn`) to be executed that extracts values for `dfreq` and `dof` from lookup tables. The tables, stored in the directory `/vnmr/nuctables`, are coded by atomic weights.

Values: In the lookup tables, typically 'H1', 'C13', 'P31', etc.

See also: *NMR Spectroscopy User Guide*

Related:	dfrq	Transmitter frequency of first decoupler (P)
	dn2	Nucleus for second decoupler (P)
	dn3	Nucleus for third decoupler (P)
	dn4	Nucleus for fourth decoupler (P)
	dof	Frequency offset for first decoupler (C)
	tn	Nucleus for observe transmitter (P)

dn2 Nucleus for second decoupler (P)

Applicability: Systems with a second decoupler.

Description: Changing the value of dn2 causes a macro (named `_dn2`) to be executed that extracts values for **dfrq2** and **dof2** from lookup tables. Otherwise, dn2 functions analogously to the parameters **tn** and **dn**. If an experiment does not use the second decoupler channel, the channel can be disabled by setting `dn2= ' '` (two single quotes with no space in between). This sets **dm2**= 'n', **dmm2**= 'c', **dmf2**=1000 (in Hz), **dfrq2**=1 (in MHz), **dof2**=0, **dpwr2**=0, **dseq2**= ' ', and **dres2**=1.

See also: *NMR Spectroscopy User Guide*

Related:	dfrq2	Transmitter frequency of second decoupler (P)
	dn	Nucleus for first decoupler (P)
	dof2	Frequency offset for second decoupler (C)
	numrfch	Number of rf channels (P)
	tn	Nucleus for observe transmitter (P)

dn3 Nucleus for third decoupler (P)

Applicability: Systems with a third decoupler.

Description: Changing the value of dn3 causes a macro (named `_dn3`) to be executed that extracts values for **dfrq3** and **dof3** from lookup tables. Otherwise, dn3 functions analogously to the parameters **tn** and **dn**. If an experiment does not use the third decoupler channel, the channel can be disabled by setting `dn3= ' '` (two single quotes with no space in between). This sets **dm3**= 'n', **dmm3**= 'c', **dmf3**=1000 (in Hz), **dfrq3**=1 (in MHz), **dof3**=0, **dpwr3**=0, **dseq3**= ' ', and **dres3**=1.

See also: *NMR Spectroscopy User Guide*

Related:	dn	Nucleus for first decoupler (P)
	dfrq3	Transmitter frequency of third decoupler (P)
	dof3	Frequency offset for third decoupler (C)
	numrfch	Number of rf channels (P)
	tn	Nucleus for observe transmitter (P)

dn4 Nucleus for fourth decoupler (P)

Applicability: Systems with a deuterium decoupler channel as the fourth decoupler.

Description: Changing the value of dn4 causes a macro (named `_dn4`) to be executed that extracts values for **dfrq4** and **dof4** from lookup tables. Otherwise, dn4 functions analogously to the parameters **tn** and **dn** except that the only valid value for dn4 is 'H2'. If an experiment does not use the fourth decoupler channel, the channel can be disabled by setting `dn4= ' '` (two single quotes with no space in between). This sets **dm4**= 'n', **dmm4**= 'c', **dmf4**=1000 (in Hz), **dfrq4**=1 (in MHz), **dof4**=0, **dpwr4**=0, **dseq4**= ' ', and **dres4**=1.

See also: *NMR Spectroscopy User Guide*

Related:	dfrq4	Transmitter frequency of fourth decoupler (P)
	dn	Nucleus for first decoupler (P)
	dof4	Frequency offset for fourth decoupler (C)
	numrfch	Number of rf channels (P)
	tn	Nucleus for observe transmitter (P)

dndfid Retrieve and process fid data from the locator (M)

Applicability: Liquids, Imaging, Solids

Description: Retrieve fid data from an item selected in the locator. Data is also processed if Process data on drag-and-drop from locator is selected in the System settings dialog in the Utilities menu.

Related:	dndjoin	Join a work space from the locator (M)
	dndpar	Retrieve a parameter set from the locator (M)
	dndshims	Retrieve a shimset set from the locator (M)
	locaction	Locator action (M)
	locprotoexec	Execute a protocol from the locator (M)
	xmmakenode	Make a new study queue node (M)

dndjoin Join a work space from the locator (M)

Description: Join the work space selected by the locator.

Related:	dndfid	Retrieve and process fid data from the locator (M)
	dndpar	Retrieve a parameter set from the locator (M)
	dndshims	Retrieve a shimset set from the locator (M)
	locaction	Locator action (M)
	locprotoexec	Execute a protocol from the locator (M)
	xmmakenode	Make a new study queue node (M)

dndpar Retrieve a parameter set from the locator (M)

Description: Retrieve a parameter set selected by the locator.

Related:	dndfid	Retrieve and process fid data from the locator (M)
	dndjoin	Join a work space from the locator (M)
	dndshims	Retrieve a shimset set from the locator (M)
	locaction	Locator action (M)
	locprotoexec	Execute a protocol from the locator (M)
	xmmakenode	Make a new study queue node (M)

dndshims Retrieve a shimset set from the locator (M)

Description: Retrieve a shimset set selected by the locator.

Related:	dndfid	Retrieve and process fid data from the locator (M)
	dndjoin	Join a work space from the locator (M)
	dndpar	Retrieve a parameter set from the locator (M)
	locaction	Locator action (M)
	locprotoexec	Execute a protocol from the locator (M)
	xmmakenode	Make a new study queue node (M)

D

- dnode** **Display list of valid limNET nodes (M,U)**
- Applicability: Systems with limNET.
- Description: Displays the contents of the user's limNET node database (i.e., all remote nodes available to limNET). Each node is listed by name, Ethernet address (6 hexadecimal bytes), and burst size
- See also: *NMR Spectroscopy User Guide*
- Related: **eaddr** Display Ethernet address (M,U)
-
- doautodialog** **Start a dialog window using def file (M)**
- Applicability: Systems with automation.
- Syntax: doautodialog
- Description: Internal macro used by **enter** to start a dialog window using the def file for an experiment in the dialoglib directory.
- Related: **enter** Enter sample information for automation run (M,U)
-
- dodialog** **Start a dialog window with dialoglib file (M)**
- Syntax: dodialog
- Description: Internal macro that starts a dialog window using a dialog file in the dialoglib directory.
-
- dof** **Frequency offset for first decoupler (P)**
- Description: Controls the frequency offset of the first decoupler. Higher numbers move the decoupler to higher frequency (toward the left side of the spectrum). The frequency accuracy of the decoupler offset is generally 0.1 Hz. The value is specified in the **config** program.
- Values: -100000 to 100000 Hz (approximate, depends on frequency), in steps of 0.1 Hz.
- See also: *NMR Spectroscopy User Guide*
- Related: **config** Display current configuration and possible change it (M)
- dof2** Frequency offset for second decoupler (P)
- dof3** Frequency offset for third decoupler (P)
- dof4** Frequency offset for fourth decoupler (P)
- tof** Frequency offset for observe transmitter (P)
-
- dof2** **Frequency offset for second decoupler (P)**
- Applicability: Systems with a second decoupler.
- Description: Controls the frequency offset for the second decoupler. dof2 functions analogously to the parameters **tof** and **dof**.
- Values: -100000 to 100000 Hz (approximate, depends on frequency), in steps of 0.1 Hz. If **dn2** = ' ' (two single quotes with no space in between) and a second decoupler channel is present in the console, dof2 assumes a default value of 0 when **go** is executed.
- See also: *NMR Spectroscopy User Guide*
- Related: **dn2** Nucleus for second decoupler (P)
- dof** Frequency offset for first decoupler (P)
- tof** Frequency offset for observe transmitter (P)

dof3 Frequency offset for third decoupler (P)

Applicability: Systems with a third decoupler.

Description: Controls the frequency offset for the third decoupler. `dof3` functions analogously to the parameters `tof` and `dof`.

Values: -100000 to 100000 Hz (approximate, depends on frequency), in steps of 0.1 Hz. If `dn3= ' '` (two single quotes with no space in between) and a third decoupler channel is present in the console, `dof3` assumes a default value of 0 when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related: `dn3` Nucleus for third decoupler (P)
`dof` Frequency offset for first decoupler (P)
`tof` Frequency offset for observe transmitter (P)

dof4 Frequency offset for fourth decoupler (P)

Applicability: Systems with a deuterium decoupler channel as the fourth decoupler.

Description: Controls the frequency offset for the fourth decoupler. `dof4` functions analogously to the parameters `tof` and `dof`.

Values: -100000 to 100000 Hz (approximate, depends on frequency), in steps of 2.384 Hz. If `dn4= ' '` (two single quotes with no space in between) and a fourth decoupler channel is present in the console, `dof4` assumes a default value of 0 when `go` is executed.

See also: *NMR Spectroscopy User Guide*

Related: `dn4` Nucleus for fourth decoupler (P)
`dof` Frequency offset for first decoupler (P)
`tof` Frequency offset for observe transmitter (P)

Doneshot Set up parameters for Doneshot pulse sequence (M)

Description: Converts a parameter set to Doneshot experiment.

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)
`fiddle` Perform reference deconvolution (M)
`setup_dosy` Set up gradient levels for DOSY experiments (M)

dopardialog Start a dialog with dialoglib/experiment def file (M)

Description: Internal macro that starts a dialog window using a `def` file in the directory `dialoglib/experiment`.

do_pcsm Calculate proton chemical shifts spectrum (C)

Syntax: `do_pcsm(<threshold><,max_cc><,max_width>)`

Description: Strips a high-resolution proton spectrum down to a list of chemical shifts. The list is saved in the file `pcsm.outpar`. If no argument is given, `do_pcsm` automatically calculates the threshold and uses default values for the maximum allowable coupling constant and the maximum width of a spin multiplet.

Arguments: `threshold` sets the level whether a point belongs to a peak or is noise.
`max_cc` is the maximum allowable coupling constant in the spectrum. Default is 20 Hz.

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`max_width` is the maximum width of a spin multiplet in the spectrum.
Default is 60 Hz.

Examples: `do_pcsm`
`do_pcsm(10)`
`do_pcsm(9, 20, 80)`

See also: *NMR Spectroscopy User Guide*

Related: `pcsm` Calculate and show proton chemical shifts spectrum (M)

dosy Process DOSY experiments (M)

Syntax: `dosy(<'prune'>, <lowerlimit, upperlimit>)`

Description: Performs a DOSY (diffusion ordered spectroscopy) analysis of the data in an array of spectra.

`dosy` uses the commands `dll` and `fp` to determine the heights of all signals above the threshold defined by the parameter `th` and then fits the decay curve for each signal to a Gaussian using the program `dosyfit`. It stores a summary of all diffusion coefficients and their estimated standard errors and various other results as follows:

- In the directory `$HOME/vnmrsys/Dosy`: `diffusion_display.inp`, `general_dosy_stats`, `calibrated_gradients`, `fit_errors`, and `diffusion_spectrum`
- In the current experiment: a second copy of `diffusion_display.inp`.

The command `showdosy` has been incorporated into `dosy`.

Arguments: `prune` starts a dialog to allow one or more spectra to be omitted from the analysis.

`lowerlimit` is the lower diffusion limit (in units of 10^{-10} m²/s) to be displayed.

`upperlimit` is the upper diffusion limit (in units of 10^{-10} m²/s) to be displayed.

Without arguments, `dosy` uses all the experimental spectra and covers the whole diffusion range seen in the experimental peaks.

See also: *NMR Spectroscopy User Guide*

Related: `ddif` Synthesize and display DOSY plot (C)
`fiddle` Perform reference deconvolution (M)
`setup_dosy` Set up gradient levels for DOSY experiments (M)

dosy2d Apptype macro for dosy 2D experiments (M)

Applicability: Liquids

Description: Performs the actions for 2D dosy protocols to set up, process, and plot experiments. It is only available if the Dosy software is installed.

Related: `apptype` Application type (PM)
`execpars` Set up the exec parameters (M)

dosyfrq Larmor frequency of phase encoded nucleus in DOSY (P)

Description: Stores the NMR frequency of the phase encoded nucleus in DOSY experiments. It is directly set by the DOSY sequences.

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)

dosygamma Gyromagnetic constant of phase encoded nucleus in DOSY (P)

Description: Stores the gyromagnetic constant of the phase encoded nucleus in DOSY experiments. It is automatically set by the DOSY sequences and used by the **dosy** macro.

See also: *NMR Spectroscopy User Guide*

Related: **dosy** Process DOSY experiments (M)

dosytimecubed Gyromagnetic constant of phase encoded nucleus in DOSY (P)

Description: Time cubed factor in the expression for diffusional attenuation. It is automatically set by the DOSY sequences and used by the **dosy** macro.

See also: *NMR Spectroscopy User Guide*

Related: **dosy** Process DOSY experiments (M)

dot1 Set up a T_1 experiment (M)

Syntax: `dot1<(min_T1_estimate,max_T1_estimate,time)>`

Description: Sets up all parameters to perform a T_1 experiment, including **d1**, **pw**, **p1**, **nt**, and an array of **d2** values, based on information entered you enter. Make sure that the parameter **pw90** is set properly and contains the correctly calibrated 90° pulse width because **dot1** uses this information. If you have not done a pulse width calibration recently, you may wish to do so now.

Minimum and maximum T_1 for the peaks of interest are estimates. Do the best you can. Your estimates are used to select optimum values of **d2**. If the T_1 does not fall between your two guesses, your experiment may not be optimum, but it should still be usable unless your estimates are extremely far off. When you are satisfied with the parameters, enter **ga** or **au** to acquire the data.

Arguments: **min_T1_estimate** is the estimated minimum expected T_1 . The default is the system prompts the user for the value.

max_T1_estimate is the estimated maximum expected T_1 . The default is the system prompts the user for the value.

time is the total time in hours that the experiment should take. The default is the system prompts the user for the value.

Examples: `dot1`
`dot1(1,2,.5)`

See also: *NMR Spectroscopy User Guide*

Related: **d1** First delay (P)
d2 Incremented delay in 1st indirectly detected dimension (P)
ga Submit experiment to acquisition and FT the result (C)
go Submit experiment to acquisition (C)
nt Number of transients (P)
p1 First pulse width (P)
pw Pulse width (P)
pw90 90° pulse width (P)

dotflag Display FID as connected dots (P)

Description: When sparse FID data points are displayed, they are displayed as unconnected dots. If **dotflag** exists and is set to 'n', the FID dots will be connected. To create **dotflag**, enter **create('dotflag','flag')**. To create **dotflag** and the FID display parameters **axisf**, **vpf**, **vpfi**, **crf**, and

`deltaf` (if the parameter set is older and lacks these parameters), enter `addpar('fid')`.

Values: 'n' sets connecting the dots. 'y' sets not connecting the dots.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to the current experiment (M)
`create` Create new parameter in a parameter tree (C)
`df` Display a single FID (C)

downsamp **Downsampling factor applied after digital filtering (P)**

Description: Specifies the downsampling factor applied after digital filtering. The spectral width of the data set after digital filtering and downsampling is `sw` divided by `downsamp`, where `sw` is the acquired spectral width. If `downsamp` does not exist in the current experiment, enter `addpar('downsamp')` to add it. `addpar('downsamp')` creates the digital filtering and downsampling parameters `downsamp`, `dscoef`, `dsfb`, `dsfsfrq`, and `filtfile`.

Values: Number for the downsampling factor. 1 sets digital filtering with a filter bandwidth specified by `dsfb` without downsampling.

'n' sets normal data processing without digital filtering.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to current experiment (M)
`digfilt` Write digitally filtered FID to another experiment (M)
`dscoef` Digital filter coefficients for downsampling (P)
`dsfb` Digital filter bandwidth for downsampling (P)
`dsfsfrq` Bandpass filter offset for downsampling (P)
`filtfile` File of FIR digital filter coefficients (P)
`pards` Create additional parameters used by downsampling (M)
`sw` Spectral width in directly detected dimension (P)

dp **Double precision (P)**

Description: Sets whether data are acquired in a 16-bit or 32-bit integer format.

Values: 'n' sets 16-bit format, 'y' sets 32-bit format. If the 200-kHz receiver option is installed (Max. Narrowband Width set to 200 kHz in the Spectrometer Configuration window), `dp` is forced to 'n' if $120000 < sw \leq 200000$. If $sw > 200000$, `dp` is forced to 'y'. On wideline systems, `dp='y'` is required when $sw > 100000$.

See also: *NMR Spectroscopy User Guide*

Related: `sw` Spectral width in directly detected dimension (P)

dpcon **Display plotted contours (C)**

Syntax: `dpcon(<options>, <levels>, <spacing>)`

Description: Produces a true contour plot display.

Arguments: `options` must precede `levels` and `spacing` in the argument list and can be one or more of the following:

- 'pos' is a keyword to limit the display to positive peaks only in phased spectra. The default is both positive and negative peaks.
- 'neg' is a keyword to limit the display to negative peaks only in phased spectra.

- 'noaxis' is a keyword to omit outlining the display and drawing the horizontal or vertical axis.

levels is the maximum number of contours to be shown. The default is 4.

spacing is the spacing by relative intensity of successive contour levels. The default is 2.

Examples: `dpcon`
`dpcon('pos', 6)`
`dpcon(15, 1.4)`

See also: *NMR Spectroscopy User Guide*

Related: `dcon` Display noninteractive color intensity map (C)
`dconi` Control display selection for the `dconi` program (P)
`dpconn` Display plotted contours without screen erase (C)
`pcon` Plot contours on plotter (C)

dpconn Display plotted contours without screen erase (C)

Syntax: `dpconn(<options>, <levels>, spacing)`

Description: Produces a true contour plot display exactly the same as the `dpcon` command, but without erasing the screen before drawing. The arguments are entered the same as `dpcon`.

See also: *NMR Spectroscopy User Guide*

Related: `dpcon` Display plotted contours (C)

dpf Display peak frequencies over spectrum (C)

Syntax: (1) `dpf(<'noll'><, 'pos'><, noise_mult><, 'top'>)>`
 (2) `dpf(<'noll'><, 'pos'><, noise_mult><, 'leader'><, length>)>`

Description: Displays peak frequencies in the graphics window, with units specified by the `axis` parameter. Only those peaks greater than `th` high are selected. If the interactive command `ds` is active, `dpf` deactivates it.

Two basic modes of label positioning are available: labels placed at the top, with *long leaders* extending down to the tops of the lines (syntax 1 using 'top' keyword) or labels positioned just above each peak, with *short leaders* (syntax 2 using 'leader' keyword). The default is short leaders.

Arguments: 'noll' is a keyword to display frequencies using last previous line listing.

'pos' (or 'noneg') is a keyword to display positive peaks only.

noise_mult is a numerical value that determines the number of noise peaks displayed for broad, noisy peaks. The default is 3. A smaller value results in more peaks, a larger value results in fewer peaks, and a value of 0.0 results in a line listing containing all peaks above the threshold `th`. Negative values of noise_mult are changed to a value of 3. The noise_mult argument is inactive when the 'noll' keyword is specified.

'top' is a keyword to display peak labels at the top with long leaders. In this mode, the height of labels is varied by changing the parameter `wc2`.

'leader' is a keyword to display labels positioned just above each peak.

length specifies the leader length, in mm, if labels are positioned just above each peak. The default is 20.

Examples: `dpf('pos')`
`dpf('leader', 30)`

```
dpf('top','noll')
dpf('pos',0.0,'leader',30)
```

See also: *NMR Spectroscopy User Guide*

Related:

<code>axis</code>	Axis label for displays and plots (P)
<code>dpir</code>	Display integral amplitudes below spectrum (C)
<code>dpirn</code>	Display normalized integral amplitudes below spectrum (M)
<code>pir</code>	Plot integral amplitudes below spectrum (C)
<code>pirn</code>	Plot normalized integral amplitudes below spectrum (M)
<code>ppf</code>	Plot peak frequencies over spectrum (M)
<code>th</code>	Threshold (P)
<code>vp</code>	Vertical position of spectrum (P)
<code>wc2</code>	Width of chart in second direction (P)

dpir **Display integral amplitudes below spectrum (C)**

Description: Displays integral amplitudes below the appropriate spectral regions.

See also: *NMR Spectroscopy User Guide*

Related:

<code>dpf</code>	Display peak frequencies over spectrum (C)
<code>dpirn</code>	Display normalized integral amplitudes below spectrum (M)
<code>pir</code>	Plot integral amplitudes below spectrum (C)
<code>pirn</code>	Plot normalized integral amplitudes below spectrum (M)
<code>ppf</code>	Plot peak frequencies over spectrum (M)

dpirn **Display normalized integral amplitudes below spectrum (M)**

Description: Equivalent to the command `dpir` except that the sum of the integrals is normalized to the value of the parameter `ins`.

See also: *NMR Spectroscopy User Guide*

Related:

<code>dpir</code>	Display integral amplitudes below spectrum (C)
<code>ins</code>	Integral normalization scale (P)
<code>pirn</code>	Plot normalized integral amplitudes below spectrum (M)

dpiv **Display integral values below spectrum (M)**

Syntax: `dpiv<(vertical_position)>`

Description: Labels integrals with a bracket below the spectrum and a vertical number indicating the integral value.

- vertical labels for narrower regions
- avoids label overlap by label shifting
- more flexible vertical positioning

The vertical position defaults to a location just underneath the scale labels, assuming there is enough room below the scale. If the vertical position is too low, the vertical position is allowed to approach the position of the spectrum up to 1 mm. If the spectral position is so low that the integral labels would overlap with the spectrum, an error message is produced (indicating the minimum `vp`), and the command aborts. No error message is produced in case of overlap with the scale. The minimum for `vp` depends on the plotter and the character size, and in the case of `dpiv` also on the size of the graphics window.

Use an optional argument to force the vertical position to any value; no checking is done, and no error message is produced in case of overlap. `piv(vp-2)` produces integral labels with the brackets ending 2 mm below the position of the spectrum.

`dpiv` follows this convention: the output is controlled by `ins` and `insref` and not by `is`. Restore the `is` integration mode by creating a (local or global) parameter `oldint` and set `oldint='y'`:

```
create('oldint','flag','global')
```

```
oldint='y'
```

`oldint='n'` (or destroy the parameter) switches back to the default integration mode.

Examples: `vp=25 dpiv`
`vp=50 pl pscale piv(0)`

Related:	<code>dpir</code>	Display integral amplitudes below spectrum (C)
	<code>dpirn</code>	Display normalized integral amplitudes below spectrum (C)
	<code>dpivn</code>	Display normalized integral amplitudes below spectrum (M)
	<code>pirn</code>	Plot normalized integral amplitudes below spectrum (C)
	<code>pir</code>	Plot integral amplitudes below spectrum (C)
	<code>piv</code>	Plot integral amplitudes below spectrum (M)
	<code>pivn</code>	Plot normalized integral amplitudes below spectrum (M)

`dpivn` Display normalized integral values below spectrum (M)

Syntax: `dpivn<(vertical_position)>`

Description: Labels integrals with a bracket below the spectrum and a vertical number indicating the integral value.

See `dpiv` for description and use.

Related:	<code>dpir</code>	Display integral amplitudes below spectrum (C)
	<code>dpirn</code>	Display normalized integral amplitudes below spectrum (C)
	<code>dpiv</code>	Display integral amplitudes below spectrum (M)
	<code>pirn</code>	Plot normalized integral amplitudes below spectrum (C)
	<code>pir</code>	Plot integral amplitudes below spectrum (C)
	<code>piv</code>	Plot integral amplitudes below spectrum (M)
	<code>pivn</code>	Plot normalized integral amplitudes below spectrum (M)

`dpl` Default plot (M)

Description: Looks for sequence-specific default plot macro (`dpl_seqfil`) and executes if one is found.

Related:	<code>dpl_seqfil</code>	Sequence-specific default plot (M)
	<code>dpr</code>	Default process (M)
	<code>dds</code>	Default display (M)

`dpl_seqfil` Sequence-specific default plot (M)

Description: Sequence-specific default plot. These macros are called by the `dpl` macro.

Examples: `dpl_NOESY1D`
`dpl_TOCSY1D`

Related:	<code>dpl</code>	Default plot (M)
	<code>dpr</code>	Default process (M)
	<code>dds</code>	Default display (M)

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dplane **Display a 3D plane (M)**

Syntax: `dplane (<plane_type, >plane_number)`

Description: Displays the 2D color map of a particular data plane from a 3D spectral data set. The 3D parameters are loaded into VnmrJ each time `dplane` is executed. The parameter `path3d` specifies the absolute path to the directory (without the `.extr` file extension) where the 2D planes extracted from the 3D spectral data set reside.

Arguments: `plane_type` is one of the keywords 'f1f3', 'f2f3', and 'f1f2' for the f₁f₃, f₂f₃, and f₁f₂ planes, respectively. If `plane_type` is specified, the parameter `plane` is updated with that new value. `plane` is then used to determine the type of 3D plane to be displayed.

`plane_number` specifies which plane of a particular type is to be displayed:

- For plane f₁f₃, the range of `plane_number` is 1 to `fn2/2`
- For plane f₂f₃, the range of `plane_number` is 1 to `fn1/2`
- For plane f₁f₂, the range of `plane_number` is 1 to `fn/2`

Examples: `dplane (3)`
`dplane ('f1f2', 2)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dsplanes</code>	Display a series of 3D planes (M)
	<code>dproj</code>	Display a 3D plane projection (M)
	<code>getplane</code>	Extract planes from a 3D spectral data set (M)
	<code>nextpl</code>	Display the next 3D plane (M)
	<code>path3d</code>	Path to currently displayed 2D planes from a 3D data set (P)
	<code>plane</code>	Currently displayed 3D plane type (P)
	<code>prevpl</code>	Display the previous 3D plane (M)
	<code>plplanes</code>	Plot a series of 3D planes (M)

dpr **Default process (M)**

Description: Looks for sequence-specific default plot macro (`dpr_seqfil`) and executes if one is found.

Related:	<code>dpr_seqfil</code>	Sequence-specific default process (M)
	<code>dpl</code>	Default plot (M)
	<code>dds</code>	Default display (M)

dpr_seqfil **Sequence-specific default process (M)**

Description: Sequence-specific default plot. These macros are called by the `dpr` macro.

Examples: `dpr_NOESY1D`
`dpr_TOCSY1D`

Related:	<code>dpr</code>	Default process (M)
	<code>dpl</code>	Default plot (M)
	<code>dds</code>	Default display (M)

dprofile **Display pulse excitation profile (M)**

Syntax: `dprofile<(axisflag<, profile<, shapefile>>)>`

Description: Displays the X, Y and Z excitation (inversion) profile for a pulse shape generated by the Pbox software. If `shapefile` is not provided, the last simulation data stored in the `shapelib/pbox.sim` file are displayed.

Arguments: The `axisflag` and `profile` arguments can be given in any order.

`axisflag` is 'y' to display the full spectrum and a frequency scale, or 'n' to suppress the scale and spectrum. The default is 'n'.

`profile` is a character string identifying the desired profile. 'xyz' selects X, Y, and Z (inversion) profiles; 'xy' selects only the excitation (transverse) profiles; 'x' selects only the X transverse excitation profile; and 'z' selects only the inversion profile. The default is 'xyz'.

`shapefile` is the name of a *.RF or *.DEC file, including the extension.

Examples: `dprofile`
`dprofile('y','xy')`
`dprofile('xy','n','softpls.RF')`

See also: *NMR Spectroscopy User Guide*

Related: `pprofile` Plot pulse excitation profile (M)
`Pbox` Pulse shaping software (U)

dproj Display a 3D plane projection (M)

Syntax: `dproj<(plane_type)>`

Description: Displays 2D color map of the 2D projection plane from a 3D spectral data set. The projection is a skyline projection. The 3D parameters are loaded into VnmrJ each time `dproj` is executed. For this macro, the parameter `path3d` specifies the directory (without the `.extr` extension) where the 2D projection resides that has been created from the 3D spectral data set.

Arguments: `plane_type` is one of the keywords 'f1f3', 'f2f3', and 'f1f2' for the f_1f_3 , f_2f_3 , and f_1f_2 planes, respectively. If `plane_type` is specified, the parameter `plane` is updated with that value. `plane` is then used to determine the type of 2D projection to be displayed.

Examples: `dproj`
`dproj('f1f2')`

See also: *NMR Spectroscopy User Guide*

Related: `dplane` Display a 3D plane (M)
`dsplanes` Display a series of 3D planes (M)
`getplane` Extract planes from a 3D spectral data set (M)
`nexttpl` Display the next 3D plane (M)
`path3d` Path to currently displayed 2D planes from a 3D data set (P)
`plane` Currently displayed 3D plane type (P)
`plplanes` Plot a series of 3D planes (M)
`prevpl` Display the previous 3D plane (M)

dps Display pulse sequence (C)

Syntax: `dps<(file),x,y,width,height>`

Description: Displays a picture of pulse sequences consisting of three to five parts. The top part is the transmitter pulse sequence (Tx). The second part is the decoupler pulse sequence (Dec). The third part might be the second or third decoupler (Dec2 or Dec3) pulse sequence or gradients (X, Y, or Z), depending on the program. The lowest part is the status.

The pulse parameters are displayed if there is enough space and if the length of the parameter name is less than thirty letters. The value of each pulse is also displayed. If the value delay or width is less than zero, a question mark (?) is displayed. The time units are displayed in color (on a color monitor). The height of pulses is scaled according to their power level.

`dps` also displays spin lock, transmitter gating, observe transmitter power, and other information.

Arguments: `file` specifies the name of the file containing the pulse sequences. The default is the file `seqfil`.

`x`, `y` specifies the start of the position with respect to the lower-left corner of the window.

`width`, `height` are in proportion to `wcmax` and `wc2max`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>pps</code>	Plot pulse sequence (C)
	<code>seqfil</code>	Pulse sequence name (P)
	<code>wc</code>	Width of chart (P)
	<code>wcmax</code>	Maximum width of chart (P)
	<code>wc2max</code>	Maximum width of chart in second direction (P)

`dpwr` Power level for first decoupler with linear amplifier (P)

Applicability: Systems with a linear amplifier.

Description: On systems equipped with a linear amplifier, a 63-dB or 79-dB attenuator between the decoupler transmitter and the amplifier controls the power level.

The system value for the attenuator upper safety limit is set in the Spectrometer Configuration window (opened by `config`). The Upper Limit entry sets this value. For broadband decoupling of ^1H nuclei, typical values range from 36 to 49 dB. For homonuclear decoupling, typical values range from 5 to 15 dB.

Values: 79 dB, -16 to +63, in steps of 1 dB.

Decoupler power greater than 2 watts in a switchable probe will damage the probe. Always carefully calibrate decoupling to avoid exceeding 2 watts. The maximum value for `dpwr` on a 200-, 300-, or 400-MHz system with a linear amplifier on the decoupler channel has been set to 49, corresponding to about 2 watts of power. Before using `dpwr=49` for continuous decoupling, ensure safe operation by measuring the output power. This should be done during system installation and checked periodically by the user.

See also: *VnmrJ Installation and Administration*

Related:	<code>cattn</code>	Coarse attenuator (P)
	<code>config</code>	Display current configuration and possibly change it (M)
	<code>dpwrf</code>	First decoupler fine power (P)
	<code>dpwr2</code>	Power level for second decoupler (P)
	<code>dpwr3</code>	Power level for third decoupler (P)
	<code>dpwr4</code>	Power level for fourth decoupler (P)
	<code>fattn</code>	Fine attenuator (P)
	<code>tpwr</code>	Power level of observe transmitter with linear amplifiers (P)
	<code>tpwrf</code>	Observe transmitter fine power (P)

`dpwr2` Power level for second decoupler with linear amplifier (P)

Applicability: Systems with a linear amplifier as the second decoupler.

Description: Controls the coarse attenuator (63 dB or 79 dB) that resides between the transmitter board and the linear amplifier associated with the second decoupler.

The system value for the attenuator upper safety limit is set in the Spectrometer Configuration window (opened by `config`).

Values: 79 dB, -16 to +63, in steps of 1 dB.

If `dn2= ' '` (two single quotes) and a second decoupler channel is present in the console, `dpwr2` assumes a default value of 0 when `go` is executed.

CAUTION: Decoupler power greater than 2 watts in a switchable probe will damage the probe. Always carefully calibrate decoupling to avoid exceeding 2 watts. The maximum value for `dpwr2` on a 200-, 300-, or 400-MHz system with a linear amplifier on the decoupler channel has been set to 49, corresponding to about 2 watts of power. Before using `dpwr2=49` for continuous decoupling, ensure safe operation by measuring the output power. This should be done during system installation and checked periodically by the user.

See also: *NMR Spectroscopy User Guide*

Related: `cattn` Coarse attenuator type (P)
`config` Display current configuration and possible change it (M)
`dn2` Nucleus for second decoupler (P)

dpwr3 Power level for third decoupler with linear amplifier (P)

Applicability: Systems with a linear amplifier as the third decoupler.

Description: Controls the coarse attenuator (63 dB or 79 dB) that resides between the transmitter board and the linear amplifier associated with the third decoupler. The system value for the attenuator upper safety limit is set in the Spectrometer Configuration window (opened by `config`).

Values: If 63-dB attenuator installed: 0 to 63 (63 is max. power), in units of dB.
 If 79-dB attenuator installed: -16 to 63 (63 is max. power), in units of dB. If `dn3= ' '` (two single quotes) and a third decoupler channel is present in the console, `dpwr3` assumes a default value of 0 when `go` is executed.

CAUTION: Decoupler power greater than 2 watts in a switchable probe will damage the probe. Always carefully calibrate decoupling to avoid exceeding 2 watts. The maximum value for `dpwr3` on a 200-, 300-, or 400-MHz system with a linear amplifier on the decoupler channel has been set to 49, corresponding to about 2 watts of power. Before using `dpwr3=49` for continuous decoupling, ensure safe operation by measuring the output power. This should be done during system installation and checked periodically by the user.

See also: *NMR Spectroscopy User Guide*

Related: `cattn` Coarse attenuator type (P)
`config` Display current configuration and possible change it (M)
`dn3` Nucleus for third decoupler (P)

dpwr4 Power level for fourth decoupler amplifier (P)

Applicability: Systems with deuterium decoupler channel as the fourth decoupler.

Description: Controls the coarse attenuator (45 dB range) that resides on the Lock Transceiver board and the amplifier associated with the fourth decoupler. The system value for the attenuator upper safety limit is set in the Spectrometer Configuration window (opened by `config`).

Values: 48-dB attenuator: 15 to 63 (63 is max. power), in units of dB.
 If `dn4= ' '` (two single quotes) and a third decoupler channel is present in the console, `dpwr4` assumes a default value of 0 when `go` is executed.

CAUTION: Decoupling power greater than 5 watts applied to a triple-resonance probe will damage the probe. The maximum value for `dpwr4` is 63, corresponding to about 35 watts to the probe. A value of `dpwr4` equal to 52 corresponds to about 5 watts and will produce approximately a 1 kHz decoupling field. Always carefully calibrate decoupling power to avoid exceeding 5 watts. Before using `dpwr4=52` continuous decoupling, ensure safe operation by measuring the output power. Measurement should be taken during system installation and checked periodically by the user.

See also: *NMR Spectroscopy User Guide*

Related: `cattn` Coarse attenuator type (P)
`config` Display current configuration and possible change it (M)
`dn3` Nucleus for third decoupler (P)

dpwrf First decoupler fine power (P)

Applicability: Systems with an optional fine attenuator on the decoupler channel.

Description: Controls the first decouple fine attenuator. Systems with this attenuator are designated within the Spectrometer Configuration window (opened by `config`) by the status of the Fine Attenuator entry. The fine attenuator is linear and spans 6 dB.

Values: 0 to 4095 (where 4095 is maximum power). If `dpwrf` does not exist in the parameter table, a value of 4095 is assumed.

See also: *User Programming, User Guide: Solids; CP/MAS Installation*,

Related: `config` Display current configuration and possibly change it (M)
`dpwr` Power level for first decoupler with linear amplifiers (P)
`dpwrf2` Second decoupler fine power (P)
`dpwrf3` Third decoupler fine power (P)
`dpwrm` First decoupler linear modulator power (P)
`fattn` Fine attenuator (P)
`tpwr` Power level of observe transmitter with linear amplifiers (P)
`tpwrf` Transmitter fine power (P)

dpwrf2 Second decoupler fine power (P)

Applicability: Systems with an optional fine attenuator on the second decoupler channel.

Description: Controls the second decoupler fine attenuator, functioning analogously to `dpwrf`.

Values: 0 to 4095 (where 4095 is maximum power). If `dpwrf2` does not exist in the parameter table, a value of 4095 is assumed.

See also: *User Programming*

Related: `dpwrf` First decoupler fine power (P)

dpwrf3 Third decoupler fine power (P)

Applicability: Systems with an optional fine attenuator on the third decoupler channel.

Description: Controls the third decoupler fine attenuator, functioning analogously to `dpwrf`.

Values: 0 to 4095 (where 4095 is maximum power). If `dpwrf3` does not exist in the parameter table, a value of 4095 is assumed.

See also: *User Programming*

Related: `dpwrf` First decoupler fine power (P)

dpwrm First decoupler linear modulator power (P)

Applicability: Systems with a first decoupler linear modulator.
The fine power control is linear and spans 0 to dpwr.

Values: 0 to 4095 (where 4095 is maximum power). If dpwrm does not exist in the parameter table, a value of 4095 is assumed.

See also: *User Programming; User Guide: Solids; CP/MAS Installation*

Related: [dpwrm2](#) Second decoupler linear modulator power (P)
[dpwrm3](#) Third decoupler linear modulator power (P)
[tpwrm](#) Observe transmitter linear modulator power (P)

dpwrm2 Second decoupler linear modulator power (P)

Applicability: Systems with a second decoupler linear modulator.

Description: Controls the second decoupler linear modulator systems.

Values: 0 to 4095 (where 4095 is maximum power). If dpwrm2 does not exist in the parameter table, a value of 4095 is assumed.

See also: *User Programming*

Related: [dpwrm](#) First decoupler linear modulator power (P)

dpwrm3 Third decoupler linear modulator power (P)

Applicability: Systems with a third decoupler linear modulator.

Description: Controls the third decoupler linear modulator systems.

Values: 0 to 4095 (where 4095 is maximum power). If dpwrm3 does not exist in the parameter table, a value of 4095 is assumed.

See also: *User Programming*

Related: [dpwrm](#) First decoupler linear modulator power (P)

Dqcosy Convert the parameter to a DQCOSY experiment (M)

Description: Convert the parameter to a double-quantum filtered (DQCOSY) experiment

See also: *NMR Spectroscopy User Guide*

Related: [cosyps](#) Set up parameters for phase-sensitive COSY (M)
[Cosy](#) Set up parameters for COSY pulse sequence (M)
[relayh](#) Set up parameters for COSY pulse sequence (M)

draw Draw line from current location to another location (C)

Syntax: `draw(<'keywords'>x,y)`

Description: Draws a line from the current location to the absolute location with coordinates given by the arguments.

Arguments: 'keywords' identifies the output device ('graphics' | 'plotter'), drawing mode ('xor' | 'normal'), and drawing capability ('newovly' | 'ovly' | 'ovlyC').

- 'graphics' | 'plotter' is a keyword for the output device. The default is 'plotter'. The output selected is passed to subsequent [pen](#), [move](#), or [draw](#) commands and remains active until a different output is specified.

- 'xor', 'normal' is a keyword for the drawing mode when using the 'graphics' output device. The default is 'normal'. In the 'xor' mode, if a line is drawn such that one or more points of the line are in common with a previous 'xor' line, the common points are erased. In the normal mode, the common points remain. The mode selected is passed to subsequent draw, pen, and move commands and remains active until a different mode is specified.
- 'newovly', 'ovly', and 'ovlyC' are keywords that specify an interactive drawing capability that is slightly slower than the 'xor' mode but more consistent in color. 'newovly' clears any previous draws, boxes, and writes made with the 'ovly' modes and draws the figure. 'ovly' draws without clearing so that multisegment figures can be created. 'ovlyC' clears without drawing.

x, y are the absolute coordinates, in mm, of the endpoint of the line to be drawn. The range of x is 0 at the left edge of the chart and wcm_{max} at the right edge. The range of y is -20 at the bottom of the chart and wc2_{max} at the top.

Examples: `draw('graphics', 'xor'.wcmmax-sc, vp+th)`
`draw(wcmmax-sc-wc*(cr-delta-sp)/wp, wc2max)`

See also: *NMR Spectroscopy User Guide*

Related:	gin	Return current mouse position and button values (C)
	move	Move to an absolute location (C)
	pen	Select a pen or color for drawing (C)
	wcm _{max}	Maximum width of chart (P)
	wc2 _{max}	Maximum width of chart in second direction (P))

dres Measure linewidth and digital resolution (C)

Syntax: `dres(<freq<, fractional_height>>) >`
`:linewidth, digital_resolution`

Description: Analyzes the line defined by the current cursor position for its linewidth (width at half-height) and digital resolution.

Arguments: freq is the frequency of the line. The default is the parameter cr. This overrides using the current cursor position as the frequency.

fractional_height is the linewidth is measured at this height.

linewidth is the value returned for the linewidth of the line.

digital_resolution is the value returned for the digital resolution of the line.

Examples: `dres:$width, $res`
`dres(cr, 0.55)`

See also: *NMR Spectroscopy User Guide; User Programming*

Related:	cr	Current cursor position (P)
	dsn	Measure signal-to-noise (C)

dres Tip-angle resolution for first decoupler (P)

Applicability: Systems with waveform generators.

Description: Controls the tip-angle resolution to be used within a waveform generator decoupling sequence on the first decoupler. The optimum value is a function of the decoupling sequence to be used: for WALTZ-16, dres=90.0; for MLEV16-240, dres=30.0; and for GARP1, dres=1.0.

Values: 1.0 to 90.0, in units of degrees. In reality, `dres` can assume values as small of 0.7 (but no smaller) and can be specified in units of 0.1°. To use this capability, change the limits of `dres` by using `destroy('dres')`
`create('dres','real') setlimit('dres',360,0.7,0.1)`.
 Making corresponding changes within the `fixpar` macro ensures that `dres` is created in the desired way with each new parameter set.

See also: *NMR Spectroscopy User Guide*

Related: `dmfadj` Adjust decoupler tip-angle resolution time (M)
`dres2` Tip angle resolution for second decoupler (P)
`dres3` Tip angle resolution for third decoupler (P)
`fixpar` Correct parameter characteristics in experiment (M)

dres2 Tip-angle resolution for second decoupler (P)

Applicability: Systems with waveform generators.

Description: Controls the tip-angle resolution to be used within a waveform generator decoupling sequence on the second decoupler. The optimum value is a function of the decoupling sequence to be used: for WALTZ-16, `dres2=90.0`; for MLEV16-240, `dres2=30.0`; and for GARP1, `dres2=1.0`.

Values: 1.0 to 90.0, in units of degrees.

See also: *NMR Spectroscopy User Guide*

Related: `dmf2adj` Adjust second decoupler tip-angle resolution time (M)
`dres` Tip-angle resolution for first decoupler (P)

dres3 Tip-angle resolution for third decoupler (P)

Applicability: Systems with waveform generators.

Description: Controls the tip-angle resolution to be used within a waveform generator decoupling sequence on the third decoupler. The optimum value is a function of the decoupling sequence to be used: for WALTZ-16, `dres3=90.0`; for MLEV16-240, `dres3=30.0`; and for GARP1, `dres3=1.0`.

Values: 1.0 to 90.0, in units of degrees.

See also: *NMR Spectroscopy User Guide*

Related: `dmf3adj` Adjust third decoupler tip-angle resolution time (M)
`dres` Tip-angle resolution for first decoupler (P)

dres4 Tip-angle resolution for fourth decoupler (P)

Applicability: Systems with deuterium decoupler channel as the fourth decoupler.

Description: Controls the tip-angle resolution to be used for the decoupling sequence on the fourth decoupler. The optimum value is a function of the decoupling sequence to be used: for WALTZ-16, `dres4=90.0`; for MLEV16-240, `dres4=30.0`; and for GARP1, `dres4=1.0`.

Values: 1.0 to 90.0, in units of degrees.

See also: *NMR Spectroscopy User Guide*

Related: `dmf4adj` Adjust fourth decoupler tip-angle resolution time (M)
`dres` Tip-angle resolution for first decoupler (P)

ds**Display a spectrum (C)**

Syntax: (1) `ds<(index)>`
 (2) `ds<(options)>`

Description: Displays a single spectrum. Parameter `intmod` controls integral display:

- `intmod='off'` turns off the integral display
- `intmod='full'` displays the entire integral
- `intmod='partial'` displays every other integral region

Parameter entry after a spectrum has been displayed with the `ds` command causes the spectrum to be updated.

Two additional parameters control the behavior of the `ds` command:

- The parameter `phasing` (in the “global” parameter set) controls the percentage of the spectrum updated during interactive phasing. This parameter can be set in the range of 10 to 100. A value of 100 causes the entire spectrum to be updated. A value of 20 causes the area between the two horizontal cursors to be updated.
- The parameter `lvltlt` (in the “current” parameter set) controls the sensitivity of the interactive `lv1` and `tlt` adjustments. `lvltlt` can be set to any positive real number. It is basically a multiplier for the sensitivity. The default value is 1.0. Larger values make the adjustments larger. Smaller values make the adjustments smaller.

For arrayed 1D spectra or for 2D spectra, a particular trace can be viewed by supplying the index number as an argument. For 2D data sets, spectra can be displayed from either the f_1 or f_2 domain by setting the parameter `trace` equal to `'f1'` or `'f2'`, respectively. After entering `ftld`, interferograms can be viewed by setting `trace='f1'` and then typing `ds`.

Spectra are scaled according to the number of completed transients `ct`. If `nt` is arrayed (`nt=1, 2, 4, 8`), each spectrum is scaled by its own `ct`.

Arguments: `index` (used with syntax 1) is the index number of a particular trace to be displayed in arrayed 1D spectra or in 2D spectra (syntax 1).

`options` (used with syntax 2) is any of the following keywords:

- `'toggle'` switches between the box and the cursor modes.
- `'restart'` redraws the cursor if it has been turned off.
- `'expand'` toggles between expanded and full view of the spectrum.
- `'spwp'` interactively adjusts start and width of the spectrum display.
- `'phase'` enters an interactive phasing mode.
- `'thresh'` interactively adjusts the threshold.
- `'z'` interactively sets integral resets.
- `'dscale'` toggles the scale below the spectrum on and off.
- `'lvltlt'` interactively adjusts the `lv1` and `tlt` parameters.
- `'scwc'` interactively adjusts the start and width of chart.
- `'noclear'` start or restart the `ds` display without clearing the graphics screen
- `'exists'` exit the `ds` display, leaving a non-interactive `dss` display.

Examples: `ds`
`ds(7)`
`ds('restart')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>crmode</code>	Current state of cursors in <code>dfid</code> , <code>ds</code> , or <code>dcon1</code> (P)
	<code>ct</code>	Completed transients (P)
	<code>exists</code>	
	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>intmod</code>	Integral display mode (P)
	<code>lp</code>	First-order phase in directly detected dimension (P)
	<code>lv1</code>	Zero-order baseline correction (P)
	<code>lv1tlt</code>	Control sensitivity of <code>lv1</code> and <code>tlt</code> adjustments (P)
	<code>nt</code>	Number of transients (P)
	<code>phasing</code>	Control update region during <code>ds</code> phasing (P)
	<code>rp</code>	Zero-order phase in directly detected dimension (P)
	<code>select</code>	Select a spectrum without displaying it (C)
	<code>tlt</code>	First-order baseline correction (P)
	<code>trace</code>	Mode for n-dimensional data display (P)
	<code>wft1d</code>	Weight and Fourier transform f_2 for 2D data (C)

ds2d Display 2D spectra in whitewash mode (C)

Syntax: `ds2d<(options)>`

Description: Displays a stacked plot of 2D spectra in whitewash mode (after the first spectra, each spectra is blanked out in regions in which it is behind an earlier spectra). Color does not represent intensity (unlike `dcon`), because intensity can be seen visually, but instead successive traces are displayed in different colors so that color represents frequency.

Arguments: `options` can be any of the following keywords:

- '`nobase`' is a keyword to activate the `th` parameter to suppress all intensity below the `th` level.
- '`fill`' is a keyword to fill in the peaks. When using '`fill`', `th` operates linearly and not logarithmically (factors of 2) as it does in the contour or color intensity displays.
- '`fillnb`' is a keyword to combine base suppression and peak filling. When using '`fillnb`', `th` operates linearly and not logarithmically (factors of 2) as it does in the contour or color intensity displays.
- '`noaxis`' is a keyword to omit outlining the display and drawing the horizontal and vertical axis.

Examples: `ds2d`
`ds2d('fillnb')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dcon</code>	Display noninteractive color intensity map (C)
	<code>dcon1</code>	Control display selection for the <code>dcon1</code> program (P)
	<code>ds2dn</code>	Display 2D spectra in whitewash mode without screen erase (C)
	<code>pl2d</code>	Plot 2D spectra in whitewash mode (C)
	<code>th</code>	Threshold (P)

ds2dn Display 2D spectra in whitewash mode without screen erase (C)

Syntax: `ds2dn<(options)>`

Description: Displays a stacked plot of 2D spectra in whitewash mode (after the first spectra, each spectra is blanked out in regions in which it is behind an earlier spectra) the same as `ds2d` but without erasing the screen before drawing. The arguments are the same as `ds2d`.

D

Examples: `ds2dn`
`ds2dn('fillnb')`

See also: *NMR Spectroscopy User Guide*

Related: `ds2d` Display 2D spectra in whitewash mode (C)

dsnarray Report statistical signal-to-noise for Cold Probes (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Report the statistical S/N of a series of repeated gNhsqc data sets acquired with a labeled protein sample.

dscale Display scale below spectrum or FID (C)

Syntax: `dscale(<rev><, axis><, label><, vp0><, sp0><, color><, pen>)` >

Description: Displays a scale under a spectrum or FID.

Arguments: `rev` – reverses the direction of the scale. That is, the smaller numbers will be at the left side of the scale. If used, 'rev' must be the first argument.

`axis` – If the letter p, h, k, etc. is supplied, it will be used instead of the current value of the parameter `axis`. For an FID scale, if the letter s, m, or u is supplied, it will be used instead of the current value of the parameter `axisf`.

`label` – If a string of 2 or more characters is supplied, it will be used as the axis label.

`vp0` – This is supplied as the first real number. It defines the vertical position where the scale is drawn. The default is 5 mm below the current value of the parameter `vp`.

`sp0` – This is supplied as the second real number. It is a modified start of plot. If, for example, the display is from 347 to 447 hz, but the scale is desired to read 0 to 100 hz., `sp0` would be input as 0.

`wp0` – This is supplied as the third real number. It is a modified width of plot. If, for example, the display is from 347 to 447 hz, but the scale is desired to read 0 to 550 Units. `sp0` would be input as 0, `wp0` would be 550, and the label would be 'Units'.

An optional color or pen number can be supplied to `dscale` or `pscale`. The available colors and pens are: 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'black', 'white', 'pen1', 'pen2', 'pen3', ..., 'pen8'

Examples: `dscale`
`dscale('rev')`
`dscale('h', 0, 'green')`
`dscale('h', vp-10, 0)`

See also: *NMR Spectroscopy User Guide*

Related: `axis` Axis label for displays and plots (P)
`axisf` Axis label for FID displays and plots (P)
`pscale` Plot scale below spectrum or FID (C)
`vp` Vertical position of spectrum (P)

dscoef Digital filter coefficients for downsampling (P)

Description: Specifies the number of coefficients used in the digital filter. This parameter does not need to be changed as the parameter `downsamp` is changed, because `dscoef` is automatically adjusted by VnmrJ to give filter cutoffs that are the same, regardless of the value of `downsamp`. This is done by using

`dscoef*downsamp/2` coefficients in the digital filter. VnmrJ always rounds `dscoef*downsamp/2` to an odd number. If `dscoef` does not exist in the current experiment, enter `addpar('downsamp')` to add it. Entering `addpar('downsamp')` creates the digital filtering and downsampling parameters `downsamp`, `dscoef`, `dsfb`, `dsfsfrq`, and `filtfile`.

Values: Number of digital filter coefficients. The default is 61. A larger number of coefficients gives a filter with sharper cutoffs; a smaller number gives a filter with more gradual cutoffs.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to current experiment (M)
	<code>downsamp</code>	Downsampling factor applied after digital filtering (P)
	<code>dsfb</code>	Digital filter bandwidth for downsampling (P)
	<code>dsfsfrq</code>	Bandpass filter offset for downsampling (P)
	<code>filtfile</code>	File of FIR digital filter coefficients (P)
	<code>pards</code>	Create additional parameters used for downsampling (M)

dseq **Decoupler sequence for first decoupler (P)**

Applicability: Systems with waveform generators.

Description: Specifies the decoupling sequence (without the `.DEC` file extension) to be used during any period of programmable decoupling on the first decoupler under status control (i.e., `dmm='p'`). The decoupling sequence must be located in the user's `shapelib` directory or in the VnmrJ system's `shapelib` directory.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dmm</code>	Decoupler modulation mode for first decoupler (P)
	<code>dseq2</code>	Decoupler sequence for second decoupler (P)
	<code>dseq3</code>	Decoupler sequence for third decoupler (P)

dseq2 **Decoupler sequence for second decoupler (P)**

Applicability: Systems with waveform generators.

Description: Specifies the decoupling sequence (without the `.DEC` file extension) to be used during any period of programmable decoupling on the second decoupler under status control (i.e., `dmm2='p'`). The decoupling sequence must be located in the user's `shapelib` directory or in the VnmrJ system `shapelib` directory.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dmm2</code>	Decoupler modulation mode for second decoupler (P)
	<code>dseq</code>	Decoupler sequence for first decoupler (P)

dseq3 **Decoupler sequence for third decoupler (P)**

Applicability: Systems with waveform generators.

Description: Specifies the decoupling sequence (without the `.DEC` file extension) to be used during any period of programmable decoupling on the third decoupler under status control (i.e., `dmm3='p'`). The decoupling sequence must be located in the user's `shapelib` directory or in the `shapelib` directory.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dmm3</code>	Decoupler modulation mode for third decoupler (P)
	<code>dseq</code>	Decoupler sequence for first decoupler (P)

D

dseq4 Decoupler sequence for fourth decoupler (P)

Applicability: Systems with waveform generators.

Description: Specifies the decoupling sequence (without the .DEC file extension) to be used during any period of programmable decoupling on the third decoupler under status control (i.e., `dmm4 = 'p'`). The decoupling sequence must be located in the user's `shapelib` directory or in the system's `shapelib` directory.

See also: *NMR Spectroscopy User Guide*

Related: `dmm4` Decoupler modulation mode for third decoupler (P)
`dseq` Decoupler sequence for first decoupler (P)

dsfb Digital filter bandwidth for downsampling (P)

Description: Specifies the bandwidth of the digital filter used for downsampling. If `dsfb` does not exist in the current experiment, enter `addpar('downsamp')` to add it. `addpar('downsamp')` creates the digital filtering and downsampling parameters `downsamp`, `dscoef`, `dsfb`, `dsfsfrq`, and `filtfile`.

Values: Number, in Hz. A smaller value rejects frequencies at the spectrum edges; a larger value aliases noise and signals at frequencies outside of $\pm sw/2$.

'n' makes `dsfb` default to the final `sw/2`.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to current experiment (M)
`downsamp` Downsampling factor applied after digital filtering (P)
`dscoef` Digital filter coefficients for downsampling (P)
`dsfsfrq` Bandpass filter offset for downsampling (P)
`filtfile` File of FIR digital filter coefficients (P)
`pards` Create additional parameters used for downsampling (M)
`sw` Spectral width in directly detected dimension (P)

dshape Display pulse shape or modulation pattern (M)

Syntax: `dshape<(pattern.ext)>`

Description: Displays the real (X) and imaginary (Y) components of a shaped pulse. Any type of waveform (.RF, .DEC or .GRD) can be displayed.

Arguments: `pattern` is the name of a shape or pattern file specified by an absolute file name, relative file name, or a simple pattern file name. `ext` is a file name extension that specifies the file type. In the case of a simple file name, `dshape` searches for the file in the local directory, then in the user's `shapelib`, and finally in the directory `/vnmr/shapelib`. If `pattern.ext` is not given, `dshape` displays the last created waveform stored in the `pbox.fid` file.

Examples: `dshape`
`dshape('Pbox.RF')`

See also: *NMR Spectroscopy User Guide*

Related: `Pbox` Pulse shaping software (U)
`pshape` Plot pulse shape or modulation pattern (M)

dshapef Display last generated pulse shape (M)

Description: Displays the real (X) and imaginary (Y) components of last generated shaped pulse, stored in `pbox.fid` file.

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)
[pshapef](#) Plot last generated pulse shape (M)

dshapei Display pulse shape or modulation pattern interactively (M)

Syntax: `dshapei<(pattern.ext)>`

Description: Displays the real (X) and imaginary (Y) components of a pulse shape, modulation pattern or gradient shape interactively. `dshapei` overwrites the existing data (FID) after the permission is granted by the user. It also asks for the duration of the waveform and displays the timescale.

Arguments: `pattern` is the name of a shape or pattern file specified by an absolute file name, relative file name, or a simple pattern file name. `ext` is a file name extension that specifies the file type. In the case of a simple file name, `dshapei` searches for the file in the local directory, then in the user's `shapelib`, and finally in the directory `/vnmr/shapelib`. If no file name is given, `dshapei` displays the last created waveform stored in the `pbox.fid` file.

Examples: `dshapei`
`dshapei('myfile.DEC')`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

dshim Display a shim “method” string (M)

Syntax: (1) `dshim<(file)>`
 (2) `dshim('method'|'help')`

Description: Looks in the user's `shimmethods` directory and then in the system `shimmethods` directory for a file and displays the file (syntax 1) or displays information about `method` strings (syntax 2).

Arguments: `file` is the name of a file to be searched for in the `shimmethods` directories. The default is to display the contents of the `shimmethods` directories.
`'method'` is a keyword to explain the structure of `method` strings.
`'help'` is a keyword to describe the `method` strings in the system's `shimmethods` directory.

Examples: `dshim`
`dshim('method')`
`dshim('help')`

See also: *NMR Spectroscopy User Guide*

Related: [method](#) Autoshim method (P)
[newshm](#) Interactively create a shim “method” with options (M)
[shim](#) Submit an Autoshim experiment to acquisition (C)
[stdshm](#) Interactively create a shim “method” (M)

dsfsfrq Bandpass filter offset for downsampling (P)

Description: For downsampling, selects a bandpass filter that is not centered about the transmitter frequency. In this way, `dsfsfrq` works much like [lsfrq](#). If `dsfsfrq` does not exist in the current experiment, add it by entering [addpar](#)('downsamp'). The command [addpar](#)('downsamp') creates

the digital filtering and downsampling parameters `downsamp`, `dscoef`, `dsfb`, `dsfsfrq`, and `filtfile`.

Values: A number, in Hz. A positive value selects a region upfield from the transmitter frequency; a negative value selects a downfield region.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to current experiment (M)
`downsamp` Downsampling factor applied after digital filtering (P)
`dscoef` Digital filter coefficients for downsampling (P)
`dsfb` Digital filter bandwidth for downsampling (P)
`filtfile` File of FIR digital filter coefficients (P)
`lsfrq` Frequency shift of the `fn` spectrum in Hz (P)
`movedssw` Set parameters for digital filtering and downsampling (M)
`pards` Create additional parameters used by downsampling (M)

dsn Measure signal-to-noise (C)

Syntax: `dsn<(low_field,high_field)>:signal_to_noise,noise`

Description: Measures the signal-to-noise ratio of the spectrum by first measuring the intensity of the largest peak in the spectral range defined by `sp` and `wp`, and then measuring the noise in the spectral region defined by the position of the two cursors. The noise value returned from `dsn` is not scaled by `vs`. The interrelations between the signal-to-noise ratio, the noise, and peak intensities can be illustrated by comparing `dsn:$sn`, `$noise` and `peak:$signal`. In this case, `$sn` is equal to $(\$signal / \$noise) / vs$.

Calculate noise by first doing a drift correction on the noise region. Noise is defined as:

$$noise = \left(\sum_{i=1}^{np} Y_i^2 / np \right)^{\frac{1}{2}}$$

Y_i^2 values are the square of the drift-corrected amplitude and `np` is the number of points in the noise region.

Arguments: `low_field` and `high_field` are the upper and lower frequencies of the noise region to be measured. The default is the position of the two cursors.

`signal_to_noise` is the calculated value of signal-to-noise ratio.

`noise` is the noise value measured within the defined spectral region.

Examples: `dsn:$ston`
`dsn(sp+sp, sp+wp-100)`
`dsn(10000, 8000):r1`

See also: *User Programming*

Related: `dres` Measure linewidth and digital resolution (C)
`peak` Find tallest peak in specified region (C)
`sp` Start of plot (P)
`vs` Vertical scale (P)
`wp` Width of plot (P)

dsnmax Calculate maximum signal-to-noise (M)

Syntax: `dsnmax<(noise_region)>`

Description: Finds the best signal-to-noise in a specified region.

Arguments: `noise_region` is the size, in Hz, of the region. The default is the region between the cursors as defined by the parameter `delta`.

Examples: `dsnmax`
`dsnmax(400)`

See also: *User Programming*

Related: `delta` Cursor difference in directly detected dimension (P)

dsp **Display calculated spectrum (C)**

Syntax: `dsp<(file<, 'nods'>)>`

Description: Using the current table of transitions and intensities, `dsp` recalculates the simulated spectrum (using the current value for the linewidth `slw`) and displays the spectrum. `dsp` can only be used after the `spins` program has been run. If only the linewidth `slw` or vertical scale `svs` have been changed, `dsp` can be used to redisplay the spectrum. If a chemical shift or coupling constant has been changed, however, `dsp` will not display a spectrum reflecting the changes in the parameter; `spins` must be run again to recalculate the new spectrum.

The number of points in the calculated spectrum is `fn/2`. To increase the number of points, change `fn` and rerun `dsp` without doing a transform.

To display a synthetic spectrum, prepare a file in the following format:

```
Freq1, Intens1, LineWidth1, GaussFrac1
Freq2, Intens2, LineWidth2, GaussFrac2
...
FreqN, IntensN, LineWidthN, GaussFracN
```

The units for frequency and line width are Hz. The Gaussian fraction, which is the percentage of the line shape that is Gaussian (the rest is Lorentzian) should be between 0 and 1 (i.e., 0 is pure Lorentzian, 1 is pure Gaussian). Units for intensity are not particularly important. Given numbers in a file `myshape`, it is only necessary to enter `dsp('myshape')` to display the synthetic spectrum. This approach is often preferred over deconvolution for quantifying small shoulders on large peaks.

Arguments: `file` is the name of a file containing spectral information that displays the result of a spectrum deconvolution. Any file in the proper format can be used to generate a display. The default is the file `spins.outdata` in the experiment directory. This file contains information about frequencies, intensities, line widths, and Gaussian/Lorentzian fractions.

'`nods`' is a keyword for `dsp` to recalculate the simulated spectrum but not to display the spectrum. The spectrum can be displayed with the `ds` or `dss` command.

Examples: `dsp`
`dsp('fitspec.outpar')`

See also: *NMR Spectroscopy User Guide*

Related: `ds` Display a spectrum (C)
`dss` Display stacked spectra (C)
`fn` Fourier number in directly detected dimension (P)
`slw` Spin simulation linewidth (P)
`spins` Perform spin simulation calculation (C)
`svs` Spin simulation vertical scale (P)

dsp **Type of DSP for data acquisition (P)**

Description: Selects the type of DSP (digital signal processing) for data acquisition:

- *Inline DSP* performs digital filtering and downsampling on the workstation immediately after each oversampled FID is transferred from the console. **sw** and **at** should be set to the values desired for the final spectrum. Only the digital filtered and downsampled data is written to the disk. Selective detection of a region of a spectrum is available using the **moveossw** macro.
- *Real-time DSP* uses optional hardware (not available on all systems) to filter the data prior to summing to memory. Real-time DSP is not compatible with pulse sequences that use explicit acquisition to acquire less than the full number of data points (**np**) in a single acquire statement (e.g., solids sequences such as BR24 and FLIPFLOP).

If either type is active, the filter bandwidth parameter **fb** is not active. The actual analog filter is active and is automatically set by the software to a value that matches $(sw/2) * oversamp$ as closely as possible.

Another type of DSP is available that allows post-processing of data. See the description of the **pards** macro for details.

Values: 'i' selects inline DSP and calls **addpar**('oversamp') to create the DSP parameters **def_osfilt**, **filtfile**, **oscoef**, **osfb**, **osfilt**, **oslsfrq**, and **oversamp**. A value of **oversamp** greater than 1 causes the next experiment run to be oversampled, digitally filtered, and downsampled back to the selected **sw** prior to saving it to disk.

'r' selects real-time DSP and calls the macro **addpar**('oversamp') to create the DSP parameters **def_osfilt**, **filtfile**, **oscoef**, **osfb**, **osfilt**, **oslsfrq**, and **oversamp** (although only **oversamp** and **osfilt** are user adjustable for real-time DSP). Use **dsp='r'** only if the optional DSP hardware is present in the system. Set **fsq='y'** to use frequency-shifted quadrature detection.

'n' (or parameter **dsp** is not present) disables both types of DSP. Set **dsp='n'** if you wish to turn off DSP on a permanent or semi-permanent basis. To turn off DSP within just a single experiment, set **oversamp='n'**.

See also: *NMR Spectroscopy User Guide*

Related:	addpar	Add selected parameters to current experiment (M)
	at	Acquisition time (P)
	def_osfilt	Default value of osfilt (P)
	fb	Filter bandwidth (P)
	filtfile	File of FIR digital filter coefficients (P)
	fsq	Frequency-shifted quadrature detection (P)
	il	Interleave arrayed and 2D experiments (P)
	moveossw	Set oversampling parameters for selected spectral region (M)
	np	Number of data points (P)
	oscoef	Digital filter coefficients for oversampling (P)
	osfb	Digital filter bandwidth for oversampling (P)
	osfilt	Oversampling filter for real-time DSP (P)
	oslsfrq	Bandpass filter offset for oversampling (P)
	oversamp	Oversampling factor for acquisition (P)
	pards	Create additional parameters used by downsampling (M)
	paros	Create additional parameters used by oversampling (M)
	ra	Resume acquisition stopped with sa command (C)
	sa	Stop acquisition (C)
	sw	Spectral width in the directly detected dimension (P)

dsplanes **Display a series of 3D planes (M)**

Syntax: `dsplanes(start_plane, stop_plane)`

Description: Produces a graphical 2D color or contour map for a subset of 3D planes. The `dconi` program is used to display the planes.

Arguments: `start_plane` specifies the number of the 3D plane with which display is to begin. It must be greater than 0.

`stop_plane` specifies the number of the 3D plane with which the display is to end. If `start_plane` is greater than `stop_plane`, only the first plane, whose number is `start_plane`, is plotted. The range of `stop_plane` depends on the value of the parameter `plane` as follows:

- If `plane='f1f3'`, range of `stop_plane` is between 0 and `fn2/2`
- If `plane='f2f3'`, range of `stop_plane` is between 0 and `fn1/2`
- If `plane='f1f2'`, range of `stop_plane` is between 0 and `fn/2`

Examples: `dsplanes(1, 3)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dconi</code>	Interactive 2D data display (C)
	<code>dplane</code>	Display a 3D plane (M)
	<code>dproj</code>	Display a 3D plane projection (M)
	<code>getplane</code>	Extract planes from 3D spectral data set (M)
	<code>nextpl</code>	Display the next 3D plane (M)
	<code>plane</code>	Currently displayed 3D plane type (P)
	<code>plplanes</code>	Plot a series of 3D planes (M)
	<code>prevpl</code>	Display the previous 3D plane (M)

dsptype **Type of DSP (P)**

Description: Indicates the existence of digital signal processing (DSP).

Values: 0 indicates no digital signal processing. 1 indicates DSP exists.

Examples: `dsptype?=0` `dsptype?=1`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dsp</code>	Type of DSP for data acquisition (P)

dss **Display stacked spectra (C)**

Syntax: `dss(<start, finish<, step>><, options>)>`

Description: Displays one or more spectra on the screen.

The display is not interactive like the command `ds`. Integral display is controlled by the parameter `intmod` when a single spectrum is displayed (see 'int' option below). The following values are accepted for `intmod`:

- `intmod='off'` turns off the integral display.
- `intmod='full'` displays the entire integral.
- `intmod='partial'` displays every other integral region.

An individual trace is displayed from and arrayed 1D spectra or 2D spectra by supplying the index number as an argument. Spectra from 2D data set are displayed from either the f_1 or f_2 domain by setting the parameter `trace` equal to 'f1' or 'f2', respectively. Enter `ft1d`, `trace='f1'`, and `dss` to view the interferogram. Multiple spectra are displayed by supplying indexes of the first and last spectra.

The position of the first spectrum is governed by the parameters **wc**, **sc**, and **vp**. For 1D data, subsequent spectra are positioned relative to the preceding spectrum by the parameters **vo** (vertical offset) and **ho** (horizontal offset). For 2D data, **ho** defines the total horizontal offset between the first and last spectrum. Also for 2D data, **vo** is inactive while the parameter **wc2** defines the total vertical offset between the first and last spectrum.

The parameter **cutoff**, if it exists and is active, defines the distance above and below the current vertical position **vp** at which peaks are truncated. By arraying **cutoff** to have two different values, the truncation limits above and below the current vertical position can be controlled independently. For example, **cutoff=50** truncates peaks at **vp+50** mm and **vp-50** mm. **cutoff=50, 10** truncates peaks at **vp+50** mm and **vp-10** mm.

Arguments: **start** is the index of the first spectra when displaying multiple spectra. It is also the index number of a particular trace to be viewed when displaying arrayed 1D spectra or 2D spectra.

finish is the index of the last spectra when displaying multiple spectra. Since the parameter **arraydim** is automatically set to the total number of spectra, it can be used to set **finish** to include all spectra (e.g., **dss(1, arraydim, 3)**).

step is the increment for the spectral index when displaying multiple spectra. The default is 1.

options can be any of the following:

- 'all' is a keyword to display all of the spectra.
- 'int' is a keyword to display only the integral, independently of the value of the parameter **intmod**
- 'top' or 'side' are keywords that cause the spectrum to be displayed either above or at the left edge, respectively, of a contour plot. This assumes that the parameters **sc**, **wc**, **sc2**, and **wc2** are those used to position the contour plot.
- 'dodc' is a keyword for all spectra to be drift corrected independently.
- 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'black', and 'white' are keywords that select a color.
- 'pen1', 'pen2', 'pen2' ... are keywords that pens.
- 'nopars' — prevents the display commands from drawing the parameters at the bottom of the graphics screen.
- 'custom' — uses the parameters **shownumx** (x position) and **shownumy** (y position), counting from bottom left of every spectrum.
- 'reverse' — rotate the text by 90° - useful if the arrayed parameter values are long with respect to the width of the individual sub-spectra.
- 'value' — The values of up to two simultaneous arrays are displayed. Diagonal arrays are allowed. The second parameter is shown in different color). The name of the arrayed parameter(s) is also shown. If used on a one-dimensional array representation of a 2D spectrum, **ni** and **phase** (in case of phase sensitive 2Ds) parameters are shown.

Examples: **dss(1, 3)**
dss(1, 12, 3, 'green')

See also: *NMR Spectroscopy User Guide*

Related:	cutoff	Data truncation limit (P)
	dssa	Display stacked spectra automatically (C)
	dssan	Display stacked spectra automatically without erasing (C)
	dssh	Display stacked spectra horizontally (C)

<code>dsshn</code>	Display stacked spectra horizontally without erasing (C)
<code>dssn</code>	Display stacked spectra without screen erase (C)
<code>dsww</code>	Display spectra in whitewash mode (C)
<code>ft1d</code>	Fourier transform along f_2 dimension (C)
<code>ho</code>	Horizontal offset (P)
<code>intmod</code>	Integral display mode (P)
<code>pl</code>	Plot spectra (C)
<code>plww</code>	Plot spectra in whitewash mode (C)
<code>sc</code>	Start of chart (P)
<code>sc2</code>	Start of chart in second direction (P)
<code>shownumx</code>	x position counting from bottom left of every spectrum (P)
<code>shownumy</code>	y position counting from bottom left of every spectrum (P)
<code>trace</code>	Mode for 2D data display (P)
<code>vo</code>	Vertical offset (P)
<code>vp</code>	Vertical position of spectrum (P)
<code>wc</code>	Width of chart (P)
<code>wc2</code>	Width of chart in second direction (P)

dssa**Display stacked spectra automatically (C)**

Syntax: `dssa(<start, finish<, step>><, options>)>`

Description: Displays one or more spectra automatically.

Integral display is controlled by the parameter `intmod` when a single spectrum is displayed (see 'int' option below). The following values are accepted for `intmod`:

- `intmod='off'` turns off the integral display.
- `intmod='full'` displays the entire integral.
- `intmod='partial'` displays every other integral region.

An individual trace is displayed from and arrayed 1D spectra or 2D spectra by supplying the index number as an argument. Spectra from 2D data set are displayed from either the f_1 or f_2 domain by setting the parameter `trace` equal to 'f1' or 'f2', respectively. Enter `ft1d`, `trace='f1'`, and `dss` to view the interferogram. Multiple spectra are displayed by supplying indexes of the first and last spectra.

The position of the first spectrum is governed by the parameters `wc`, `sc`, and `vp`. For 1D data, subsequent spectra are positioned relative to the preceding spectrum by the parameters `vo` (vertical offset) and `ho` (horizontal offset). For 2D data, `ho` defines the total horizontal offset between the first and last spectrum.

Also for 2D data, `vo` is inactive while the parameter `wc2` defines the total vertical offset between the first and last spectrum. To display spectra “automatically,” the command `dssa` adjusts the parameters `vo` and `ho` to fill the screen in a lower left to upper right presentation (`wc` must be set to less than full screen width for this to work)

The parameter `cutoff`, if it exists and is active, defines the distance above and below the current vertical position `vp` at which peaks are truncated. By arraying `cutoff` to have two different values, the truncation limits above and below the current vertical position can be controlled independently. For example, `cutoff=50` truncates peaks at `vp+50` mm and `vp-50` mm. `cutoff=50, 10` truncates peaks at `vp+50` mm and `vp-10` mm.

Arguments: `start` is the index of the first spectra when displaying multiple spectra. It is also the index number of a particular trace to be viewed when displaying arrayed 1D spectra or 2D spectra.

`finish` is the index of the last spectra when displaying multiple spectra.

step is the increment for the spectral index when displaying multiple spectra. The default is 1.

options can be any of the following:

- 'all' is a keyword to display all of the spectra.
- 'int' is a keyword to only display the integral, independently of the value of the parameter `intmod`
- 'dodc' is a keyword for all spectra to be drift corrected independently.
- 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'black', and 'white' are keywords that select a color.
- 'pen1', 'pen2', 'pen2' ... are keywords that pens.
- 'nopars' — prevents the display commands from drawing the parameters at the bottom of the graphics screen.

Examples: `dssa(1,3)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>cutoff</code>	Data truncation limit (P)
	<code>dss</code>	Display stacked spectra (C)
	<code>dssan</code>	Display stacked spectra automatically without erasing (C)
	<code>dssh</code>	Display stacked spectra horizontally (C)
	<code>dsshn</code>	Display stacked spectra horizontally without erasing (C)
	<code>dssn</code>	Display stacked spectra without screen erase (C)
	<code>dsww</code>	Display spectra in whitewash mode (C)
	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>ho</code>	Horizontal offset (P)
	<code>intmod</code>	Integral display mode (P)
	<code>pl</code>	Plot spectra (C)
	<code>plww</code>	Plot spectra in whitewash mode (C)
	<code>sc</code>	Start of chart (P)
	<code>sc2</code>	Start of chart in second direction (P)
	<code>shownumx</code>	x position counting from bottom left of every spectrum (P)
	<code>shownumy</code>	y position counting from bottom left of every spectrum (P)
	<code>trace</code>	Mode for 2D data display (P)
	<code>vo</code>	Vertical offset (P)
	<code>vp</code>	Vertical position of spectrum (P)
	<code>wc</code>	Width of chart (P)
	<code>wc2</code>	Width of chart in second direction (P)

dssan Display stacked spectra automatically without erasing (C)

Syntax: `dssan(<start, finish<, step>><, options>)` >

Description: Functions the same as the command `dssa` except the graphics window is not erased before starting the display. This allows composite displays of many spectra to be created. The arguments are the same as `dssa`.

Examples: `dssan(1,3)`

See also: *NMR Spectroscopy User Guide*

Related: `dssa` Display stacked spectra automatically (C)

dssh Display stacked spectra horizontally (C)

Syntax: `dssh(<start, finish<, step>><, options>)` >

Description: Displays one or more spectra horizontally.

Integral display is controlled by the parameter `intmod` when a single spectrum is displayed (see 'int' option below). The following values are accepted for `intmod`:

- `intmod='off'` turns off the integral display.
- `intmod='full'` displays the entire integral.
- `intmod='partial'` displays every other integral region.

An individual trace is displayed from an arrayed 1D spectra or 2D spectra by supplying the index number as an argument. Spectra from 2D data set are displayed from either the f_1 or f_2 domain by setting the parameter `trace` equal to 'f1' or 'f2', respectively. Enter `ftld, trace='f1'`, and `dss` to view the interferogram. Multiple spectra are displayed by supplying indexes of the first and last spectra.

The position of the first spectrum is governed by the parameters `wc`, `sc`, and `vp`. For 1D data, subsequent spectra are positioned relative to the preceding spectrum by the parameters `vo` (vertical offset) and `ho` (horizontal offset). For 2D data, `ho` defines the total horizontal offset between the first and last spectrum. Also for 2D data, `vo` is inactive while the parameter `wc2` defines the total vertical offset between the first and last spectrum. To display spectra horizontally, the command `dssh` causes `vo` to be set to zero and for `ho`, `sc`, and `wc` to be adjusted to fill the screen from left to right with the entire array.

The parameter `cutoff`, if it exists and is active, defines the distance above and below the current vertical position `vp` at which peaks are truncated. By arraying `cutoff` to have two different values, the truncation limits above and below the current vertical position may be controlled independently. For example, `cutoff=50` truncates peaks at `vp+50` mm and `vp-50` mm, and `cutoff=50,10` truncates peaks at `vp+50` mm and `vp-10` mm.

Arguments: `start` is the index of the first spectra when displaying multiple spectra. It is also the index number of a particular trace to be viewed when displaying arrayed 1D spectra or 2D spectra.

`finish` is the index of the last spectra when displaying multiple spectra.

`step` is the increment for the spectral index when displaying multiple spectra. The default is 1.

`options` can be any of the following:

- 'all' is a keyword to display all of the spectra.
- 'int' is a keyword to only display the integral, independently of the value of the parameter `intmod`
- 'dodc' is a keyword that causes all spectra to be drift corrected independently.
- 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'black', and 'white' are keywords that select a color.
- 'pen1', 'pen2', 'pen2' ... are keywords that pens.
- 'nopars' — prevents the display commands from drawing the parameters at the bottom of the graphics screen.

Examples: `dssh(1,3)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>cutoff</code>	Data truncation limit (P)
	<code>dss</code>	Display stacked spectra (C)
	<code>dssa</code>	Display stacked spectra automatically (C)
	<code>dssan</code>	Display stacked spectra automatically without erasing (C)
	<code>dsshn</code>	Display stacked spectra horizontally without erasing (C)
	<code>dssn</code>	Display stacked spectra without screen erase (C)

<code>dsww</code>	Display spectra in whitewash mode (C)
<code>ft1d</code>	Fourier transform along f_2 dimension (C)
<code>ho</code>	Horizontal offset (P)
<code>intmod</code>	Integral display mode (P)
<code>pl</code>	Plot spectra (C)
<code>plww</code>	Plot spectra in whitewash mode (C)
<code>sc</code>	Start of chart (P)
<code>sc2</code>	Start of chart in second direction (P)
<code>shownumx</code>	x position counting from bottom left of every spectrum (P)
<code>shownumy</code>	y position counting from bottom left of every spectrum (P)
<code>trace</code>	Mode for 2D data display (P)
<code>vo</code>	Vertical offset (P)
<code>vp</code>	Vertical position of spectrum (P)
<code>wc</code>	Width of chart (P)
<code>wc2</code>	Width of chart in second direction (P)

dsshn Display stacked spectra horizontally without erasing (C)

Syntax: `dsshn(<start, finish<, step>><, options>)` >

Description: Functions the same as the command `dssh` except the graphics window is not erased before starting the display. This allows composite displays of many spectra to be created. The arguments are the same as `dssh`.

Examples: `dssh(1, 3)`

See also: *NMR Spectroscopy User Guide*

Related: `dssh` Display stacked spectra horizontally (C)

dssl Label a display of stacked spectra (M)

Syntax: `dssl(<options>)`

Description: Displays a label for each element in a set of stacked spectra. The label is an integer value from 1 up to the number of spectra in the display or the values of parameters up to 2 dimensions.

Labels can appear at incorrect positions if `wysiwyg='n'`. The positions are empirically determined for a large screen display and are not guaranteed to be correct for all displays.

Arguments: `options` control the display (more than one option can be entered as long as the options do not conflict with each other):

- `'center', 'left', 'right', 'top', 'bottom', 'above', and 'below'` are keywords setting the position of the displayed index relative to each spectrum.
- `'custom'` — uses the parameters `shownumx` (x position) and `shownumy` (y position), counting from bottom left of every spectrum.
- `'list=xxx'` produces a display of the values contained in the arrayed parameter `xxx`.
- `'format=yyy'` uses the format `yyy` to control the display of each label. See the `write` command for information about formats.
- `'reverse'` — rotate the text by 90° - useful if the arrayed parameter values are long with respect to the width of the individual sub-spectra.
- `'value'` —The values of up to two simultaneous arrays are displayed. Diagonal arrays are allowed. The second parameter is shown in different color). The name of the arrayed parameter(s) is also shown. If used on a

one-dimensional array representation of a 2D spectrum, ni and phase (in case of phase sensitive 2Ds) parameters are shown.

Examples: `dssl`
`dssl('top','left')`
`dssl('value','format=%3.1f') pssl`

See also: *NMR Spectroscopy User Guide*

Related: `dss` Display stacked spectra (C)
`shownumx` x position counting from bottom left of every spectrum (P)
`shownumy` y position counting from bottom left of every spectrum (P)
`write` Write formatted text to a device (C)

dssn Display stacked spectra without screen erase (C)

Syntax: `dssn(<start,finish<,step>><,options>)>`

Description: Functions the same as the command `dss` except the graphics window is not erased before starting the display. This allows composite displays of many spectra to be created. The arguments are the same as `dss`.

Examples: `dssn(1,3)`

See also: *NMR Spectroscopy User Guide*

Related: `dss` Display stacked spectra (C)

dsvast Display VAST data in a stacked 1D-NMR matrix format (M)

Applicability: Systems with the VAST accessory.

Syntax: `dsvast<(display order,number of columns displayed)>`

Description: `dsvast` will arrange and display the traces from a reconstructed 2D data set (see `vastglue`) as an array of 1D spectra in a matrix of 1D spectra. If no arguments are provided, the number of rows and columns will be determined by the periodicity of the display order based on the `doneQ`. For example, if a block of 96 spectra (typical for a microtiter-plate) have been acquired using VAST automation, the spectra will be displayed in a matrix 8 rows and 12 columns with the well label using the format `[A->H][1->12]`.

The spectra can be plotted using the macro `plvast`.

Arguments: `display order` is optional and its default value is the glue order as listed in `glueorderarray`. A `display order` can be defined using the `plate_glue` program.

`number of columns displayed`. The default value of is deduced by examining the periodicity of the requested display order. The `number of columns displayed` can entered as the second argument or as the first argument if the default `display order` is used.

Examples: `dsvast`
`dsvast(12)`
`dsvast('glue_file', 4)`

See also: *NMR Spectroscopy User Guide*

Related: `dsast2d` Display VAST data in a pseudo-2D format (M)
`plvast` Plot VAST data in a stacked 1D-NMR matrix (M)
`plvast2d` Plot VAST data in a pseudo-2D format (M)
`plate_glue` Define a display order (U)

D

dsvast2d Display VAST data in a pseudo-2D format (M)

Applicability: Systems with the VAST accessory.

Syntax: `dsvast2d (number)`

Description: If an array of 1D spectra have been acquired (in particular if a block of 96 spectra has been acquired using VAST automation, especially in a microtiter-plate format), and if these spectra have been glued into a reconstructed 2D dataset (see [vastglue](#)), this macro will arrange and display them (on the screen) in a convenient pseudo-2D format (almost like an LC-NMR chromatogram). Well labels are not attached to the spectra and spectra are plotted with 8 spectra per row.

Arguments: The default is to display all the spectra (from 1 through `arraydim`) with 8 columns (spectra) and 12 rows. An optional argument `dsvast2d (number)` allows specifying that only spectra from 1 through *number* should be plotted. The number of spectra displayed is rounded up to the nearest multiple of 8.

Related: [dsast](#) Display VAST data in a 1D-NMR matrix format (M)
[plvast](#) Plot VAST data in a stacked 1D-NMR matrix (M)
[plvast2d](#) Plot VAST data in a pseudo-2D format (M)

dsww Display spectra in whitewash mode (C)

Syntax: `dsww(<start,finish<,step>><,'int'>)>`

Description: Displays one or more spectra in whitewash mode (after the first spectra, each spectra is blanked out in regions in which it is behind a prior spectra).

Arguments: *start* is the index of the first spectra when displaying multiple spectra. It is also the index number of a particular trace to be viewed when displaying arrayed 1D spectra or 2D spectra; default is to display all spectra.

finish is the index of the last spectra when displaying multiple spectra.

step is the increment for the spectral index when displaying multiple spectra. The default is 1.

'int' is a keyword to display only the integral, independently of the value of the parameter [intmod](#)

Examples: `dsww(1,3)`

Related: [dss](#) Display stacked spectra (C)
[dssa](#) Display stacked spectra automatically (C)
[dssan](#) Display stacked spectra automatically without erasing (C)
[dssh](#) Display stacked spectra horizontally (C)
[dsshn](#) Display stacked spectra horizontally without erasing (C)
[dssn](#) Display stacked spectra without screen erase (C)
[pl](#) Plot spectra (C)
[plww](#) Plot spectra in whitewash mode (C)

dtext Display a text file in graphics window (M)

Syntax: `dtext<(file,x,y)><:$x_next,$y_next,$increment>`

Description: Displays a text file in the graphics window.

Arguments: *file* is the name of a text file. The default is the current experiment text file.
x and *y* are coordinates of the first line of text. This positions the location of the output. The default is the upper left-hand corner of the screen.

`$x_next` and `$y_next` are the coordinates where the start of the next line would have been displayed. This is useful for subsequent character display.

`$increment` is the increment between lines.

Examples: `dtext`
`dtext (userdir+' /exp3/text ')`
`dtext (100,100)`
`dtext :$x,$y,$dy`

Related:	<code>plttext</code>	Plot a text file (M)
	<code>ptext</code>	Print out a text file (M)
	<code>text</code>	Display text or set new text for current experiment (C)
	<code>write</code>	Write formatted text to a device (C)

dtrig **Delay to wait for another trigger or acquire a spectrum (P)**

Applicability: Systems with LC-NMR accessory.

Description: If `nttrig` is greater than 0 after a trigger is detected, a pulse sequence waits for `dtrig` seconds before either waiting for another trigger or acquiring a spectrum. Typically, after the LC has positioned the sample in the NMR probe and stopped the pump, there is a small time (30 seconds) during which conditions (pressure, etc.) in the NMR probe are still settling; better NMR performance is obtained if an appropriate delay is inserted using `dtrig`. If `dtrig` does not exist, a value of 0 is assumed. If `dtrig` does not exist, the `parlc` macro can create it.

Related:	<code>nttrig</code>	Number of trigger signals to wait before acquisition (P)
	<code>parlc</code>	Create LC-NMR parameters (M)

dutyc **Duty cycle for homodecoupling (optional) (P)**

Applicability: VNMRs systems, 400 MR

Syntax: `dutyc=<value>`

Description: Sets the rf duty cycle fraction (0.0-0.4) for rf on part of homonuclear decoupling. The duty cycle default is 0.1 (or 10% rf on) if the `dutyc` does not exist. Homonuclear decoupling delay before and after the rf on period. `homorof1`, `homorof2`, and `homorof3`, are equivalent to `rof1`, `rof2` and `rof3` and all default to 2 μ sec.

Values: 0.0 to 0.4 — default is 0.1

Examples: `dutyc=0.2` sets a 20% duty cycle

Related:	<code>homo</code>	Homodecoupling control for observe channel (P)
	<code>hdof</code>	Frequency offset for homodecoupling (P)
	<code>hdpwr</code>	Sets the rf attenuator to control the power for homonuclear decoupling (P)
	<code>hdmf</code>	modulation frequency for the band selective homonuclear decoupling (P)
	<code>hdpwrf</code>	Sets the rf linear modulator fine power for homonuclear decoupling (P)
	<code>hdres</code>	Sets the tip angle resolution (P)
	<code>hdseq</code>	Sets the decoupler waveform filename (P)
	<code>homorof1</code>	Delay before turning on homo decoupling rf (P)
	<code>homorof2</code>	Delay after blanking the amplifier and setting T/R switch to receive (P)

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<code>homorof3</code>	Delay between setting T/R switch to receive gating on the receiver (P)
<code>tn</code>	Nucleus for observe transmitter (P)

G

<code>g2pul_ecc</code>	Setup macro for eddy current compensation parameters (M)
<code>ga</code>	Submit experiment to acquisition and FT the result (M)
<code>gain</code>	Receiver gain (P)
<code>gap</code>	Find gap in the current spectrum (M)
<code>gaussian</code>	Set up unshifted Gaussian window function (M)
<code>gcal</code>	Gradient calibration constant (P)
<code>gcoil</code>	Current gradient coil (P)
<code>Gcosy</code>	Convert the parameter to a gradient COSY experiment (M)
<code>gdiff</code>	Diffusion gradient level (P)
<code>Gdqcosy</code>	Convert the parameter to a gradient DQCOSY experiment (M)
<code>get1d</code>	Select a 1D experiment for processing (M)
<code>get2d</code>	Select a 2D experiment for processing (M)
<code>getdim</code>	Return dimensionality of experiment (M)
<code>getfile</code>	Get information about directories and files (C)
<code>getlimit</code>	Get the limits of a variable in a tree (C)
<code>getll</code>	Get intensity and line frequency of line (C)
<code>getparam</code>	Retrieve parameter from probe file (M)
<code>getplane</code>	Extract planes from a 3D spectral data set (M)
<code>getreg</code>	Get frequency limits of a specified region (C)
<code>getsn</code>	Get signal-to-noise estimate of a spectrum (M)
<code>gettoken</code>	Utility macro to separate a string into tokens (M)
<code>gettxt</code>	Get text file from VnmrJ data file (C)
<code>gettype</code>	Get the type of a variable (C)
<code>getvalue</code>	Get value of parameter in a tree (C)
<code>gf</code>	Prepare parameters for FID/spectrum display in acqi (M)
<code>gf</code>	Gaussian function in directly detected dimension (P)
<code>gf1</code>	Gaussian function in 1st indirectly detected dimension (P)
<code>gf2</code>	Gaussian function in 2nd indirectly detected dimension (P)
<code>gflow</code>	Flow encoding gradient level (P)
<code>gfs</code>	Gaussian shift const. in directly detected dimension (P)
<code>gfs1</code>	Gaussian shift const. in 1st indirectly detected dimension (P)
<code>gfs2</code>	Gaussian shift const. in 2nd indirectly detected dimension (P)
<code>Ghmbc</code>	Convert the parameter to a gradient HMBC experiment (M)
<code>ghmqc</code>	Set up a PFG HMQC pulse sequence (M)
<code>Ghmqc</code>	Convert the parameter to a gradient HMQC experiment (M)
<code>gHMQC15</code>	Set up parameters for ¹⁵ N gHMQC experiment (M)
<code>gHMQC_d2</code>	Set up parameters for ¹⁵ N gHMQC experiment using dec. 2 (M)
<code>gHMQC_d213</code>	Set up parameters for ¹³ C gHMQC experiment using dec. 2 (M)
<code>ghmqcps</code>	Set up a PFG HMQC phase-sensitive pulse sequence (M)
<code>ghsqc</code>	Set up a PFG HSQC pulse sequence (M)
<code>Ghsqc</code>	Convert the parameter to a gradient HSQC experiment (M)
<code>gHSQC15</code>	Set up parameters for ¹⁵ N gHSQC experiment (M)
<code>gHSQC_d2</code>	Set up parameters for ¹⁵ N gHSQC experiment using dec. 2 (M)

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<code>gHSQC_d213</code>	Set up parameters for ^{13}C gHSQC experiment using dec. 2 (M)
<code>Ghsqctoxy</code>	Convert parameters for gradient HSQCTOXY experiment (M)
<code>gilson</code>	Open the Gilson Liquid Handler window (C)
<code>gin</code>	Return current mouse position and button values (C)
<code>globalauto</code>	Automation directory name (P)
<code>glue</code>	Create a pseudo-2D dataset (M)
<code>gmapshim</code>	Start gradient autoshimming (M)
<code>gmapshim_au</code>	Start acquisition with gradient shimming (M)
<code>gmapspin</code>	Enable or disable spinning during gradient shimming (P)
<code>gmapsys</code>	Run gradient autoshimming, set parameters, map shims (M)
<code>gmapz</code>	Get parameters and files for gmapz pulse sequence (M)
<code>gmap_findtof</code>	Gradient shimming flag to first find tof (P)
<code>gmap_z1z4</code>	Gradient shimming flag to first shim z1-z4 (P)
<code>gmax</code>	Maximum gradient strength (P)
<code>gmqcosy</code>	Set up PFG absolute-value MQF COSY parameter set (M)
<code>gnoesy</code>	Set up a PFG NOESY parameter set (M)
<code>go</code>	Submit experiment to acquisition (M)
<code>go_</code>	Pulse sequence setup macro called by go, ga, and au (M)
<code>gpat-gpat3</code>	Gradient shape (P)
<code>gplan</code>	Start interactive image planning (C)
<code>gradientdisable</code>	Disable PFG gradients (P)
<code>gradientshaping</code>	Activate shaping on the gradient pulses (P)
<code>gradstepsz</code>	Gradient step size (P)
<code>gradtype</code>	Gradients for X, Y, and Z axes (P)
<code>graphis</code>	Return the current graphics display status (C)
<code>grayctr</code>	Gray level window adjustment (P)
<code>graysl</code>	Gray level slope (contrast) adjustment (P)
<code>grecovery</code>	Eddy current testing (M)
<code>grid</code>	Draw a grid on a 2D display (M)
<code>groupcopy</code>	Copy parameters of group from one tree to another (C)
<code>gspoil</code>	Spoiler gradient level (P)
<code>gsspat</code>	Slice-select gradient shape (P)
<code>gttnoesy</code>	Set up a PFG TNNNOESY parameter set (M)
<code>gtnoesy</code>	Set up a PFG absolute-value ROESY parameter set (M)
<code>gtotlimit</code>	Gradient total limit (P)
<code>gtrim</code>	Trim gradient level (P)
<code>gxmax, gymax, gzmax</code>	Maximum gradient strength for each axis (P)
<code>gzlvl</code>	Pulsed field gradient strength (P)
<code>gzsize</code>	Number of z-axis shims used by gradient shimming (P)
<code>gzwin</code>	Spectral width percentage used for gradient shimming (P)

g2pul_ecc Setup macro for eddy current compensation parameters (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Setup macro for pulse sequence used to determine the eddy current compensation parameters.

ga **Submit experiment to acquisition and FT the result (M)**

Syntax: `ga(<'nocheck'><,<'next'><,<'wait'>>>`

Description: Performs experiment described by the current acquisition parameters, checking parameters `loc`, `spin`, `gain`, `wshim`, `load`, and `method` to determine the necessity to perform various actions in addition to simple data acquisition. This may involve a single FID or multiple FIDs, as in the case of arrays or 2D experiments. `ga` causes the data to be automatically weighted and Fourier transformed (`wft`) at the end of each FID data acquisition.

Before starting the experiment, `ga` executes two user-created macros if they exist. The first is `usergo`, a macro that allows the user to set up general conditions for the experiment. The second is a macro whose name is formed by `go_` followed by the name of the pulse sequence (from `seqfil`) to be used (e.g., `go_s2pul`, `go_dept`). The second macro allows a user to set up experiment conditions suited to a particular sequence.

Arguments: `'nocheck'` is a keyword to override checking if there is insufficient free disk space for the complete 1D or 2D FID data set to be acquired.

`'next'` is a keyword to put the experiment started with `ga('next')` at the head of the queue of experiments to be submitted to acquisition.

`'wait'` is a keyword to stop submission of experiments to acquisition until `wexp` processing of the experiment, started with `ga('wait')`, is finished.

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (M)
	<code>change</code>	Submit a change sample experiment to acquisition (M)
	<code>gain</code>	Receiver gain (P)
	<code>go</code>	Submit experiment to acquisition (M)
	<code>go_</code>	Pulse sequence setup macro called by <code>go</code> , <code>ga</code> , and <code>au</code> (M)
	<code>load</code>	Load status of displayed shims (P)
	<code>loc</code>	Location of sample in tray (P)
	<code>lock</code>	Submit an Autolock experiment to acquisition (C)
	<code>method</code>	Autoshim method (P)
	<code>sample</code>	Submit change sample, Autoshim experiment to acquisition (M)
	<code>seqfil</code>	Pulse sequence name (P)
	<code>shim</code>	Submit an Autoshim experiment to acquisition (C)
	<code>spin</code>	Submit a spin setup experiment to acquisition (C)
	<code>spin</code>	Sample spin rate (P)
	<code>su</code>	Submit a setup experiment to acquisition (M)
	<code>usergo</code>	Experiment setup macro called by <code>go</code> , <code>ga</code> , and <code>au</code> (M)
	<code>wft</code>	Weight and Fourier transform 1D data (C)
	<code>wshim</code>	Conditions when shimming is performed (P)

gain **Receiver gain (P)**

Description: Sets receiver gain or, by setting `gain='n'`, enables Autogain for automatic adjustment of gain. Low gain in multiline, high-dynamic-range samples can cause a number of problems, including intermodulation distortions and extra lines in the spectrum. Too high a gain, on the other hand, can cause receiver overload and consequent baseline distortions. Autogain capability allows the observe channel to be set optimally for detecting and digitizing NMR signals from a wide variety of samples.

Autogain adjusts the observe channel gain such that the NMR signal takes about 50 percent of the maximum range of the ADC. This setting allows a comfortable leeway for variations in signal. The program begins acquisition in the normal manner but the first transient (after any requested steady state transients) is

examined for signal level. If the intensity is too low or too high, the gain is changed and the process is repeated until the intensity is within the proper range, and then normal acquisition commences. The final gain value used for the experiment is stored and when the experiment is finished, setting `gain='y'` results in the value being displayed in the `dgs` parameter group.

If the gain is reduced by the Autogain procedure such that the noise does not trigger the least significant 1 or 2 bits in the ADC and the signal still overloads either the receiver or ADC, the system stops and displays a message indicating Autogain failure.

Values: 0 to 60, in steps of 2 dB (60 represents highest possible receiver gain and 0 lowest). On 500-750-MHz systems, low-band gain is limited from 18 to 60.

'n' enables Autogain, in which the gain is automatically adjusted at the start of acquisition for an optimum value. After the acquisition is finished, setting `gain='y'` then allows the value of gain to be read. `gain='n'` may not be used for arrayed experiments.

See also: *NMR Spectroscopy User Guide*

Related: `dgs` Display group of special/automation parameters (M)
`gf` Prepare parameters for FID/spectrum display in `acqi` (M)

gap Find gap in the current spectrum (M)

Syntax: `gap(gap,height):found,position,width`

Description: Looks for a gap between the lines of the currently displayed spectrum. It can be used to automatically place inserts, parameter printouts, trace labels, etc. The search starts on the left side (low-field end) of the spectrum.

Arguments: `gap` is the width of the desired gap.

`height` is the starting height (same as the lower limit for the insert).

`found` is a return value that is set to 1 if the search is successful, or set to 0 if unsuccessful.

`position` is a return value that is set to the distance from the left edge of the chart (not the plot) to the left end of the gap (3 mm from the nearest peak to the left, positioning with "left gravity") if the search is successful, or set to the position (no spacing to the nearest line) of the largest gap found if unsuccessful.

`width` is a return value set to the total width of the first gap if the search is successful, or set to the width of largest gap found if unsuccessful.

Examples: `gap(120,80);$1,$2,$3`

See also: *User Programming*

gaussian Set up unshifted Gaussian window function (M)

Syntax: `gaussian(<t1_inc>,<t2_inc>)>`

Description: Sets up an unshifted Gaussian window function in 1, 2, or 3 dimensions. The macro checks whether the data is 1D, 2D, and 3D.

Arguments: `t1_inc` is the number of t1 increments. The default is `ni`.
`t2_inc` is the number of t2 increments. The default is `ni2`.

See also: *NMR Spectroscopy User Guide*

Related: `ni` Number of increments in 1st indirectly detected dimension (P)
`ni2` Number of increments in 2nd indirectly detected dimension (P)
`pi3ssbsq` Set up pi/3 shifted sinebell-squared window function (M)
`pi4ssbsq` Set up pi/4 shifted sinebell-squared window function (M)

`sqcosine` Set up unshifted cosine-squared window function (M)
`sqsinbell` Set up unshifted sinebell-squared window function (M)

gcal Gradient calibration constant (P)

Applicability: Systems with the pulsed field gradient or the imaging module.

Description: Stores the proportionality constant between the parameter values (DAC units) controlling the desired gradient and the intensity of the gradient expressed in gauss/cm. The gradients generated in the magnet require calibration of the gain on the gradient compensation board so that coordinate data, slice positions, and the field of view can be set up accurately. `gcal` should be located in each user's `vnmr/sys/global` file.

Values: Number that is probe dependent, in gauss/cm-DAC unit. On the Performer I PFG module, 0.00028 to 0.00055 gauss/cm-DAC unit is nominal; On the Performer II, 0.0014 to 0.0025 gauss/cm-DAC unit is nominal.

See also: *VnmrJ Imaging NMR*

Related `setgcal` Set gradient calibration constant (M)

gcoil Current gradient coil (P)

Description: Reserved parameter that specifies which physical gradient set is currently installed. This allows convenient updating of important gradient characteristics when one gradient set is interchanged for another. When set, `gcoil` reads the gradient table file of the same name in `/vnmr/imaging/gradtables` and sets the gradient calibration parameters.

`gcoil` is local to each individual experiment. It is normally set the same as `sysgcoil` for acquiring new data, but can be set to other gradient names when working with saved data or data from another instrument. Each possible gradient name should have an associated file of that name located in the directory `/vnmr/imaging/gradtables`. Look at any file in this directory for an example of the proper `gradtable` format, or use the macro `createtable` to make new `gradtables` entries.

If the parameter `gcoil` does not exist in a parameter set and a user wants to create it, you must set the protection bit that causes the macro `_gcoil` to be executed when the value for `gcoil` is changed. There are two ways to create `gcoil`:

- Use the macro `updtgcoil`, which will create the `gcoil` parameter if it does not exist and set the correct protection bits.
- Enter the following commands:

```
create('gcoil','string')
setprotect('gcoil','set',9)
```

`gcoil` and the associated gradient calibration parameter `gmax` is updated with the values listed in the table on the right each time a parameter set is retrieved, or when an experiment is joined. In the rare case that a `gradtables` file is modified, but the value of `gcoil` is not changed, manually force an update of the calibration parameters. Updating may be accomplished either by setting `gcoil` to itself, for example, `gcoil=gcoil`, or by using the macro `_gcoil`.

Variable Name	Value
boresize	22.50 cm
gmax	5.00 gauss/cm
trise	0.000500 sec

Be aware that if an old dataset is returned and processed, gradient parameters associated with that dataset will replace any new `gcoil` parameters.

The table is a gradient table (gradient coil name: asg33) for a horizontal imaging system with all three axes set to the same maximum gradient strength.

On the right is a gradient table (gradient coil name: tc203) for a three-axis gradient set with unequal maximum gradient strength.

Variable Name	Value
boresize	5.10 cm
trise	0.000200 sec
gxmax	29.00 gauss/cm
gymax	27.00 gauss/cm
gzmax	70.00 gauss/cm

See also: *User Programming*

Related:	<code>gmax</code>	Maximum gradient strength (P)
	<code>setgcoil</code>	Assign sysgcoil configuration parameter (M)
	<code>sysgcoil</code>	System gradient coil (P)
	<code>updtgcoil</code>	Update gradient coil (M)

Gcosy Convert the parameter to a gradient COSY experiment (M)

Applicability: Systems with the pulsed field gradient or the imaging module.

Description: Converts a 1D standard two-pulse sequence parameter set into a set ready to run a PFG (pulsed field gradient) absolute-value COSY experiment.

See also: *NMR Spectroscopy User Guide*

gdif Diffusion gradient level (P)

Description: Predefined parameter available for use in setting a diffusion gradient level, often paired with the timing parameters `tdiff` or `tdelta`.

Gdqcosy Convert the parameter to a gradient DQCOSY experiment (M)

Description: Convert the parameter to a gradient `Dqcosy` experiment

get1d Select a 1D experiment for processing (M)

Syntax: `get1d<(experiment)>`

Description: In nonautomation mode, the macros `hcosy`, `hcapt`, `capt`, `hcdept`, and `cdept` all acquire two or more data sets in the experiment in which the macro was executed. These data sets are stored, complete with Fourier transformed data. The data sets are also stored directly in the experiment. The `get1d` macro is used to select which data set should be active for processing in that experiment. After `get1d` is executed, data can be stored in the conventional way with the `svf` command (e.g., when `hcosy` completes, `get1d` can be used to process the 1D data set).

Arguments: `experiment` is the 1D data set to be used for processing. The default is the 'H1' experiment.

Examples: `get1d`
`get1d('apt')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>capt</code>	Automated carbon and APT acquisition (M)
	<code>cdept</code>	Automated carbon and DEPT acquisition (M)
	<code>get2d</code>	Select a 2D experiment for processing (M)
	<code>hcapt</code>	Automated proton, carbon, and APT acquisition (M)
	<code>hcdept</code>	Automated proton, carbon, and DEPT acquisition (M)

hcosy Automated proton and COSY acquisition (M)
svf Save FIDs in current experiment (C)

get2d Select a 2D experiment for processing (M)

Syntax: `get2d<(experiment)>`

Description: In nonautomation mode, the macros **hcosy**, **hcapt**, **capt**, **hcdept**, and **cdept** all acquire two or more data sets in the experiment in which the macro was executed. These data sets are stored complete with Fourier transformed data. The data sets are also stored directly in the experiment. The `get2d` macro is used to select which data set should be active for processing in that experiment. After entering `get2d`, data may be stored in the conventional way with the **svf** command. For example, following completion of **hcosy**, `get2d` can be used to process the 2D data set.

Arguments: `experiment` is the 2D data set that should be used for processing. The default is the 'relayh' experiment.

Examples: `get2d('hetcor')`

See also: *NMR Spectroscopy User Guide*

Related: **get1d** Select a 1D experiment for processing (M)
svf Save FIDs in current experiment (C)

getdim Return dimensionality of experiment (M)

Syntax: `getdim:dimensions`

Description: Used in other macros to determine the number of dimensions of the current data set. Many macros make decisions based on whether a data set is multidimensional or 1D. `getdim` makes it easier to access this information.

Arguments: `dimensions` is a return variable giving the number of dimensions of the data. If `ni3` is 2 or greater, `dimensions` is set to 4; if `ni2` is 2 or greater, `dimensions` is set to 3; if `ni` is 2 or greater, `dimensions` is set to 2; and if `ni` is less than 2 or undefined, `dimensions` is 1.

Examples: `getdim:r1`

See also: *NMR Spectroscopy User Guide*

Related: **ni** Number of increments in 1st indirectly detected dimension (P)
ni2 Number of increments in 2nd indirectly detected dimension (P)
ni3 Number of increments in 3rd indirectly detected dimension (P)

getfile Get information about directories and files (C)

Syntax: (1) `getfile(directory):$number_files`
 (2) `getfile(directory,file_index):$file,$extension`

Description: Returns information about the number of files in a directory or about a particular file in a directory.

Arguments: `directory` is the name of the directory for which information is desired.
`number_files` is the number of files in the directory, with dot files (e.g., `.login`) ignored.
`file_index` is the number of file for which information is desired (the order is UNIX-dependent).
`file` is the name of the file, excluding any extension, identified by the `index` (see examples below).

extension is the extension of the file name identified by the `file_index`. For example, if `file_index` points to the file named `s2pul.fid`, `getfile` returns the string `s2pul` to `$file` and the string `fid` to `$extension`. If the file name pointed to has no extension (e.g., `dummy`), no value is returned to `$extension`. If the file name has more than one extension, only the last extension is returned to `$extension` (e.g., the file `fid.tmp.par` returns `fid.tmp` to `$file` and `par` to `$extension`).

Complete paths (full file names) can be reconstructed like this:

```
getfile('dir',i):$filename,$ext
if ($ext='') then $path='dir'+'/'+$filename
else $path='dir'+'/'+$filename+'.'+$ext
endif
```

Paths for the `rt` command can be reconstructed like this:

```
$path='dir'+'/'+$filename.
```

Examples:

```
getfile('dir'):$entries
$temp = 0
while ($temp < $entries)
    $temp = $temp + 1
    getfile('dir',$temp):$filename,$ext
    ...
endwhile
```

See also: *User Programming*

getlimit **get the limits of a variable in a tree (C)**

Syntax: `getlimit (name [, tree]) : $max, $min, $step, $index`

Description: `getlimit` displays or returns the limits of a variable in a tree.

The returned values are the max value, min. value, step size, and index. The fourth argument will return a 0 if the parameter is not using an indexed table lookup for the maximum, minimum, and step size. If the parameter is using the table lookup mechanism, the fourth argument will be set to the index for that table.

The variable trees are `current` (the default), `global`, `processed`, or `systemglobal`.

Arguments: `name` — the name of the variable

`tree` — the variable tree: `current` (the default), `global`, `processed`, or `systemglobal`.

Examples:

```
getlimit('np'):$max,$min,$step,$index
sets $max to 128000, $min to 32, $step to 2 and $index to 0
getlimit('lockfreq','systemglobal'):$max
sets $max to 160
getlimit('dpwr'):$max,$min,$step,$index
sets $max to 49, $min to 0 $step to 1 and $index to 9
```

Related:	<code>setlimit</code>	Set limits of a parameter in a tree (C)
	<code>setprotect</code>	Set protection mode of a parameter (C)

getll **Get intensity and line frequency of line (C)**

Syntax: `getll(line_number)<:height,frequency>`

Description: Finds the height and frequency of line from a line listing. It assumes a previous line list using `dll`.

Arguments: `line_number` is the number of the line in the line list.
`height` is the intensity of the specified line.
`frequency` is the line frequency with units defined by the parameter `axis`.

See also: *User Programming*

Related: `axis` Axis label for displays and plots (P)
`dll` Display listed line frequencies and intensities (C)
`fp` Find peak heights (C)
`nll` Find line frequencies and intensities (C)

getparam Retrieve parameter from probe file (M)

Syntax: `getparam(param<,nucleus>):$value`

Description: Retrieves the value of a parameter from the current probe file. The name of the probe file is referenced from the parameter `probe`.

Arguments: `param` is the name of the parameter to be retrieved.
`nucleus` is the nucleus to be retrieved from the probe file. The default is the current value of the parameter `tn`
`value` is a return variable with the value of the retrieved parameter.

Examples: `getparam('tpwr'):tpwr`
`getparam('dmf','H1'):$dmf`

See also: *NMR Spectroscopy User Guide*

Related: `addnucleus` Add new nucleus to existing probe file (M)
`addparams` Add parameter to current probe file (M)
`addprobe` Create new probe directory and probe file (M)
`probe` Probe type (P)
`setparams` Write parameter to current probe file (M)
`tn` Nucleus for the observe transmitter (P)
`updateprobe` Update probe file (M)

getplane Extract planes from a 3D spectral data set (M)

Syntax: `getplane(<data_dir><,plane_dir><,plane_type>)>`

Description: Executes the program `getplane` in the VnmrJ system bin directory (`$vnmrsystem/bin`). `getplane` checks whether there is sufficient file space on the disk partition to accommodate the extracted planes. If space is insufficient, `getplane` writes an error to the VnmrJ text window and aborts. `getplane` does not delete the output plane directory if it is run multiple times to individually extract different plane types.

Arguments: `data_dir` specifies the directory (without the `/data` subdirectory) containing the input 3D spectral data. The first non-keyword argument to `getplane` is always taken to be `data_dir`.
`plane_dir` specifies the directory (without the `/extr` subdirectory) in which the extracted planes are to be stored. The second non-keyword argument to `getplane` is always taken to be `plane_dir`. If `plane_dir` is not specified, `data_dir` also specifies the output plane directory. If both `data_dir` and `plane_dir` are not specified, the input data directory and the output plane directory are set to `curexp/datadir3d`. The parameter `plane` is always set equal to the output plane directory.
`plane_type` can be any of the following keywords:

- 'xall' is a keyword to extract all three 2D plane types: f1f3, f2f3, f1f2.
- 'f1f3', 'f2f3', 'f1f2' are keywords to extract their respective 2D planes.
- Any of these keywords can be submitted more than once to the `getplane` macro, but the `getplane` program displays an error and aborts if any one plane type is defined for extraction more than once.

Examples: `getplane`
`getplane('data3d.inp','data3d.planes','f1f3','f2f3')`

See also: *NMR Spectroscopy User Guide*

Related:

<code>dplane</code>	Display a 3D plane (M)
<code>dproj</code>	Display a 3D plane projection (M)
<code>dsplanes</code>	Display a series of 3D planes (M)
<code>ft3d</code>	Perform a 3D Fourier transform (M)
<code>nextpl</code>	Display the next 3D plane (M)
<code>path3d</code>	Path to currently displayed 2D planes from a 3D data set (P)
<code>plane</code>	Currently displayed 3D plane type (P)
<code>plplanes</code>	Plot a series of 3D planes (M)
<code>prevpl</code>	Display the previous 3D plane (M)

getreg Get frequency limits of a specified region (C)

Syntax: `getreg(region_number)<:minimum,maximum>`

Description: Returns the frequency limits of a region. The spectrum should have been previously divided into regions with the `region` command.

Arguments: `region_number` specifies the number of the region.
`minimum,maximum` are return values set to the frequency limits, in Hz, of the specified region.

Examples: `getreg(1):$a,$b`
`getreg($4):cr,$lo`
`getreg(R1-1):r2,r3`

See also: *User Programming*

Related:

<code>cz</code>	Clear integral reset points (C)
<code>ds</code>	Display a spectrum (C)
<code>numreg</code>	Return the number of regions in a spectrum (C)
<code>region</code>	Divide spectrum into regions (C)
<code>z</code>	Add integral reset point at cursor position (C)

getsn Get signal-to-noise estimate of a spectrum (M)

Syntax: `getsn:current_sn,predicted_sn`

Description: Estimates spectrum signal-to-noise using the following algorithm:

- Measures four adjacent 5-percent portions at the left edge of the spectrum, finding the root-mean-square noise, and taking the smallest of the four values. By measuring four different values and finding root-mean-square noise instead of peak noise, the result should be reliable even if several signals are present in the selected regions.
- Next, estimates the signal level using the vertical scale adjustment macros: `vsadjh` for proton, `vsadjc` for carbon, and `vsadj` for other nuclei. For carbon spectra, this algorithm ignores solvent lines and TMS. For proton spectra, in addition to ignoring the largest line in the spectrum, if the tallest line is greater than three times the height of the second tallest line, the

second highest line is be used instead. For other nuclei, `getsn` uses the tallest line in the spectrum.

- Finally, estimates the signal-to-noise at the end of the experiment by a simple extrapolation (multiplying by the square root of `nt/ct`).

Arguments: `current_sn` is a return value set to the current signal-to-noise level.

`predicted_sn` is a return value set to the predicted signal-to-noise level at the end of the experiment.

See also: *NMR Spectroscopy User Guide*

Related:	<code>ct</code>	Completed transients (P)
	<code>nt</code>	Number of transients (P)
	<code>testsn</code>	Test signal-to-noise ratio (M)
	<code>vsadj</code>	Adjust vertical scale (M)
	<code>vsadjc</code>	Adjust vertical scale for carbon spectra (M)
	<code>vsadjh</code>	Adjust vertical scale for proton spectra (M)

gettoken **Utility macro to separate a string into tokens (M)**

Syntax: `gettoken(input_string<,delimiter>):output_string, next_location`

Description: Gets the first occurrence of a substring in `input_string` which is delimited by `delimiter`, or by the default delimiter ' \$ '. The substring is returned in `output_string`. The next location in the string after the second delimiter is returned as a real in `next_location`. If there are not both one occurrence of each of the beginning delimiter and the second delimiter - in other words, if the delimiters are not paired - an empty string is returned in `output_string`, and -1 is returned in `next_location`. If the delimited substring is the last substring in `input_string`, then the substring is returned as expected, but `next_location` returns -1.

Arguments: `input_string`

The string to be tokenized `delimiter` is the delimiter for the tokens (default is \$)

Examples: `gettoken($mydirname):$mytoken, $next_location`

`gettoken($mydirname,'%'): $mytoken, $next_location`

Related: `reqpartest` Tests whether required parameters are set (M)

gettxt **Get text file from VnmrJ data file (C)**

Syntax: `gettxt(file)`

Description: Copies text from a data file to the current experiment.

Arguments: `file` is the name of a VnmrJ data file saved from an experiment (i.e., a directory with a `.fid` or `.par` suffix). Do not include the file name suffix.

Examples: `gettxt('/vnmr/fidlib/fid1d')`

See also: *NMR Spectroscopy User Guide*

Related: `puttxt` Put text file into another file (C)

gettype **Get the type of a variable (C)**

Syntax: `gettype(name[, tree])<:index, name>`

Description: Displays or returns the type of an existing variable.

Arguments: A “string” variable can return type 'string' or 'flag'. A “real” variable can return type 'real', 'delay', 'frequency', 'pulse', or 'integer'. `gettype` returns one or two values to a macro. The first value is an integer corresponding to the parameter type. The second value is the name of the parameter type. `name` can be used in commands such as `settype` and `create`.

An optional `tree` argument can be given. Variables are 'current', 'global', 'processed', and 'systemglobal'.

The default is to search for the parameter in the 'current', 'global', and 'systemglobal' trees, in that order.

Examples: `gettype('dmm'):$int,$name` sets `$int` to 4 and `$name` to 'flag'.

See also: `gettype('pw'):$int,$name` sets `$int` to 6 and `$name` to 'pulse'.

getvalue **Get value of parameter in a tree (C)**

Syntax: `getvalue(parameter<,>,index<>,>,tree<>)`

Description: Gets the value of any parameter in a tree. The value of most parameters can be accessed simply by using their name in an expression. For example, `sw?` or `r1=np` accesses the value of `sw` and `np`, respectively. However, parameters in the processed tree cannot be accessed that way; `getvalue` can be used to get the value of a parameter in the processed tree.

Arguments: `parameter` is the name of an existing parameter.

`index` is the number of a single element in an arrayed parameter. Default is 1.

`tree` is one of the keywords 'global', 'current', 'processed', or 'systemglobal'. The default is 'processed'. Refer to the `create` command for more information on the types of parameter trees.

Examples: `getvalue('arraydim')`

See also: *User Programming*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>setgroup</code>	Set group of a parameter in a tree (C)
	<code>setlimit</code>	Set limits of a parameter in a tree (C)
	<code>setprotect</code>	Set protection mode of a parameter (C)
	<code>settype</code>	Change type of a parameter (C)
	<code>setvalue</code>	Set value of any parameter in a tree (C)

gf **Prepare parameters for FID/spectrum display in acqi (M)**

Description: Provided as a model for preparing parameters for the FID and spectrum display in `acqi`. The unmodified version of this macro turns off phase cycling, autoshimming, autolocking, spin control, temperature control, sample changer control, and autogain. It also selects the current pulse sequence and parameter set by issuing the command `go('acqi')` and the command `acqi('par')`. The automation parameters `cp`, `wshim`, `alock`, `spin`, `temp`, `loc`, and `gain` are then reset to their original values. Users can customize `gf` by copying it into their private `maclib` directory and editing that version to suit their needs.

See also: *NMR Spectroscopy User Guide*

Related:	<code>acqi</code>	Interactive acquisition display process (C)
	<code>alock</code>	Automatic lock status (P)
	<code>cp</code>	Cycle phase (P)
	<code>dmgf</code>	Absolute-value display of FID data and spectrum in <code>acqi</code> (P)
	<code>gain</code>	Receiver gain (P)

<code>go</code>	Submit an experiment to acquisition (C)
<code>loc</code>	Location of sample in tray (P)
<code>spin</code>	Sample spin rate (P)
<code>temp</code>	Sample temperature (P)
<code>wshim</code>	Conditions when shimming performed (P)

gf **Gaussian function in directly detected dimension (P)**

Description: Defines a Gaussian time constant of the form $\exp(-(t/gf)^2)$ along the directly detected dimension. This dimension is referred to as the f_2 dimension in 2D data sets, the f_3 dimension in 3D data sets, etc.

Values: Number, in seconds. Typical value is `gf='n'`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>gf1</code>	Gaussian function in 1st indirectly detected dimension (P)
	<code>gf2</code>	Gaussian function in 2nd indirectly detected dimension (P)
	<code>gfs</code>	Gaussian shift constant in directly detected dimension (P)

gf1 **Gaussian function in 1st indirectly detected dimension (P)**

Description: Defines a Gaussian time constant of the form $\exp(-(t/gf1)^2)$ along the first indirectly detected dimension. This dimension is referred to as the f_1 dimension of a multidimensional data set. `gf1` works analogously to the parameter `gf`. The “conventional” parameters, such as `lb` and `gf`, operate on the detected FIDs, while this “2D” parameter is used during processing of the interferograms.

Values: Number, in seconds.

See also: *NMR Spectroscopy User Guide*

Related:	<code>gf</code>	Gaussian function in directly detected dimension (P)

gf2 **Gaussian function in 2nd indirectly detected dimension (P)**

Description: Defines a Gaussian time constant of the form $\exp(-(t/gf2)^2)$ along the second indirectly detected dimension. This dimension is referred to as the f_2 dimension of a multidimensional data set. `gf2` works analogously to the parameter `gf`. The `wti` program can be used to set `gf2` on the 2D interferogram data.

Values: Number, in seconds.

See also: *NMR Spectroscopy User Guide*

Related:	<code>gf</code>	Gaussian function in directly detected dimension (P)
	<code>wti</code>	Interactive weighting (C)

gflow **Flow encoding gradient level (P)**

Description: Predefined parameter available for use in setting a flow encoding gradient level, often paired with the timing parameter `tflow`.

See also: *VnmrJ Imaging NMR*

gfs **Gaussian shift const. in directly detected dimension (P)**

Description: Working in combination with the `gf` parameter, `gfs` allows shifting the center of the Gaussian function $\exp(-(t-gfs)/gf)^2$ along the directly

detected dimension. This dimension is referred to as the f_2 dimension in 2D data sets, the f_3 dimension in 3D data sets, etc. Typical value is `gfs='n'`.

See also: *NMR Spectroscopy User Guide*

Related: `gf` Gaussian function in directly detected dimension (P)
`gfs1` Gaussian shift const. in 1st indirectly detected dimension (P)
`gfs2` Gaussian shift const. in 2nd indirectly detected dimension (P)

gfs1 Gaussian shift const. in 1st indirectly detected dimension (P)

Description: Working in combination with the `gf1` parameter, `gfs1` allows shifting the center of the Gaussian function $\exp(-(t-gfs1)/gf1)^2)$ along the first indirectly detected dimension. This dimension is referred to as the f_1 dimension in multidimensional data sets. `gfs1` works analogously to the parameter `gfs`. The “conventional” parameters (i.e., `lb`, `gf`, etc.) operate on the detected FIDs, while this “2D” parameter is used during processing of the interferograms.

See also: *NMR Spectroscopy User Guide*

Related: `gf` Gaussian function in directly detected dimension (P)
`gf1` Gaussian function in 1st indirectly detected dimension (P)
`gfs` Gaussian shift const. in directly detected dimension (P)

gfs2 Gaussian shift const. in 2nd indirectly detected dimension (P)

Description: Working in combination with the `gf2` parameter, `gfs2` allows shifting the center of the Gaussian function $\exp(-(t-gfs2)/gf2)^2)$ along the second indirectly detected dimension. This dimension is referred to as the f_2 dimension in multidimensional data sets. `gfs2` works analogously to the parameter `gfs`. The `wti` program can be used to set `gfs2` on the 2D interferogram data.

See also: *NMR Spectroscopy User Guide*

Related: `gf` Gaussian function in directly detected dimension (P)
`gf2` Gaussian function in 2nd indirectly detected dimension (P)
`gfs` Gaussian shift const. in directly detected dimension (P)
`wti` Interactive weighting (C)

Ghmhc Convert the parameter to a gradient HMBC experiment (M)

Applicability: Systems with a pulsed field gradient module.

Description: Prepares an experiment for a PFG (pulsed field gradient) HMQC.

Arguments: *NMR Spectroscopy User Guide*

ghmqc Set up a PFG HMQC pulse sequence (M)

Applicability: Systems with a pulsed field gradient module.

Description: Prepares an experiment for a PFG (pulsed field gradient) HMQC using the sequence GHMQC. The sequence sets three gradients, all separately.

Arguments: *NMR Spectroscopy User Guide*

Ghmqc Convert the parameter to a gradient HMQC experiment (M)

Description: Convert the parameter to a gradient HMQC experiment

- gHMQC15** **Set up parameters for ^{15}N gHMQC experiment (M)**
 Description: Converts the current parameter set to a gHMQC experiment for ^{15}N .
- gHMQC_d2** **Set up parameters for ^{15}N gHMQC experiment using dec. 2 (M)**
 Description: Converts the current parameter set to a gHMQC experiment for ^{15}N with decoupler 2 as ^{15}N .
- gHMQC_d213** **Set up parameters for ^{13}C gHMQC experiment using dec. 2 (M)**
 Description: Converts the current parameter set to a gHMQC experiment for ^{13}C with decoupler 2 as ^{13}C .
- ghmqcps** **Set up a PFG HMQC phase-sensitive pulse sequence (M)**
 Applicability: Systems with a pulsed field gradient module.
 Description: Prepares an experiment for a PFG (pulsed field gradient) HMQC, phase-sensitive version.
 See also: *NMR Spectroscopy User Guide*
- ghsqc** **Set up a PFG HSQC pulse sequence (M)**
 Applicability: Systems with a pulsed field gradient module.
 Syntax: `ghsqc<(nucleus)>`
 Description: Converts a 1D standard two-pulse sequence parameter set into a parameter set ready to run a PFG (pulsed field gradient) HSQC experiment, either absolute value or phase sensitive.
 Arguments: `nucleus` is ^{13}C or ^{15}N . The default is ^{13}C .
 See also: *NMR Spectroscopy User Guide*
- Ghsqc** **Convert the parameter to a gradient HSQC experiment (M)**
 Description: Convert the parameter to a gradient HSQC experiment.
- gHSQC15** **Set up parameters for ^{15}N gHSQC experiment (M)**
 Description: Converts the current parameter set to a gHSQC experiment for ^{15}N .
- gHSQC_d2** **Set up parameters for ^{15}N gHSQC experiment using dec. 2 (M)**
 Description: Converts the current parameter set to a gHSQC experiment for ^{15}N with decoupler 2 as ^{15}N .
- gHSQC_d213** **Set up parameters for ^{13}C gHSQC experiment using dec. 2 (M)**
 Description: Converts the current parameter set to a gHSQC experiment for ^{13}C with decoupler 2 as ^{13}C .
- Ghsqctoxy** **Convert parameters for gradient HSQCTOXY experiment (M)**
 Description: Convert the parameter to a gradient HSQCTOXY experiment

G

gilson **Open the Gilson Liquid Handler window (C)**

Syntax: `gilson`

Description: Opens the Gilson Liquid Handler window, which enables setup, configuration, and operation of the VAST automatic sampler changer accessory.

See also: *NMR Spectroscopy User Guide*

gin **Return current mouse position and button values (C)**

Applicability: All

Syntax: `gin<(Bn_<press><release>)>:$x,$y,$b1,$b2,$b3`

Description: The `gin` command reports the pointer position in relationship to the graphics window and is often used with the `move` and `draw` commands. The variables `$x` and `$y` are the x and y positions hold the pointer in millimeters. The variables `$b1`, `$b2`, and `$b3` hold the values for the state of the left, middle, and right mouse buttons.

Values: `$x` is the value in the x direction, in millimeters, of the pointer. The range of x is 0 at the left edge of the chart and `wcmax` at the right edge. A value of -1 is returned if the pointer position is outside the graphics window along the x axis.

`$y` is the position of the pointer along the y axis. The range of y is -20 at the bottom of the chart to `wc2max` at the top. A value of 10000 is returned if the pointer position is outside the graphics window along the y axis.

`$b1` is the state of left button; returns the value 0 if released and 1 if pressed.

`$b2` is the of middle button; returns the value 0 if released and 1 if pressed.

`$b3` is the of right button; returns the value 0 if released and 1 if pressed.

Arguments: `no` argument, returns current mouse positions and button values.

`Bn_press, n=a, 1, 2, or 3`. Wait for mouse button (any, 1, 2, or 3) or any key to be pressed.

`Bn_release, n=a, 1, 2, or 3`. Wait for mouse button (any, 1, 2, or 3) to be released or any key to be pressed.

Examples: `gin('B3_press'):$x,$y,$b1,$b2,$b3`
 wait until button 3 or any key is pressed
`gin('Ba_press'):$x,$y,$b1,$b2,$b3`
 wait until any button or any key is pressed
`gin('B1_release'):$x,$y,$b1,$b2,$b3`
 wait until button 1 is released or any key pressed
`gin('B2_release'):$x,$y,$b1,$b2,$b3`
 wait until button 2 is released or any key pressed

See also: *User Programming*

Related:	<code>box</code>	Draw a box on a plotter or graphics display (C)
	<code>draw</code>	Draw line from current location to another location (C)
	<code>move</code>	Move to an absolute location to start a line (C)

globalauto **Automation directory name (P)**

Applicability: *VnmrJ Walkup* and systems with automation such as sample handling.

Description: A global parameter that specifies the name of a directory in which the daily automation directories or study directories are saved. This parameter is created and used by the `walkup` macro and the VnmrJ Walkup interface.

See also: *NMR Spectroscopy User Guide*; *VnmrJ Walkup*

Related: [cqinit](#) Initialize liquids study queue (M)
[walkup](#) Walkup automation (M)

glue Create a pseudo-2D dataset (M)

Applicability: Systems with the LC-NMR accessory.

Syntax: `glue<(num_scans)>`

Description: Steps through the series of FIDs, putting them into `exp5` one by one as an array, and then jumps to `exp5` and changes the parameters `arraydim`, `ni`, and `fn1`, so that the data appear to the user to be a 2D experiment, which can then be processed and displayed with standard 2D commands (`wft2d`, `dconi`, etc.). The parameter `savefile` should exist and should contain the base file name to which a series of FIDs have been saved as `savefile.001`, `savefile.002`, etc.

Arguments: `num_scans` is the number of FIDs copied into the `exp5` array. Typically, `num_scans` is used if the experiment was aborted prematurely, so that the complete `num_scans` worth of FIDs were not actually acquired.

See also: *NMR Spectroscopy User Guide*

Related: [savefile](#) Base file name for saving FIDs or data sets (P)

gmapshim Start gradient autoshimming (M)

Applicability: Systems with gradient shimming installed.

Syntax: `gmapshim<('files'|'mapname'|'quit')>`

Description: Starts gradient autoshimming if no arguments are used. It can also retrieve a shimmap file or quit gradient autoshimming. When the `gmapshim` macro is done, it automatically exits, and the previous data set is retrieved.

Arguments: `'files'` is a keyword to enter the gradient autoshimming files menu.

`'mapname'` is a keyword to display the current mapname.

`'quit'` is a keyword to exit from gradient autoshimming and retrieve the previous data set.

See also: *NMR Spectroscopy User Guide*

Related: [gmapsys](#) Run gradient autoshimming, set parameters, map shims (M)
[gmapz](#) Get parameters and files for `gmapz` pulse sequence (M)

gmapshim_au Start acquisition with gradient shimming (M)

Applicability: Systems with gradient shimming installed.

Description: If `wshim` is not set to `'n'`, `gmapshim_au` checks the probe file for a lock gradient map name. If the name exists, `gmapshim_au` executes `gmapshim('glideau')` to start gradient shimming followed by acquisition. If the map name does not exist, `gmapshim_au` starts acquisition by running `au('wait')`.

gmapspin Enable or disable spinning during gradient shimming (P)

Description: Specifies whether or not sample spinning during gradient shimming is enabled. If spinning is enabled during gradient shimming, the pulses and delays *must* also be synchronized with the rotor period.

Values: 'n' disable spinning during gradient shimming.
'y' enable spinning during gradient shimming.

Related: **gmapz** Get parameters and files for gmapz pulse sequence (M)
gmapsys Run gradient autoshimming, set parameters, map shims (M)
gzsize Number of z-axis shims used by gradient shimming (P)
spin Sample spin rate (P)

gmapsys Run gradient autoshimming, set parameters, map shims (M)

Applicability: Systems with gradient shimming installed.

Syntax: (1) `gmapsys<(option)>`
 (2) `gmapsys('shimmap'<,shimmap_option>)`

Description: Enters the Gradient Shimming Setup panel for setting parameters, mapping the shims, and performing autoshimming. This is the only entry point to the gradient shimming Setup panel.

If the **gmapz** pulse sequence is not loaded, retrieve parameters from the last shimmap used (or current mapname) or from `gmapz.par` if no shimmap exists.

Arguments: `option` is one of the following keywords:

- 'addpar' adds gradient shimming parameters to the current parameter set.
- 'findgzlvl' runs an experiment to calibrate `gzlvl`, `gzwin`, and `tof` to optimize the spectral window.
- 'findgzwin' runs an experiment to calibrate `gzwin` and `tof` to optimize the spectral window.
- 'findtof' runs an experiment to center `tof` to optimize the spectral window.
- 'rec' displays the record of shim adjustments from the previous gradient shimming run.
- 'shim' start autoshimming (same as Gradient Autoshim on Z button).
- 'vi' edits the file `gshim.list`, which is used for editing shim offsets, mapname, or selecting coarse and fine shims.
- 'writeb0' displays the b0 plot calculated from the first two array elements.

'shimmap' is a keyword to run a shim mapping experiment and save the results (same as Make Shimmap button).

`shimmap_option` is one of the following values:

- 'auto' is a keyword to calibrate `gzwin` and then make a shimmap (same as Automake Shimmap button).
- 'manual' is a keyword to use shim offset values set manually from the file `gshim.list` and not the default values to make a shimmap.
- 'overwrite' is a keyword to make a shimmap and overwrite the current mapname if it exists.
- mapname is the prefix of the shimmap file name. The default is the user is queried for mapname before running the experiment.

See also: *NMR Spectroscopy User Guide*

Related: **gmapshim** Start gradient autoshimming (M)
gmapz Get parameters and files for gmapz pulse sequence (M)

<code>gradtype</code>	Gradients for X, Y, Z axes (P)
<code>gzwin</code>	Spectral width percentage used for gradient shimming (P)
<code>seqfil</code>	Pulse sequence name (P)
<code>gmap_z1z4</code>	Gradient shimming flag to first shim z1-z4 (P)
<code>gzsize</code>	Number of z-axis shims used by gradient shimming (P)

gmapz Get parameters and files for gmapz pulse sequence (M)

Applicability: Systems with gradient shimming installed.

Syntax: `gmapz < (mapname) >`

Description: Retrieves gradient shimming parameters to set up a gradient shimming experiment.

Arguments: `mapname` is the name of a gradient shimmap file that must exist in the `shimmaps` directory. `gmapz` retrieves parameters and loads the shimmap file from `mapname`. The default is to retrieve standard gradient shimming parameters from the file `gmapz.par`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>gmapshim</code>	Start gradient autoshimming (M)
	<code>gmapsys</code>	Run gradient autoshimming, set parameters, map shims (M)
	<code>gmap_z1z4</code>	Gradient shimming flag to first shim z1-z4 (P)

gmap_findtof Gradient shimming flag to first find tof (P)

Applicability: Systems with gradient shimming installed.

Description: When the flag is set to 'y', gradient shimming first performs a calibration to find `tof` before the start of shimming. This action is recommended for only homospoil deuterium gradient shimming with different solvents. The default value is 'n'.

Values: 'y' turns on the flag.
'n' turns off the flag.

See also: *NMR Spectroscopy User Guide*

Related:	<code>gmapshim</code>	Start gradient autoshimming (M)
	<code>gmapsys</code>	Run gradient autoshimming, set parameters, map shims (M)
	<code>gmapz</code>	Get parameters and files for gmapz pulse sequence (M)
	<code>tof</code>	Frequency offset for observe transmitter (P)

gmap_z1z4 Gradient shimming flag to first shim z1-z4 (P)

Applicability: Systems with gradient shimming installed.

Description: When the flag is set to 'y', if `gzsize` is greater than 4, gradient shimming first shims on z1-z4, and then uses all shims specified by `gzsize`. When the flag is set to 'n' (default), all shims specified by `gzsize` are used.

Values: 'y' turns on the flag.
'n' turns off the flag.

See also: *NMR Spectroscopy User Guide*

Related:	<code>gmapshim</code>	Start gradient autoshimming (M)
	<code>gmapsys</code>	Run gradient autoshimming, set parameters, map shims (M)
	<code>gmapz</code>	Get parameters and files for gmapz pulse sequence (M)
	<code>gzsize</code>	Number of z-axis shims used by gradient shimming (P)

gmax Maximum gradient strength (P)

Description: The allowed maximum gradient level (absolute value) in gauss/cm. gmax is one of the calibration entries in a gradtables file. gxmax, gymax, and gzmax are used when the maximum gradient level is different for each axis in gauss/cm, which is the case for triple-axis PFG coils.

See also: *VnmrJ Installation and Administration; VnmrJ Imaging NMR*

Related: [gcoil](#) Current gradient coil (P)
[gxmax,gymax,gzmax](#) Maximum gradient strength for each axis (P)
[sysgcoil](#) System gradient coil (P)

gmqcosy Set up PFG absolute-value MQF COSY parameter set (M)

Applicability: Systems with the pulsed field gradient module.

Description: Converts a 1D standard two-pulse sequence parameter set into a parameter set ready to run a PFG (pulsed field gradient) absolute-value MQF COSY experiment.

See also: *NMR Spectroscopy User Guide*

gnoesy Set up a PFG NOESY parameter set (M)

Applicability: Systems with the pulsed field gradient module.

Description: Converts a 1D standard two-pulse sequence parameter set into a parameter set ready to run a PFG (pulsed field gradient) NOESY experiment, either absolute value or phase sensitive.

See also: *NMR Spectroscopy User Guide*

go Submit experiment to acquisition (M)

Syntax: `go(<'acqi'><,'nocheck'><,'nosafe'><,'next'>
<,'sync'><,'wait'>)>`

Description: Performs the experiment described by the current acquisition parameters, checking parameters [loc](#), [spin](#), [gain](#), [wshim](#), [load](#), and [method](#) to determine the necessity to perform various actions in addition to data acquisition. This may involve a single FID or multiple FIDs, as in the case of arrays or 2D experiments. go acquires the FID and performs no processing. If free disk space is insufficient for the complete 1D or 2D FID data set to be acquired, go prompts the user with an appropriate message and aborts the acquisition initiation process.

Before starting the experiment, go executes two user-created macros if they exist. The first is [usergo](#), a macro that allows the user to set up general conditions for the experiment. The second is a macro whose name is formed by [go_](#) followed by the name of the pulse sequence (from [seqfil](#)) to be used (e.g., [go_s2pul](#), [go_dept](#)). The second macro allows a user to set up experiment conditions suited to a particular sequence.

Arguments: 'acqi' is a keyword to submit an experiment for display by the [acqi](#) program. All operations explained above are performed, except acquisition of data is not initiated. The instructions to control data acquisition are stored so that [acqi](#) can acquire the data when the FID button is clicked. The [gf](#) macro is recommended instead of running `go('acqi')` directly. Using [gf](#) prevents certain acquisition events from occurring, such as spin control and temperature change. See the description of [gf](#) for more information.

'nocheck' is a keyword to override checking if there is not enough free disk space for the complete 1D or 2D FID data set to be acquired.

'nosafe' is a keyword to disable probe protection during the experiment.

'next' is a keyword to put the experiment started with `go('next')` at the head of the queue of experiments to be submitted to the acquisition system. If `go('next')` is entered, the `go` macro remains active until the experiment is submitted to the acquisition system, and no other VnmrJ commands are processed until the `go` macro finishes.

'sync' is a keyword in nonautomation mode that accomplishes the same effect as `go('next')` in synchronizing VnmrJ command execution with the submission of experiments to the acquisition system. The difference is that 'sync' does not put the experiment at the head of the queue.

'wait' is a keyword to stop submission of experiments to acquisition until `wexp` processing of the experiment, started with `go('wait')`, is finished.

Examples: `go`
`go('nosafe')`
`go('next')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>acqi</code>	Interactive acquisition display process (C)
	<code>au</code>	Submit experiment to acquisition and process data
	<code>change</code>	Submit a change sample experiment to acquisition (M)
	<code>gain</code>	Receiver gain (P)
	<code>ga</code>	Submit experiment to acquisition and FT the result (C)
	<code>gf</code>	Prepare parameters for FID/spectrum display in <code>acqi</code> (M)
	<code>go_</code>	Pulse sequence setup macro called by <code>go</code> , <code>ga</code> , and <code>au</code> (M)
	<code>load</code>	Load status of displayed shims (P)
	<code>loc</code>	Location of sample in tray (P)
	<code>lock</code>	Submit an Autolock experiment to acquisition (C)
	<code>method</code>	Autoshim method (P)
	<code>probe_protection</code>	Probe protection control (P)
	<code>sample</code>	Submit change sample, Autoshim exp. to acquisition (M)
	<code>seqfil</code>	Pulse sequence name (P)
	<code>shim</code>	Submit an Autoshim experiment to acquisition (C)
	<code>spin</code>	Submit a spin setup experiment to acquisition (C)
	<code>spin</code>	Sample spin rate (P)
	<code>su</code>	Submit a setup experiment to acquisition (M)
	<code>usergo</code>	Experiment setup macro called by <code>go</code> , <code>ga</code> , and <code>au</code> (M)
	<code>vnmrjcmd()</code>	Commands to invoke the GUI popup (C)
	<code>wshim</code>	Conditions when shimming is performed (P)

go_ **Pulse sequence setup macro called by go, ga, and au (M)**

Syntax: `go_macro`

Description: Called by the macros `go`, `ga`, or `au` before starting an experiment. The user typically creates this macro to set up general experiment conditions. The name of the macro is formed by combining `go_` with the name of the pulse sequence macro (from `seqfil`) to be used.

Examples: `go_dept`
`go_noesy`
`go_s2pul`

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (M)
	<code>ga</code>	Submit experiment to acquisition and FT the result (M)

<code>go</code>	Submit experiment to acquisition (M)
<code>seqfil</code>	Pulse sequence name (P)
<code>usergo</code>	Experimental setup macro called by <code>go</code> , <code>ga</code> , and <code>au</code> (M)

gpat-gpat3 Gradient shape (P)

Description: Predefined string parameters available to specify gradient shapes.

See also: *VnmrJ Imaging NMR*

gplan Start interactive image planning (C)

Syntax: `gplan(function_name, arg1, arg2, ...)`

Description: In VnmrJ, starts an image planning session.

Arguments: 'function_name', path is the name of an image planning function surrounded by single quotation marks.

`arg1, arg2, ...` are arguments for the function, if relevant.

Examples: `gplan 'clearStacks()'`
`get 'PrevStacks()'`

See also: *NMR Spectroscopy User Guide*

gradientdisable Disable PFG gradients (P)

Description: `gradientdisable` is an optional global parameter for disabling the gradient pulses. If `gradientdisable` parameter is set to 'y', the psg software sets the gradient dac values to 0. The gradient parameters in VnmrJ and pulse sequence are not altered. This feature works in both C psg and SpinCAD Jpsg.

To use this feature, create `gradientdisable` as a global parameter of type 'flag'. If `gradientdisable` is set to 'y', the gradient amplitude values will be set to 0; if set to 'n' the gradient amplitudes will be the expected values determined by the gradient parameters and pulse sequence calculations. This feature is typically used in experiments involving Cold Probes. This feature is only effective for gradient configurations, `gradtypes` of 'l', 'p', and 't'.

Related: `pfgon` Pulsed field gradient amplifiers on/off control (P)
`gradtype` Gradients for X, Y, and Z axes (P)

gradientshaping Activate shaping on the gradient pulses (P)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Activate shaping on the gradient pulses in the pulse sequence without changing the pulse sequence source program. This feature works only the Z gradient pulses, specified using the `zgradpulse(. .)` PSG statement. `gradientshaping` is a global parameter.

Values: `gradientshaping='y'` enables this feature and produces a WURST shaping of gradient amplitudes.
`gradientshaping='n'` or destroy the parameter disables this feature and produces rectangular gradients amplitudes.

gradstepsz Gradient step size (P)

Description: The maximum gradient DAC value. `gradstepsz` determines the type of gradient DAC board used in the system: 12-bit or 16-bit. It is used internally to convert gauss/cm gradient levels to the proper hardware DAC level.

Values: Systems with 12-bit DACs (older SISCO spectrometers without gradient waveform capabilities): -2047 to +2047 units, in integer steps.

Systems with 16-bit DACs (SISCO spectrometers with gradient waveform capabilities): -32767 to +32767 units, in integer steps.

See also: *VnmrJ Installation and Administration*; *VnmrJ Imaging NMR*

gradtype **Gradients for X, Y, and Z axes (P)**

Applicability: Systems with pulsed field gradient (PFG) or imaging capability.

Description: Configuration parameter for systems with optional gradients for axes. The value is set using the label X Axis, Y Axis, Z Axis in the Spectrometer Configuration window (opened from [config](#)). The values available for each axis are None, WFG + GCU, Performa I, Performa II/III, Performa II/III + WFG, Performa XYZ, Performa XYZ + WFG, SIS (12 bit), Homospoil, and Shim DAC. WFG stands for the waveform generator; GCU stands for the gradient compensation unit; and Performa I, II, III, and XYZ are types of PFG modules.

Values: String of three characters (e.g., 'nnp'). The first character is the gradient for the X axis, second for the Y axis, and third for the Z axis. Each axis has value 'n' (None choice in Spectrometer Configuration window), 'w' (WFG+GCU), 'l' (Performa I), 'p' (Performa II/III), 'q' (Performa II/III + WFG), 't' (Performa XYZ), 'u' (Performa XYZ + WFG), 's' (SIS (12 bit), or 'h' (Homospoil). Homospoil is functional only for the Z axis.

See also: *VnmrJ Installation and Administration*; *NMR Spectroscopy User Guide*

Related: [config](#) Display current configuration and possibly change it (M)
[pfgon](#) PFG amplifiers on/off control (P)

graphis **Return the current graphics display status (C)**

Syntax: (1) `graphis:$display_command`
 (2) `graphis(command):$yes_no`

Description: Determines what command currently controls the graphics window.

Arguments: `$display_command` is a return value set to the name of the currently controlling command.

`command` is the name of a command to be checked.

`$yes_no` is a return value set to 1 if the command name given by the `command` argument is controlling the graphics window, or set to 0 if it is not controlling the window.

Examples:

```
graphis:$display
if ($display='ds') then
...
endif

graphis('ds'):$ds_on
if ($ds_on) then
...
endif
```

See also: *User Programming*

Related: [textis](#) Return the current text display status (C)

grayctr **Gray level window adjustment (P)**

Description: Controls the grayscale display available in **dcon**. In the **dconi** program, the center mouse button controls the grayscale bar, which changes the mean gray level and hence the value of **grayctr**. The **grayctr** parameter (along with the parameter **graysl**) records the current settings of the gray bar as the interaction changes; the value can also be set directly. The right mouse button controls the data level of the maximum data intensity. To create **grayctr**, enter **create('grayctr','real')**
setgroup('grayctr','display')
setlimit('grayctr',64,0,1).

To create the set of imaging parameters **grayctr**, **dcrmv** and **graysl**, and in the current experiment, enter **addpar('image')**.

Values: 0 to 64 (typically 32)

See also: *NMR Spectroscopy User Guide*

Related:	addpar	Add selected parameters to the current experiment (M)
	dcon	Display noninteractive color intensity map (C)
	dconi	Interactive 2D contour display (C)
	graysl	Gray level slope (contrast) adjustment (P)

graysl **Gray level slope (contrast) adjustment (P)**

Description: Controls the grayscale display available in **dcon**. In the **dconi** program, the center mouse button controls the grayscale slope as applied to the data changes and hence the value of **graysl**. Negative values of **graysl** will invert black and white; however, negative values can be set only from the keyboard. **graysl** (along with the parameter **grayctr**) records the current settings of the gray bar as the interaction changes; the value can also be set directly. The right mouse button controls the data level of the maximum data intensity. To create **graysl**, enter the following command:

```
create('graysl','real') setgroup('graysl','display')  

setlimit('graysl',10,-10,0.1)
```

To create the set of imaging parameters **graysl**, **dcrmv**, and **grayctr** in the current experiment, enter **addpar('image')**.

Values: -10 to +10 (-100 to +100, typically 1)

See also: *NMR Spectroscopy User Guide*

Related:	addpar	Add selected parameters to the current experiment (M)
	dcon	Display noninteractive color intensity map (C)
	dconi	Interactive 2D contour display (C)
	grayctr	Gray level window adjustment (P)

grecovery **Eddy current testing (M)**

Applicability: Systems with pulsed field gradient.

Description: Conditions an experiment for eddy current testing so that it is compatible with standard installation procedures.

See also: *Pulsed Field Gradient Modules Installation, NMR Spectroscopy User Guide*

grid **Draw a grid on a 2D display (M)**

Syntax: (1) **grid(<spacing>,<,><color>)>**
 (2) **grid(<start_f2,incr_f2,start_f1,incr_f1,<color>)>**

Description: Draws grid lines over a 2D display. Grid lines are drawn on the graphics screen in the XOR mode—entering a second `grid` command with identical arguments erases (not redraws) the grid displayed by the first command.

Arguments: `spacing` specifies the approximate spacing of the grid lines, in cm. The default is intervals of approximately 1 cm, rounded so that the intervals fall at a multiple of 1, 2, or 5 (in Hz), or 1p, 2p, or 5p (in ppm).

`color` specifies the color of the grid lines and is one of the following keywords: 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'black', or 'white'. The default is 'blue'.

`start_f2`, `incr_f2`, `start_f1`, `incr_f1` define a grid by supplying the starting and increment frequencies for f2 and f1. Add the p suffix to a value to enter it in ppm (see third example below).

Examples: `grid`
`grid(1.5, 'red')`
`grid(1p, 0.5p, 3p, 0.5p)`

See also: *NMR Spectroscopy User Guide*

Related: `plgrid` Plot a grid on a 2D plot (M)

groupcopy Copy parameters of group from one tree to another (C)

Syntax: `groupcopy(from_tree, to_tree, group)`

Description: Copies a set of parameters of a group from one parameter tree to another.

Arguments: `from_tree`, `to_tree` are two different parameter trees, each given by the one of the keywords 'global', 'current', or 'processed'. Refer to the `create` command for more information on trees.

`group` is the set of parameters to be copied and is one of the keywords 'all', 'sample', 'acquisition', 'processing', and 'display'.

Examples: `groupcopy('processed', 'current', 'acquisition')`

See also: *User Programming*

Related: `create` Create new parameter in a parameter tree (C)
`destroy` Destroy a parameter (C)
`destroygroup` Destroy parameters of a group in a tree (C)
`display` Display parameters and their attributes (C)
`setgroup` Set group of a parameter in a tree (C)

gspoil Spoiler gradient level (P)

Description: Predefined parameter to set a spoiler gradient level.

gsspat Slice-select gradient shape (P)

Description: Predefined string parameter to specify a slice-select gradient shape.

gttnoesy Set up a PFG TNNOSY parameter set (M)

Applicability: Systems with the pulsed field gradient (PFG) module.

Description: Converts a 1D standard two-pulse sequence parameter set into a parameter set ready to run a PFG NOESY experiment (either absolute value or phase sensitive) or a `gttnoesy` experiment.

G

gtnroesy	Set up a PFG absolute-value ROESY parameter set (M)	
Applicability:	Systems with the pulsed field gradient (PFG) module.	
Description:	Converts a 1D standard two-pulse sequence parameter set into a parameter set ready to run a PFG absolute-value ROESY experiment or a gtnroesy experiment.	
gtotlimit	Gradient total limit (P)	
Applicability:	Systems with three-axis gradients	
Description:	Sets the gradient limit, in gauss/cm, of the x, y, and z axes, summed together. This parameter is taken from an entry of the same name in a gradient table and should only exist if a gradient amplifier limits the combined output of all three gradient axis.	
Related:	gcoil	Read data from gradient calibration tables (P)
gtrim	Trim gradient level (P)	
Description:	Predefined parameter to set a trim gradient level.	
gxmax, gymax, gzmax	Maximum gradient strength for each axis (P)	
Applicability:	Systems with three-axis gradients.	
Description:	Defines the maximum gradient strength, in gauss/cm, for each gradient axis. These values are read in from the selected system gradient table whenever the parameter set is retrieved or the gradient coil defined by gcoil has changed. When the values are read in, gmax is set to the lowest value of the three. The parameters gxmax, gymax, and gzmax are used instead of gmax when the gradients strengths are not equal for each axis. Unequal gradient strengths per axis are generally true for systems with three-axis PFG coils, which have a strong z gradient, and can be true for microimaging systems. Horizontal-bore imaging systems usually have gradients set to the same maximum value, and gmax can be used.	
See also:	<i>NMR Spectroscopy User Guide; User Programming, VnmrJ Imaging NMR</i>	
Related:	gcoil gmax	Read data from gradient calibration tables (P) Maximum gradient strength (P)
gzlvl	Pulsed field gradient strength (P)	
Applicability:	Systems with gradient shimming installed.	
Description:	Specifies the pulsed field gradient DAC value.	
Values:	Range from +2047 to –2048 for 12-bit gradient module, and from +32767 to –32768 for a 16-bit gradient module.	
Related:	gzsize gzwin	Number of z-axis shims used by gradient shimming (P) Spectral window percentage used for gradient shimming (P)
gzsize	Number of z-axis shims used by gradient shimming (P)	
Applicability:	Systems with gradient shimming installed.	

Description: Specifies the number of z-axis shims used by gradient shimming. For example, `gzsize` set to 4 means that gradient shimming uses shims z1 to z4. By default, coarse shims are used if present, as determined by the `shimset` value

Values: Integer from 1 to 8.

Related:

<code>gmapshim</code>	Start gradient autoshimming (M)
<code>gmapsys</code>	Run gradient autoshimming, set parameters, map shims (M)
<code>gmapz</code>	Get parameters and files for <code>gmapz</code> pulse sequence (M)
<code>gzlvl</code>	Pulsed field gradient strength (P)
<code>gzwin</code>	Spectral width percentage used by gradient shimming (P)
<code>shimset</code>	Type of shimset (P)
<code>gmap_z1z4</code>	Gradient shimming flag to first shim z1-z4 (P)

gzwin

Spectral width percentage used for gradient shimming (P)

Applicability: Systems with gradient shimming installed.

Description: Specifies the percentage of the spectral width `sw` used by gradient shimming for shimmap calculations. The value is set automatically with the buttons Find `gzlvl/gzwin` and Find `gzwin` in the gradient shimming system menu opened by `gmapsys`.

Values: A real number between 0 and 100. The typical value is 50.

Related:

<code>gmapshim</code>	Start gradient autoshimming (M)
<code>gmapsys</code>	Run gradient autoshimming, set parameters, map shims (M)
<code>gmapz</code>	Get parameters and files for <code>gmapz</code> pulse sequence (M)
<code>gzlvl</code>	Pulsed field gradient strength (P)
<code>gzsize</code>	Number of z-axis shims used by gradient shimming (P)
<code>sw</code>	Spectral width in directly detected dimension (P)
<code>tof</code>	Frequency offset for observe transmitter (P)

H

<code>h1</code>	Automated proton acquisition (M)
<code>h1freq</code>	Proton frequency of spectrometer (P)
<code>h1p</code>	Process 1D proton spectra (M)
<code>h2cal</code>	Calculate strength of the decoupler field (C)
<code>halt</code>	Abort acquisition with no error (C)
<code>hc</code>	Automated proton and carbon acquisition (M)
<code>hcapt</code>	Automated proton, carbon, and APT acquisition (M)
<code>hcchtocsy</code>	Set up parameters for HCCHTOCSY pulse sequence (M)
<code>hccorr</code>	Automated proton, carbon, and HETCOR acquisition (M)
<code>hcdept</code>	Automated proton, carbon, and DEPT acquisition (M)
<code>hcosy</code>	Automated proton and COSY acquisition (M)
<code>hdmf</code>	Modulation frequency for the band selective homonuclear decoupling (P)
<code>hcmult</code>	Execute protocol actions of apptype hcmult (M)
<code>hdof</code>	Frequency offset for homodecoupling (P)
<code>hdpwr</code>	Power level for homodecoupling (P)
<code>hdpwrf</code>	Homodecoupling fine power (optional) (P)
<code>hdres</code>	Sets the tip angle resolution (P)
<code>hdseq</code>	Sets the decoupler waveform filename (P)
<code>hdwshim</code>	Hardware shimming (P)
<code>hdwshimlist</code>	List of shims for hardware shimming (P)
<code>het2dj</code>	Set up parameters for HET2DJ pulse sequence (M)
<code>HETCOR</code>	Change parameters for HETCOR experiment (M)
<code>hetcor</code>	Set up parameters for HETCOR pulse sequence (M)
<code>hetcorcpl</code>	Set up parameters for solids HETCOR pulse sequence (M)
<code>hetcorps</code>	Set up parameters for HETCORPS pulse sequence (M)
<code>hetero2d</code>	Execute protocol actions of apptype hetero2d (M)
<code>hidecommand</code>	Execute macro instead of command with same name (C)
<code>hipwrampenable</code>	High Power Amplifier Enable (P)
<code>Hmbc</code>	Convert the parameter to a HMBC experiment (M)
<code>Hmqc</code>	Convert the parameter to a HMQC experiment (M)
<code>HMQC15</code>	Set up parameters for ¹⁵ N HMQC experiment (M)
<code>HMQC_d2</code>	Set up parameters for ¹⁵ N HMQC experiment using dec. 2 (M)
<code>HMQC_d213</code>	Set up parameters for ¹³ C HMQC experiment using dec. 2 (M)
<code>hmqcr</code>	Set up parameters for HMQCR pulse sequence (M)
<code>Hmqctoxy</code>	Convert the parameter to a HMQCTOXY experiment (M)
<code>HMQCTOXY15</code>	Set up parameters for ¹⁵ N HMQCTOXY experiment (M)
<code>HMQCTOXY_d2</code>	Set up parameters for ¹⁵ N HMQCTOXY using decoupler 2 (M)
<code>HMQCTOXY_d213</code>	Set up parameters for ¹³ C HMQCTOXY using decoupler 2 (M)
<code>hmqctoxy3d</code>	Set up parameters for HMQC-TOCSY 3D pulse sequence (M)
<code>ho</code>	Horizontal offset (P)
<code>hom2dj</code>	Set up parameters for HOM2DJ pulse sequence (M)
<code>homo</code>	Homodecoupling control for the observe channel (P)

H

HOMODEC	Change parameters for HOMODEC experiment (M)
homo2d	Execute protocol actions of apptype homo2d (M)
homorof1	Delay before turning on homo decoupling rf (P)
homorof2	Delay after blanking the amp and setting T/R to receive (P)
homorof3	Delay between setting T/R switch to receive and gating the recvr on (P)
hoult	Set parameters alfa and rof2 according to Hoult (M)
hpa	Plot parameters on special preprinted chart paper (C)
Hprescan	Proton prescan (P)
hregions	Select integral regions in proton spectrum (M)
hs	Homospoil pulses (P)
Hsqc	Convert the parameter to a HSQC experiment (M)
HSQC15	Set up parameters for ¹⁵ N HSQC experiment (M)
HSQC_d2	Set up parameters for ¹⁵ N HSQC experiment using dec. 2 (M)
HSQC_d213	Set up parameters for ¹³ C HSQC experiment using dec. 2 (M)
hsqcHT	Set up the hsqcHT experiment (M)
Hsqctoxy	Convert parameters to a HSQCTOXY experiment (M)
HSQCTOXY15	Set up parameters for ¹⁵ N HSQCTOXY experiment (M)
HSQCTOXY_d2	Set up parameters for ¹⁵ N HSQCTOXY using decoupler 2 (M)
HSQCTOXY_d213	Set up parameters for ¹³ C HSQCTOXY using decoupler 2 (M)
hsqctoxySE	Set up parameters for HSQC-TOCSY 3D pulse sequence (M)
hsrotor	Display rotor speed for solids operation (P)
hst	Homospoil time (P)
htbitrev	Hadamard bit reversal flag (P)
htbw1	Hadamard pulse excitation bandwidth in ni (P)
htcall	RF calibration flag for Hadamard waveforms in ni (P)
htfrq1	Hadamard frequency list in ni (P)
htofs1	Hadamard offset in ni (P)
htpwr1	Power level for RF calibration of Hadamard waveforms in ni (P)
htss1	Stepsize for Hadamard waveforms in ni (P)
hzmm	Scaling factor for plots (P)
hztomm	Convert locations from Hz or ppm to plotter units (C)

h1 Automated proton acquisition (M)

Syntax: `h1<(solvent)>`

Description: Prepares parameters for automatically acquiring a standard ¹H spectrum. The parameter **wexp** is set to 'procplot' for standard processing. If h1 is used as the command for automation via the **enter** command, then **au** is supplied automatically and should not be entered on the MACRO line of the **enter** program. However, it is possible to customize h1 on the MACRO line by following it with additional commands and parameters. (e.g., entering h1 nt=1 uses the standard h1 setup but with only one transient).

Arguments: **solvent** is the name of the solvent. In automation mode, the solvent is supplied by the **enter** program. The default is 'CDCl3'.

Examples: `h1`
`h1('DMSO')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (M)
	<code>enter</code>	Enter sample information for automation run (C)
	<code>h1p</code>	Process 1D proton spectra (M)
	<code>procplot</code>	Automatically process FIDs (M)
	<code>wexp</code>	When experiment completes (P)

h1freq Proton frequency of spectrometer (P)

Description: Configuration parameter for the resonance frequency of ^1H as determined by the field strength of the magnet. The value is set using the label Proton Frequency in the Spectrometer Configuration window.

Values: 085, 100, 200, 300, 400, 500, 600, 700, 750, 800, 900 (in MHz); 3T, 4T.

See also: *VnmrJ Installation and Administration*

Related:	<code>config</code>	Display current configuration and possibly change it (M)

h1p Process 1D proton spectra (M)

Description: Processes non-arrayed 1D proton spectra using standard macros. `h1p` is called by `procl1d`, but can also be used directly. Fully automatic processing (up to a point where a spectrum could be plotted) is provided: Fourier transformation (using preset weighting functions), automatic phasing (`aphx` macro), select integral regions (`hregions` macro), adjust integral size (`integrate` macro), vertical scale adjustment (`vsadjc` macro), avoiding excessive noise (`noislm` macro), threshold adjustment (if required, `thadj` macro), and referencing to the TMS signal if present (`setref` macro, then `tmsref` macro).

See also: *NMR Spectroscopy User Guide*

Related:	<code>aphx</code>	Perform optimized automatic phasing (M)
	<code>h1</code>	Automated proton acquisition (M)
	<code>hregions</code>	Select integral regions for proton spectra (M)
	<code>integrate</code>	Automatically integrate 1D spectrum (M)
	<code>noislm</code>	Avoids excessive noise (M)
	<code>procl1d</code>	Processing macro for simple (non-arrayed) spectra (M)
	<code>setref</code>	Set frequency referencing for proton spectra (M)
	<code>thadj</code>	Adjust threshold (M)
	<code>tmsref</code>	Reference spectrum to TMS line (M)
	<code>vsadjh</code>	Adjust vertical scale for proton spectra (M)

h2cal Calculate strength of the decoupler field (C)

Syntax: `h2cal<(j1r,j2r<,j0>)><:gammah2,pw90,frequency>`

Description: Calculates the strength of the decoupler field. It uses the results from two experiments: one with the decoupler off-resonance at a lower frequency and the other with the decoupler off-resonance at a higher frequency than the frequency of the peak being decoupled.

Arguments: `j1r` is the frequency of the decoupler during these two experiments;. The default is that `h2cal` prompts for a value. If the parameter `dof` is arrayed and has two values, `h2cal` assumes these two values represent the decoupler frequencies; if `dof` is arrayed and has more than two values, `h2cal` prompts for the two decoupler frequencies.

`j2r` is the reduced coupling constants from the two experiments. The default is that `h2cal` prompts for a value

`j0` is the full coupling constant that results when no decoupling is done. The default is a value of 142 Hz, the constant for the standard sample dioxane, or 15 Hz for the methyl iodide sample.

`gammaH2` is a return value set to the strength of the decoupler field.

`pw90` is a return value set to the pulse width of a 90° pulse from the decoupler. It is related to the value of parameter `dmf` through the equation `dmf=1/pw90`.

`frequency` is a return value set to the coalescence point (i.e., frequency at which single-frequency decoupling would collapse the dioxane to a singlet).

See also: *NMR Spectroscopy User Guide*

Related: `dmf` Decoupler modulation frequency for first decoupler (P)
`dof` Frequency offset for first decoupler (P)

halt **Abort acquisition with no error (C)**

Syntax: `halt`

Description: Aborts an experiment that has been submitted to acquisition. If the experiment is active, it is aborted immediately, all data is discarded, and the experiment is interpreted as complete. Any data collected from an earlier block size transfer is retained. If any `wexp` processing is defined, that processing then occurs, followed by any queued experiments. The login name, and the FID directory path in `file` are used as keys to find the proper experiment to abort.

Under some circumstances, there is a delay between the time `go` is entered and the acquisition is started. During this time, instructions based on the selected pulse sequence are being generated. This is signified by the letters “PSG” appearing in the upper left corner of the status window. A `halt` command issued under these circumstances reports that no acquisition is active but it instead stops the instruction generation process and displays “PSG aborted”.

See also: *NMR Spectroscopy User Guide*

Related: `aa` Abort acquisition with error (C)
`file` File name of parameter set (P)
`go` Submit experiment to acquisition (C)
`wexp` Specify action when experiment completes (C)
`wexp` When experiment completes (P)

hc **Automated proton and carbon acquisition (M)**

Syntax: `hc<(solvent)>`

Description: Combines the operation of the `h1` and `c13` macros. In non-automation mode, both spectra are acquired in the experiment in which the `hc` macro was entered. After the completion of the acquisition, `rttmp` can be used for further processing of the two spectra.

Arguments: `solvent` is the solvent name. In automation mode, the `enter` program supplies the value. In non-automation mode, the default is '`cdcl3`'.

Examples: `hc`
`hc('dmsd')`

See also: *NMR Spectroscopy User Guide*

Related: `c13` Automatic carbon acquisition (M)
`enter` Enter sample information for automation run (M,U)
`h1` Automated proton acquisition (M)
`rttmp` Retrieve experiment data from experiment subfile (M)

hcapt Automated proton, carbon, and APT acquisition (M)

Syntax: `hcapt<(solvent)>`

Description: Combines the operation of the `h1` and `c13` macros and the APT experiment. In non-automation mode, all spectra are acquired in the experiment in which the `hcapt` macro was entered. After acquisition completes, `rttmp` can be used for further processing of the three spectra.

Arguments: `solvent` is the solvent name. In automation mode, the `enter` program supplies the value. In non-automation mode, the default is `'cdcl3'`.

Examples: `hcapt`
`hcapt('dmsd')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>Apt</code>	Set up parameters for APT experiment (M)
	<code>c13</code>	Automatic carbon acquisition (M)
	<code>enter</code>	Enter sample information for automation run (M,U)
	<code>h1</code>	Automated proton acquisition (M)
	<code>rttmp</code>	Retrieve experiment data from experiment subfile (M)

hcchtocsy Set up parameters for HCCHTOCSY pulse sequence (M)

Description: Used for sidechain assignments in fully ^{13}C -enriched molecules.

See also: *NMR Spectroscopy User Guide*

hccorr Automated proton, carbon, and HETCOR acquisition (M)

Syntax: `hccorr<(solvent)>`

Description: Combines the operation of the `h1` and `c13` macros and the HETCOR experiment. In non-automation mode, all spectra are acquired in the experiment in which `hccorr` is entered. After acquisition completes, `rttmp` can be used for further processing of the three spectra.

Arguments: `solvent` is the solvent name. In automation mode, the `enter` program supplies the value. In non-automation mode, the default is `'cdcl3'`.

Examples: `hccorr`
`hccorr('dmsd')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>c13</code>	Automated carbon acquisition (M)
	<code>enter</code>	Enter sample information for automation run (M,U)
	<code>h1</code>	Automated proton acquisition (M)
	<code>hetcor</code>	Set up parameters for HETCOR experiment (M)
	<code>rttmp</code>	Retrieve experiment data from experiment subfile (M)

hcdept Automated proton, carbon, and DEPT acquisition (M)

Syntax: `hcdept<(solvent)>`

Description: Combines the operation of the `h1` and `c13` macros and the DEPT experiment. In non-automation mode, all spectra are acquired in the experiment in which `hcdept` was entered. After the completion of the acquisition, `rttmp` can be used for further processing of the three spectra.

Arguments: `solvent` is the solvent name. In automation mode, the `enter` program supplies the value. In non-automation mode, the default is `'cdcl3'`.

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Examples: `hcdept`
`hcdept ('dmsd')`

See also: *NMR Spectroscopy User Guide*

Related: `c13` Automatic carbon acquisition (M)
`Dept` Set up parameters for DEPT experiment (M)
`enter` Enter sample information for automation run (M,U)
`h1` Automated proton acquisition (M)
`rttmp` Retrieve experiment data from experiment subfile (M)

hcosy Automated proton and COSY acquisition (M)

Syntax: `hcosy<(solvent)>`

Description: Combines the operation of the `h1` macro and the COSY experiment. In non-automation mode, both spectra are acquired in the experiment in which `hcosy` is entered. After acquisition completes, `rttmp` can be used for further processing of the two spectra.

Arguments: `solvent` is the solvent name. In automation mode, the `enter` program supplies the value. In non-automation mode, the default is '`cdcl3`'.

Examples: `hcosy`
`hcosy ('dmsd')`

See also: *NMR Spectroscopy User Guide*

Related: `enter` Enter sample information for automation run (C)
`h1` Automated proton acquisition (M)
`rttmp` Retrieve experiment data from experiment subfile (M)

hdmf Modulation frequency for homonuclear decoupling (P)

Applicability: VNMR5 liquids, 400 MR

Syntax: `hdmf=<value>`

Description: Sets the modulation frequency for the band selective homonuclear decoupling. The parameter specifies 1/pw90 at the power value, `hdpwr`, used for homonuclear decoupling. The parameter is not used with single frequency homonuclear decoupling.

Related: `dutyc` The rf duty cycle fraction for homonuclear decoupling (P)
`hdof` Frequency offset for homodecoupling (P)
`hdpwr` Sets the rf attenuator to control the power for homonuclear decoupling (P)
`hdpwrf` Sets the rf linear modulator fine power for homonuclear decoupling (P)
`hdres` Sets the tip angle resolution (P)
`hdseq` Sets the decoupler waveform filename (P)
`homo` Homodecoupling control for observe channel (P)
`homorof1` Delay before turning on homo decoupling rf (P)
`homorof2` Delay after blanking the amplifier and setting T/R switch to receive (P)
`homorof3` Delay between setting T/R switch to receive gating on the receiver (P)
`tn` Nucleus for observe transmitter (P)

hcmult Execute protocol actions of apptype hcmult (M)

Description: This macro is used to execute the protocol actions of the hcmult apptype.

Examples: `hcmult('setup')` – execute hcmult experimental setup
`hcmult('process')` – execute hcmult processing
`hcmult('plot')` – execute hcmult plotting

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related: `apptype` Application type (P)
`execpars` Set up the exec parameters (M)

hdo f Frequency offset for homodecoupling (P)

Applicability: VNMRs systems

Syntax: `hdo f=<value>`

Description: Sets the irradiation frequency offset for homonuclear decoupling and similar to how `to f`, and `do f` determine the frequency. The parameter is not used if `hdseq` is set to a filename.

Values: –100000 to 100000 Hz in steps of 0.1 Hz.

Related: `dutyc` The rf duty cycle fraction for homonuclear decoupling (P)
`hdmf` modulation frequency for the band selective homonuclear decoupling (P)
`hdpwr` Sets the rf attenuator to control the power for homonuclear decoupling (P)
`hdpwrf` Homodecoupling fine power (optional) (P)
`hdres` Sets the tip angle resolution (P)
`hdseq` Sets the decoupler waveform filename (P)
`homo` Homodecoupling control for observe channel (P)
`homorof1` Delay before turning on homo decoupling rf (P)
`homorof2` Delay after blanking the amplifier and setting T/R switch to receive (P)
`homorof3` Delay between setting T/R switch to receive gating on the receiver (P)
`tn` Nucleus for observe transmitter (P)

hdpwr Power level for homodecoupling (P)

Applicability: VNMRs systems, 400 MR

Syntax: `hdpwr=<value>`

Description: Sets the rf attenuator to control the power for homonuclear decoupling. The `dutyc` parameter must be accounted for when setting `hdpwr`.

Values: –16 to 50 dB

CAUTION: Homodecoupling power greater than 2 watts in a switchable probe will damage the probe. Always carefully calibrate homodecoupling to avoid exceeding 2 watts. The maximum value for `hdpwr` is set to 49, corresponding to about 2 watts of power. The actual power delivered depends on the CW duty cycle. Before using close to the maximum value of power or duty cycle, ensure safe operation by measuring the output power.

Related: `dutyc` The rf duty cycle fraction for homonuclear decoupling (P)
`hdmf` modulation frequency for the band selective homonuclear decoupling (P)
`hdo f` Frequency offset for homodecoupling (P)
`hdpwrf` Homodecoupling fine power (optional) (P)
`hdres` Sets the tip angle resolution (P)
`hdseq` Sets the decoupler waveform filename (P)

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<code>homo</code>	Homodecoupling control for observe channel (P)
<code>homorof1</code>	Delay before turning on homo decoupling rf (P)
<code>homorof2</code>	Delay after blanking the amplifier and setting T/R switch to receive (P)
<code>homorof3</code>	Delay between setting T/R switch to receive gating on the receiver (P)
<code>tn</code>	Nucleus for observe transmitter (P)

hdpwrf Homodecoupling fine power (optional) (P)

Applicability: VNMR5 liquids systems

Syntax: `hdpwrf=<value>`

Description: Sets the rf linear modulator fine power for homonuclear decoupling. The default is 4095 if the variable does not exist. Attenuation is added to the attenuation set by `hdpwr`.

Values: 0-4095

Related:	<code>dutyc</code>	The rf duty cycle fraction for homonuclear decoupling (P)
	<code>hdmf</code>	Modulation frequency for the band selective homonuclear decoupling (P)
	<code>hdof</code>	Frequency offset for homodecoupling (P)
	<code>hdpwr</code>	Sets the rf attenuator to control the power for homonuclear decoupling (P)
	<code>hdres</code>	Sets the tip angle resolution (P)
	<code>hdseq</code>	Sets the decoupler waveform filename (P)
	<code>homo</code>	Homodecoupling control for observe channel (P)
	<code>homorof1</code>	Delay before turning on homo decoupling rf (P)
	<code>homorof2</code>	Delay after blanking the amplifier and setting T/R switch to receive (P)
	<code>homorof3</code>	Delay between setting T/R switch to receive gating on the receiver (P)
	<code>tn</code>	Nucleus for observe transmitter (P)

hdres Sets the tip angle resolution (P)

Applicability: VNMR5 liquids systems

Syntax: `hdres=<value>`

Description: Sets the tip angle resolution to be used for the band selective waveform mode of homonuclear decoupling. The parameter is not used with single frequency homonuclear decoupling.

Values: 1 to 90 in units of degrees with 1 degree resolution

Related:	<code>dutyc</code>	The rf duty cycle fraction for homonuclear decoupling (P)
	<code>hdmf</code>	Modulation frequency for the band selective homonuclear decoupling (P)
	<code>hdof</code>	Frequency offset for homodecoupling (P)
	<code>hdpwr</code>	Sets the rf attenuator to control the power for homonuclear decoupling (P)
	<code>hdpwrf</code>	Sets the rf linear modulator fine power for homonuclear decoupling (P)
	<code>hdseq</code>	Sets the decoupler waveform filename (P)
	<code>homo</code>	Homodecoupling control for observe channel (P)
	<code>homorof1</code>	Delay before turning on homo decoupling rf (P)
	<code>homorof2</code>	Delay after blanking the amplifier and setting T/R switch to receive (P)
	<code>homorof3</code>	Delay between setting T/R switch to receive gating on the receiver (P)
	<code>tn</code>	Nucleus for observe transmitter (P)

hdseq Waveform filename for band selective decoupling (P)

Applicability: VNMR5 liquids systems

Syntax: `hdseq= ' filename ' — the file must have a .DEC. extension.`

Description: Sets the decoupler waveform filename (.DEC extension) for the band selective waveform mode. The irradiation frequency is determined by the transmitter offset last applied to the observe channel in the pulse sequence (typically `tof`) and any additional frequency offset from any phase modulation programmed implicitly into the waveform .DEC file.

Examples: `hdseq= ' ' or does not exist — single frequency decoupling is used.`

Related:

- `dutyc`
- `hdmf` modulation frequency for the band selective homonuclear decoupling (P)
- `hdof` Frequency offset for homodecoupling (P)
- `hdpwr` Sets the rf attenuator to control the power for homonuclear decoupling (P)
- `hdpwrf` Sets the rf linear modulator fine power for homonuclear decoupling (P)
- `hdres` Sets the tip angle resolution (P)
- `homo` Homodecoupling control for observe channel (P)
- `homorof1` Delay before turning on homo decoupling rf (P)
- `homorof2` Delay after blanking the amplifier and setting T/R switch to receive (P)
- `homorof3` Delay between setting T/R switch to receive gating on the receiver (P)
- `tn` Nucleus for observe transmitter (P)

hdwshim Hardware shimming (P)

Applicability: Systems with additional Z1 shimming hardware.

Description: Allows `go`, `su`, `au`, etc., to turn on and off shimming hardware. Hardware shimming is automatically suspended during software autoshimming. Hardware shimming is only active during acquisition (`go`, `ga`, `au`). `hdwshim` is a global parameter, so it affects all experiments.

Values: `'y'` turns hardware shimming on.

`'p'` turns hardware shimming on during presaturation pulse (power level change followed by pulse).

`'n'` turns shimming off.

See also: *NMR Spectroscopy User Guide*

Related:

- `au` Submit experiment to acquisition and process data (C)
- `go` Submit experiment to acquisition (C)
- `su` Submit a setup experiment to acquisition (M)
- `ga` Submit experiment to acquisition and FT the result (M)

hdwshimlist List of shims for hardware shimming (P)

Description: A global parameter that sets the shims to use during hardware shimming. If it does not exist, hardware shimming uses `z1` by default. To create the parameter, use `create('hdwshimlist', 'string', 'global')`.

Values: Any string composed of `z1`, `z1c`, `z2`, `z2c`, `x1`, `y1`. Commas and blank space are ignored. Shimming is done in the order `z1`, `z2`, `x1`, `y1`, regardless of the order in the string.

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Examples: `hdwshimlist='z1'`
`hdwshimlist='z1z2x1y1'`

See also: *NMR Spectroscopy User Guide*

Related: [create](#) Create new parameter in a parameter tree (C)
[hdwshim](#) Hardware shimming (P)

het2dj Set up parameters for HET2DJ pulse sequence (M)

Description: Sets up a HET2DJ (heteronuclear 2D-J) experiment.

See also: *NMR Spectroscopy User Guide*

Related: [foldj](#) Fold J-resolved 2D spectrum about $f1=0$ axis (C)

HETCOR Change parameters for HETCOR experiment (M)

Description: Converts the current parameter set to a HETCOR experiment. This is a phase-sensitive, multiplicity-selected experiment.

hetcor Set up parameters for HETCOR pulse sequence (M)

Syntax: `hetcor<(exp_number)>`

Description: Sets up a HETCOR (heteronuclear chemical shift correlation) experiment.

Arguments: `exp_number` is the number of the experiment, from 1 to 9, in which a proton spectrum of the sample already exists.

See also: *NMR Spectroscopy User Guide*

Related: [plhxcor](#) Plot X,H-correlation 2D spectrum (M)
[ppcal](#) Proton decoupler pulse calibration (M)

hetcorcp1 Set up parameters for solids HETCOR pulse sequence (M)

Applicability: Systems with the solids module.

Description: Sets up a parameter set, obtained with XPOLAR1, for HETCORCP1, the solid-state heteronuclear correlation experiment.

See also: *User Guide: Solid-State NMR*

Related: [xpolar1](#) Set up parameters for XPOLAR1 pulse sequence (M)

hetcorps Set up parameters for HETCORPS pulse sequence (M)

Description: Sets up parameters for a heteronuclear chemical shift correlation experiment (absolute value and phase sensitive).

See also: *NMR Spectroscopy User Guide*

hetero2d Execute protocol actions of apptype hetero2d (M)

Applicability: Liquids

Description: Perform the actions for Homonuclear 2D protocols to set up, process, and plot experiments.

Examples: `hetero2d('setup')` execute hetero2d experimental setup
`hetero2d('process')` execute hetero2d processing
`hetero2d('plot')` execute hetero2d plotting

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related: [apptype](#) Application type (P)
[execpars](#) Set up the exec parameters (M)

hidecommand Execute macro instead of command with same name (C)

Syntax: (1) `hidecommand(command_name) <:$new_name>`
 (2) `hidecommand(' ? ')`

Description: Renames (or hides) a built-in VnmrJ command so that a macro with the same name as the built-in command is executed instead of the built-in command.

Arguments: `command_name` is the name of the command to be renamed. To reset the built-in command back to its original name, enter `hidecommand` with the hidden name as the argument.

`$new_name` returns the new name of the built-in command. By using this new name, access is still available to the built-in command.

`' ? '` is a keyword to display a list of all of the renamed built-in commands and their original names.

Examples: `hidecommand('sys'):$newname`
`hidecommand('Sys')`
`hidecommand(' ? ')`

See also: *System Administration; User Programming*

Related: [which](#) Display which macro or command is used (M)

hipwrampenable High Power Amplifier Enable (P)

Applicability: VNMRs solids and systems with high power amplifiers.

Description: This parameter controls the High/Low Power Relay. If the parameter does not exist low power is used. If the parameter exists and the field corresponding to the physical channel is 'n' then low power is used. If the parameter exists and the field corresponding to the physical channel is 'y' then high power is used. The parameter is created in the current tree as a flag with `create('hipwrampenable', 'flag')`.

Values: 'y' Enable high power
 'n' Enable low power and disable high power

Examples: `hipwrampenable='yny'`
 Physical channel 1 and 3 are high power enabled. Physical channel 2 is low power.

Hmbc Convert the parameter to a HMBC experiment (M)

Description: Convert the parameter to a HMBC experiment.

See also: *NMR Spectroscopy User Guide*

Hmqc Convert the parameter to a HMQC experiment (M)

Description: Convert the parameter to a HMQC experiment.

HMQC15 Set up parameters for ¹⁵N HMQC experiment (M)

Description: Converts the current parameter set to a HMQC experiment for ¹⁵N.

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HMQC_d2	Set up parameters for ^{15}N HMQC experiment using dec. 2 (M)
Description:	Converts the current parameter set to a HMQC experiment for ^{15}N with decoupler 2 as ^{15}N .
HMQC_d213	Set up parameters for ^{13}C HMQC experiment using dec. 2 (M)
Description:	Converts the current parameter set to a HMQC experiment for ^{13}C with decoupler 2 as ^{13}C .
hmqcr	Set up parameters for HMQCR pulse sequence (M)
Applicability:	Not needed in current systems. Normally was used in systems with a ^1H only decoupler.
Description:	Sets up a HMQC (heteronuclear multiple-quantum coherence) experiment with “reverse” configuration.
See also:	<i>NMR Spectroscopy User Guide</i>
Hmqctoxy	Convert the parameter to a HMQCTOXY experiment (M)
Description:	Convert the parameter to a HMQCTOXY experiment.
HMQCTOXY15	Set up parameters for ^{15}N HMQCTOXY experiment (M)
Description:	Converts the current parameter set to a HMQCTOXY experiment for ^{15}N .
HMQCTOXY_d2	Set up parameters for ^{15}N HMQCTOXY using decoupler 2 (M)
Description:	Converts the current parameter set to a HMQCTOXY experiment for ^{15}N with decoupler 2 as ^{15}N .
HMQCTOXY_d213	Set up parameters for ^{13}C HMQCTOXY using decoupler 2 (M)
Description:	Converts the current parameter set to a HMQCTOXY experiment for ^{13}C with decoupler 2 as ^{13}C .
hmqctoxy3d	Set up parameters for HMQC-TOCSY 3D pulse sequence (M)
Description:	Sets up parameters for a HMQC-TOCSY 3D experiment with a presaturation option.
ho	Horizontal offset (P)
Description:	Horizontal offset of the each spectrum in a “stacked display” with respect to the previous spectrum,. For 1D data sets, the parameter vo sets the vertical offset. For 2D data sets, the parameter wc2 sets the vertical distance (in mm) between the first and last traces.
Values:	Number, in mm, for offset size. For a “left-to-right” presentation, ho is typically negative; for “bottom-to-top” presentation, vo or wc2 is positive.
hom2dj	Set up parameters for HOM2DJ pulse sequence (M)
Description:	Sets up a HOM2DJ (homonuclear J-resolved 2D) experiment.
See also:	<i>NMR Spectroscopy User Guide</i>

homo Homodecoupling control for the observe channel (P)

Applicability: VNMR5 liquids systems

Description: Homonuclear decoupling irradiates a single frequency if `hdseq = ''` (or if `hdseq` does not exist) or a frequency band if `hdseq = 'filename'`. Pulse sequences do not require explicit homonuclear gating commands (`homo` function is similar to `dm`). A single RF channel, the observe channel, is used. The `homo = 'y'` setting cannot be used with pulse sequences containing explicit acquire commands.

Syntax: `homo=<'y' or 'n'>`

Values: `'y'` homonuclear decoupling rf and receiver gating is turned on during the acquisition time. Provides single frequency or band selective (`hdseq = 'filename'`) decoupling.

`'n'` homonuclear decoupling rf and receiver gating is turned off.

Related:	<code>hdof</code>	Frequency offset for homodecoupling (P)
	<code>hdpwr</code>	Power level for homodecoupling (P)
	<code>hdpwrf</code>	Homodecoupling fine power (P)
	<code>dutyc</code>	Duty cycle for homodecoupling (optional) (P)
	<code>tn</code>	Nucleus for observe transmitter (P)
	<code>homorof1</code>	Delay before turning on homo decoupling rf (P)
	<code>homorof2</code>	Delay after blanking the amplifier and setting T/R switch to receive (P)
	<code>homorof3</code>	Delay between setting T/R switch to receive gating on the receiver (P)

HOMODEC Change parameters for HOMODEC experiment (M)

Description: Converts the current parameter set to a HOMODEC experiment. A 1D proton spectrum is displayed to do peak selection.

homo2d Execute protocol actions of apptype homo2d (M)

Applicability: Liquids

Description: Perform the actions for Heteronuclear 2D protocols to set up, process, and plot experiments.

Examples: `homo2d('setup')` execute homo2d experimental setup
`homo2d('process')` execute homo2d processing
`homo2d('plot')` execute homo2d plotting

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related:	<code>apptype</code>	Application type (P)
	<code>execpars</code>	Set up the exec parameters (M)

homorof1 Delay before turning on homo decoupling rf (P)

Applicability: VNMR5 liquids systems

Description: Optional parameter for delay before turning on homonuclear decoupling after gating the receiver off. The amplifier is un-blanked and T/R switch set to transmit mode during `homorof1` delay (in μ sec. units). A default delay of 2 μ sec. is used if the parameter does not exist.

Values: 2 to 5 μ sec. are typical.

Related:	dutyc	The rf duty cycle fraction for homonuclear decoupling (P)
	hdmf	Modulation frequency for the band selective homonuclear decoupling (P)
	hdof	Frequency offset for homodecoupling (P)
	hdpwr	Sets the rf attenuator to control the power for homonuclear decoupling (P)
	hdpwrf	Sets the rf linear modulator fine power for homonuclear decoupling (P)
	hdseq	Sets the decoupler waveform filename (P)
	hdres	Sets the tip angle resolution (P)
	homo	Homodecoupling control for observe channel (P)
	homorof2	Delay after blanking the amplifier and setting T/R switch to receive (P)
	homorof3	Delay between setting T/R switch to receive gating on the receiver (P)
	tn	Nucleus for observe transmitter (P)

homorof2 Delay after blanking the amp and setting T/R switch to recv (P)

Applicability: VNMR5 liquids systems

Description: Optional parameter for delay after the transmitter is gated off, the amplifier is blanked, and before the T/R switch is set to receive. A default delay of 2 μ sec. is used if the parameter does not exist.

Values: 2 to 5 μ sec. are typical.

Related:	dutyc	The rf duty cycle fraction for homonuclear decoupling (P)
	hdmf	Modulation frequency for the band selective homonuclear decoupling (P)
	hdof	Frequency offset for homodecoupling (P)
	hdpwr	Sets the rf attenuator to control the power for homonuclear decoupling (P)
	hdpwrf	Sets the rf linear modulator fine power for homonuclear decoupling (P)
	hdseq	Sets the decoupler waveform filename (P)
	hdres	Sets the tip angle resolution (P)
	homo	Homodecoupling control for observe channel (P)
	homorof1	Delay before turning on homo decoupling rf (P)
	homorof3	Delay between setting T/R switch to receive gating on the receiver (P)
	tn	Nucleus for observe transmitter (P)

homorof3 Delay between setting T/R to receive and gating the recvr on (P)

Applicability: VNMR5 liquids systems

Description: Optional parameter for delay after the T/R switch is set to receive and before the receiver gate is gated on. A default delay of 2 μ sec. is used if the parameter does not exist.

Values: 2 to 5 μ sec. are typical

Related:	dutyc	The rf duty cycle fraction for homonuclear decoupling (P)
	hdmf	Modulation frequency for the band selective homonuclear decoupling (P)
	hdof	Frequency offset for homodecoupling (P)
	hdpwr	Sets the rf attenuator to control the power for homonuclear decoupling (P)
	hdpwrf	Sets the rf linear modulator fine power for homonuclear decoupling (P)
	hdseq	Sets the decoupler waveform filename (P)
	hdres	Sets the tip angle resolution (P)
	homo	Homodecoupling control for observe channel (P)
	homorof1	Delay before turning on homo decoupling rf (P)
	homorof2	Delay after blanking the amplifier and setting T/R switch to receive (P)
	tn	Nucleus for observe transmitter (P)

- hoult** **Set parameters alfa and rof2 according to Hoult (M)**
- Description: Sets the values of `alfa` and `rof2` according to a prescription advanced by D. I. Hoult (*J. Magn. Reson.* **51**, 110 (1983)). These parameters set the times that follow the final pulse, which can be important where the flatness of the baseline is of concern.
- See also: *NMR Spectroscopy User Guide*
- Related: `alfa` Set `alfa` delay before acquisition (P)
`calfa` Recalculate `alfa` so that first-order phase is zero (M)
`rof2` Receiver gating time following pulse (P)
- hpa** **Plot parameters on special preprinted chart paper (C)**
- Description: Plots a predetermined list of parameters by “filling in the blanks” at the bottom of the preprinted chart paper available for Hewlett-Packard 7475- and 7550-series plotters.
- See also: *NMR Spectroscopy User Guide*
- Related: `apa` Plot parameters automatically (M)
`x0` X-zero position of HP plotter or Postscript device (P)
`y0` Y-zero position of HP plotter or Postscript device (P)
- Hprescan** **Proton prescan (P)**
- Applicability: *VnmrJ Walkup*
- Description: This parameter is used to keep track of the type and status of the Proton prescan. It is used for Proton, Presat, Wet1d, and Minsw protocols.
- See also: *VnmrJ Walkup*
- Related: `xmHprescan` Set up and process Proton prescans (M)
- hregions** **Select integral regions in proton spectrum (M)**
- Description: Selects integral regions, a critical step in automatic processing of proton spectra. It is critical not only because of aesthetic reasons (some people like many small integrals, others prefer a few large regions), but also because other commands, such as `bc`, depend on the correct integration: `bc` can either fail or it can make broad, unintegrated lines disappear from the spectrum. `hregions` was specifically designed for proton spectra and should not be used for other types of spectra. The result of `hregions` also depends on the lineshape and the signal-to-noise ratio of a spectrum
- See also: *NMR Spectroscopy User Guide*
- Related: `bc` 1D and 2D baseline correction (C)
`integrate` Automatically integrate 1D spectrum (M)
- hs** **Homospoil pulses (P)**
- Description: Turns on homospoil pulses at various times in different pulse sequences. Homospoil is a process by which the homogeneity is temporarily made very bad (“spoiled”) to cause any transverse magnetizations present at that time to decay rapidly to zero. `hst` controls the length of any homospoil pulse.
- Values: In a standard two-pulse sequence, homospoil pulses can be inserted during periods A and B (delays `d1` and `d2`): `hs= ' yn '` gives a homospoil pulse at the beginning of `d1`, `hs= ' ny '` gives a pulse during `d2`, and `hs= ' yy '` gives

homospoil pulses during both **d1** and **d2**. The desired value is generally `hs= 'nn'`.

See also: *NMR Spectroscopy User Guide*

Related: **d1** First delay (P)
d2 Incremented delay in 1st indirectly detected dimension (P)
hst Homospoil time (P)

Hsqc Convert the parameter to a HSQC experiment (M)

Description: Convert the parameter to a HSQC experiment.

HSQC15 Set up parameters for ¹⁵N HSQC experiment (M)

Description: Converts the current parameter set to a HSQC experiment for ¹⁵N.

HSQC_d2 Set up parameters for ¹⁵N HSQC experiment using dec. 2 (M)

Description: Converts the current parameter set to a HSQC experiment for ¹⁵N with decoupler 2 as ¹⁵N.

HSQC_d213 Set up parameters for ¹³C HSQC experiment using dec. 2 (M)

Description: Converts the current parameter set to a HSQC experiment for ¹³C with decoupler 2 as ¹³C.

hsqcHT Set up the hsqcHT experiment (M)

Description: Sets up parameters for a Hadamard-encoded hsqc experiment.

See also: *NMR Spectroscopy User Guide*

Related: **htofs1** Hadamard frequency list in **ni** (P)
htfrq1 Hadamard offset in **ni** (P)
fn1 Fourier number in 1st indirectly detected dimension (P)
ni Number of increments in 1st indirectly detected dimension (P)
ft2d Fourier transform 2D data (C)
sethtfrq1 Set a Hadamard frequency list from a line list (M)
Hsqc Set up parameters for HSQC experiment (M)

Hsqctoxy Convert parameters to a HSQCTOXY experiment (M)

Description: Convert the parameter to a HSQCTOXY experiment.

HSQCTOXY15 Set up parameters for ¹⁵N HSQCTOXY experiment (M)

Description: Converts the current parameter set to a HSQCTOXY experiment for ¹⁵N.

HSQCTOXY_d2 Set up parameters for ¹⁵N HSQCTOXY using decoupler 2 (M)

Description: Converts the current parameter set to a HSQCTOXY experiment for ¹⁵N with decoupler 2 as ¹⁵N.

HSQCTOXY_d213 Set up parameters for ¹³C HSQCTOXY using decoupler 2 (M)

Description: Converts the current parameter set to a HSQCTOXY experiment for ¹³C with decoupler 2 as ¹³C.

hsqctoxySE Set up parameters for HSQC-TOCSY 3D pulse sequence (M)

Description: Sets up parameters for a HSQC -TOCSY 3D experiment.

hsrotor Display rotor speed for solids operation (P)

Applicability: Systems equipped with the rotor synchronization module.

Description: Controls display of rotor speed. Depending on whether the rotor synchronization module is present (set by the Rotor Synchronization label in the Spectrometer Configuration window, parameter **rotorsync** is set to 1 or 0. The **xpolar1** macro in turn uses this to create **hsrotor**, which is set to 'y' if rotor synchronization is present. If the parameter **srates** exists, it is updated to the spin speed of the rotor at the end of the experiment. The interlock function specified by parameter **in** also changes. If **hsrotor**= 'y' and **in**= 'y', the experiment is terminated if rotor speed deviates more than 100 Hz.

hst Homospoil time (P)

Description: Controls pulse length if homospoil is activated by the **hs** parameter.

Values: 0 to 20 ms (limited by hardware).

Values: 'n' makes **srates** unmodified by acquisition and turns off the rotor speed display in **Acqstat**.

'y' makes the hardware information from the rotor synchronization board update **srates** and displays the rotor speed in the **Acqstat** status display.

See also: *User Guide: Solid-State NMR*

Related:	Acqstat	Bring up the acquisition status display (U)
	config	Display current configuration and possibly change it (M)
	in	Interlock (P)
	rotorsync	Rotor synchronization (P)
	srates	Spinning speed (P)
	xpolar1	Set up parameters for XPOLAR1 pulse sequence (M)

htbitrev Hadamard bit reversal flag (P)

Description: A flag to enable or disable bit reversal of the Hadamard matrix. The flag should be the same for both acquisition and processing for the Hadamard transform to be successful.

Values: 'y' enable Hadamard bit reversal
 'n' disable Hadamard bit reversal
 Default value is 'n'.

See also: *NMR Spectroscopy User Guide*

Related:	htfrq1	Hadamard frequency list in ni (P)

htbw1 Hadamard pulse excitation bandwidth in ni (P)

Description: The excitation bandwidth used to generate the frequencies contained in the shaped pulses used by the Hadamard matrix. If a single value is specified, the same bandwidth is used for all frequencies. If the parameter is arrayed, the bandwidth array element is used by the corresponding array element in **htfrq1**.

Values: Default value is 20.0 if the parameter does not exist.

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See also: *NMR Spectroscopy User Guide*

Related: [htfrq1](#) Hadamard frequency list in [ni](#) (P)
[ni](#) Number of increments in 1st indirectly detected dimension (P)

htcal1 RF calibration flag for Hadamard waveforms in ni (P)

Description: A flag to allow power optimization of Hadamard waveforms in the 1st indirect dimension.

Values: 0 power optimization using [htpwr1](#) is disallowed
>0 power optimization using [htpwr1](#) is allowed
Default value is 0.

See also: *NMR Spectroscopy User Guide*

Related: [htfrq1](#) Hadamard frequency list in [ni](#) (P)
[htpwr1](#) Power level for rf calibration of Hadamard waveforms in [ni](#) (P)
[ni](#) Number of increments in 1st indirectly detected dimension (P)

htfrq1 Hadamard frequency list in ni (P)

Description: A list of frequencies used in Hadamard spectroscopy, used for creating the Hadamard pulse shapes, and for placing the transformed traces at the correct frequencies in the indirect dimension.

Values: Typical values are an arrayed set of frequencies between $-sw1/2$ and $sw1/2$.

See also: *NMR Spectroscopy User Guide*

Related: [htofs1](#) Hadamard offset in [ni](#) (P)
[fn1](#) Fourier number in 1st indirectly detected dimension (P)
[ni](#) Number of increments in 1st indirectly detected dimension (P)
[sethtfrq1](#) Set Hadamard frequency list from a line list (M)
[procl](#) Type of processing on [ni](#) interferogram (P)
[sw1](#) Spectral width in 1st indirectly detected dimension (P)

htofs1 Hadamard offset in ni (P)

Description: The number of array elements to skip in [ni](#) when doing the Hadamard transform. The first element of the Hadamard matrix typically has all positive values (++++), and is usually not useful in constructing the Hadamard data.

Values: Default value is 0. Typical values are 1 or 2.

See also: *NMR Spectroscopy User Guide*

Related: [htfrq1](#) Hadamard frequency list in [ni](#) (P)
[fn1](#) Fourier number in 1st indirectly detected dimension (P)
[ni](#) Number of increments in 1st indirectly detected dimension (P)
[ft2d](#) Fourier transform 2D data (C)
[procl](#) Type of processing on [ni](#) interferogram (P)

htpwr1 Power level for RF calibration of Hadamard waveforms in ni (P)

Description: Power level for optimizing Hadamard waveforms in the 1st indirect dimension.

Values: -16 to 63 dB in steps of 1 dB.

See also: *NMR Spectroscopy User Guide*

Related: [htfrq1](#) Hadamard frequency list in [ni](#) (P)
[htcal1](#) RF calibration flag for Hadamard waveforms in [ni](#) (P)
[ni](#) Number of increments in 1st indirectly detected dimension (P)

htssl Stepsize for Hadamard waveforms in ni (P)

Description: Sets the stepsize during Hadamard waveform creation. Typically, this parameter is not needed, and a default stepsize is used.

Values: Does not exist - default stepsize is used.
 0 default stepsize is used.
 >0 stepsize in microseconds.

See also: *NMR Spectroscopy User Guide*

Related: [htfrq1](#) Hadamard frequency list in ni (P)
[ni](#) Number of increments in 1st indirectly detected dimension (P)

hzmm Scaling factor for plots (P)

Description: Contains the quotient of [wp](#) divided by [wc](#), a scaling factor useful for plotting. hzmm applies to 1D only.

See also: *NMR Spectroscopy User Guide*

Related: [wc](#) Width of chart (P)
[wp](#) Width of plot (P)

hztomm Convert locations from Hz or ppm to plotter units (C)

Syntax: (1) `hztomm(x_position)<:xmm>`
 (2) `hztomm(x_position,y_position)<:xmm,ymm>`
 (3) `hztomm(<'box',><'plotter'|'graphics',>x_left, x_right,y_bottom,y_top)<:x1mm,x2mm,y1mm,y2mm>`

Description: Converts locations from Hz, or ppm, to plotter units.

Arguments: `x_position` in syntax 1 is a location along the 1D axis, in Hz or ppm, to be converted to plotter units using the current values of parameters [sp](#) and [wp](#). Plotter units are mm on most plots and are scaled for graphics display. For ppm entries, use the `p` suffix following numerical values (see first example below).

`x_position,y_position` in syntax 2 is a coordinate, in Hz or ppm, on a 2D plot to be converted to plotter units, using the parameters [sp](#) and [wp](#) to convert the horizontal position and the parameters [sp1](#) and [wp1](#) to convert the vertical position.

`x_left,x_right,y_bottom,y_top` in syntax 3 are box edges, in Hz or ppm, on a 2D plot to be converted to plotter units, using the parameters [sp](#) and [wp](#) to convert the left and right edges, and parameters [sp1](#) and [wp1](#) to convert the top and bottom edges.

'`box`' is a keyword to draw a box and to make the first two return arguments, if supplied, give the location of the upper left corner of the box, in plotter units.

'`plotter`' is a keyword to select the plotter. The default is '`graphics`'.

'`graphics`' is a keyword to select the graphics screen. This is the default.

`x1mm,x2mm,y1mm,y2mm` are return arguments giving values in plotter units. If return arguments are not supplied, the results are displayed instead.

Examples: `hztomm(20p)`
`hztomm(xpos,ypos):xmm,ymm`
`hztomm('box','plotter',20,50,10,30)`

See also: *NMR Spectroscopy User Guide*

Related: [box](#) Draw a box on a plotter or graphics display (C)
[sp](#) Start of plot in directly detected dimension (P)
[sp1](#) Start of plot in 1st indirectly detected dimension (P)

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<code>wp</code>	Width of plot in directly detected dimension (P)
<code>wp1</code>	Width of plot in 1st indirectly detected dimension (P)

i	Insert sample (M)
ihwinfo	Hardware status of console (U)
il	Interleave arrayed and 2D experiments (P)
ilfid	Interleave FIDs during data processing (C)
imagefile	Display an image file (M)
imagemath	Fit images to an specified function (M)
imageprint	Plot non interactive gray scale image (M)
imconi	Display 2D data in interactive grayscale mode (M)
in	Lock and spin interlock (P)
inadqt	Set up parameters for INADEQUATE pulse sequence (M)
index2	Projection or 3D plane index selected (P)
inept	Set up parameters for INEPT pulse sequence (M)
initialize_iterate	Set iterate string to contain relevant parameters (M)
input	Receive input from keyboard (C)
ins	Integral normalization scale (P)
ins2	2D volume value (P)
insref	Fourier number scaled value of an integral (P)
ins2ref	Fourier number scaled volume of a peak (P)
insert	Insert sample (M)
inset	Display an inset spectrum (C)
integ	Find largest integral in a specified region (C)
integrate	Automatically integrate 1D spectrum (M)
intmod	Integral display mode (P)
intvast	Produces a text file of integral regions (M)
io	Integral offset (P)
is	Integral scale (P)
isadj	Automatic integral scale adjustment (M)
isadj2	Automatic integral scale adjustment by powers of two (M)
isreal	Utility macro to determine a parameter type (M)
isstring	Utility macro to determine a parameter type (M)
iterate	Parameters to be iterated (P)

i	Insert sample (M)
Description:	Turns off the eject air, waits for sample to slowly drop, and then turns off the slow drop air. The macro insert functions the same as i .
See also:	<i>NMR Spectroscopy User Guide</i>
Related:	e Eject sample (M) eject Eject sample (M) insert Insert sample (M)

ihwinfo **Hardware status of console (U)**

Syntax: `(From UNIX) ihwinfo('startup' | 'abort')`

Description: Displays status of digital hardware in the console. The output is intended for service personnel and probably not meaningful to users.

Arguments: 'startup' is a keyword to display the status at the conclusion of the last console startup (powerup, reboot, etc.).
'abort' is a keyword to display the status the last time an acquisition was aborted or the console rebooted from the host computer (**abortallacqs**). In this context, exiting from either the FID display or lock display of **acqi** counts as an abort. Only the status from the last abort can be displayed.

Examples: `ihwinfo('startup')`
`ihwinfo('abort')`

See also: *NMR Spectroscopy User Guide*

Related: **abortallacqs** Reset acquisition computer in a drastic situation (C)
showconsole Show console configuration parameters (U)

il **Interleave arrayed and 2D experiments (P)**

Applicability: Interleaving is not currently supported for the VNMR5 or MR400 system.

ilfid **Interleave FIDs during data processing (C)**

Description: Converts a multiple FID element into a single FID. It is possible to effectively extend the Nyquist frequency (i.e., increase the effective spectral width **sw**) by acquiring a number of FIDs with different **tau2** values and then reprocessing the data. **ilfid** does the necessary processing of time-domain data to achieve this extension, assuming that a pulse sequence (not supplied) has been written to generate the required data.

When invoked in an experiment of **nf** FIDs, each of **np** points, **ilfid** sorts the data into a single FID of **np*nf** points that can then be transformed. The interleaving takes the first complex point of each of the **nf** FIDs and places them in sequential order in the new FID. It then takes the second complex point from each of the **nf** FIDs and appends them sequentially to the new FID. This operation is repeated for all complex points. Although **ilfid** adjusts **np** and **nf**, it does not alter other parameters such as **sw**.

CAUTION: Because **ilfid** alters the data irrevocably, it is strongly recommended that you save the FID before using **ilfid**.

Examples: Illustrated below is the interleaving of an FID with **nf**=3 and **np**=4. Each point is represented by two digits. The first digit is the **nf** number and the second digit is the sequential point for that **nf** value. Data before the **ilfid** command:

11, 12, 13, 14; 21, 22, 23, 24; 31, 32, 33, 34

Data after the **ilfid** command:

11, 21, 31, 12, 22, 32, 13, 23, 33, 14, 24, 34

See also: *NMR Spectroscopy User Guide*

Related: **nf** Number of FIDs (P)
np Number of data points (P)
sw Spectral width in directly detected dimension (P)

imagefile **Display an image file (M)**

Applicability: Imaging

Syntax: `imagefile('output_option', 'imagefile'<,x,y,w,h,'mol'>)`

Description: Display or plot an imagefile at default location and size or, optionally, at location and size specified by: x (x-position), y (y-position), w (width), h (height), and mol if it is an image file of a molecular structure. Display all, plot all, or clear all images for the current experiment.

Arguments: output_option choices are:

- clear, clear all images for the current experiment
- display, display imagefile
- displayall, displays all images for the current experiment
- plot, plot imagefile
- plotall, plot all images for the current experiment

imagefile, name of image file to display or plot

x, x position

y, y position

w, width

h, height

mol molecular structure image file

Examples: imagefile('clear') clear all images for the current experiment.

imagefile('displayall') display all images for the current experiment.

imagemath Fit images to an specified function (M)

Applicability: Imaging Systems

Syntax: imagemath(fit_type, fit_var, dir_flag)

Description: Calls standalone Linux program to fit data to the specified function (fit_type), either T2, or DIFF for a T2 map or diffusion calculation.

Data is fitted to a single exponential with the ADC or T2 options. The output is given in two images:

A computed $S(0)$ image (filename S0)

A map of either ADC or T2 (filenameADC or filenameT2).

The diffcalc linux program is invoked with the DIFF option. The output depends on the number of diffusion directions applied.

The argument dir_flag (if supplied) or the parameter aipData (if dir_flag is not supplied), determines where the program reads and writes data; if aipData or dir_flag = 'saved', it uses the parameter file to determine the input directory (e.g., sems_01.img), and appends the name of the fit type to the directory name (e.g., sems_01_ADC.img) for the output directory; if aipData or dir_flag = 'processed', it uses curexp/recon as the input directory and curexp/<fit_type> as the output directory. Calling imagemath from the Current viewport, using the current data, reads the data from/written to curexp.

See the *VnmrJ Imaging User's Guide* manual for information on the image math programs fdffit or diffcalc.

Arguments:

fit_type	'ADC', 'T2', or 'DIFF'; default is 'ADC'
fit_var	Name of the parameter that holds the independent variable. Defaults to: 'bvalue' for ADC fit 'te' for T2 fit blank string for DIFF fit

dir_flag optional string argument that mimics `aipSave`.
The macro `imagemath` looks at `aipSave` if no `dirflag` argument is given.

Examples:

```
imagemath('ADC','bvalue','saved')
imagemath('T2','te')
imagemath('DIFF')
imagemath('DIFF','','saved')
```

See also: *VnmrJ Imaging User's Guide*

imageprint Plot non interactive gray scale image (M)

Description: Sends to the plotter a **dcon** color intensity map with linear instead of logarithmic increments and with grayscale instead of colors.

See also: *NMR Spectroscopy User Guide*

Related: **dcon** Display noninteractive color intensity map (C)

imconi Display 2D data in interactive grayscale mode (M)

Description: Calls the **dconi** program with the arguments required for grayscale image display: `dcon('dcon','gray','linear')`.

in Lock and spin interlock (P)

Description: Controls error handling based on lock level and spin speed, and specifies action based on lock level failure or spinner failure. The action can be to generate an error and halt acquisition, or to generate a warning and continue acquisition.

Values: Can be set to one or two characters:

- If set to two characters, the first character specifies the action for lock failure and the second character specifies the action for spinner failure.
- If set to only one character, that character specifies the same action for either lock or spinner failure.

'n' stops any system checking so that acquisition continues regardless of the lock level or spin speed.

'w' makes the system check the lock level and the spin speed. A warning message is added to the log file if the lock level falls below a preset hardware level (about 20 on the lock meter) or if **spin** is set to a particular value and the spin speed goes out of regulation; however, acquisition is not stopped.

'y' makes the system check the lock level and spin speed. Acquisition is halted if the lock level falls below a preset hardware level (about 20 on the lock meter) or if **spin** is set to a particular value and the spin speed goes out of regulation.

See also: *NMR Spectroscopy User Guide*

Related: **spin** Sample spin rate (P)

inadqt Set up parameters for INADEQUATE pulse sequence (M)

Description: Sets up parameters for 2D INADEQUATE (Incredible Natural Abundance Double-Quantum Transfer Experiment).

See also: *NMR Spectroscopy User Guide*

Related: **foldcc** Fold INADEQUATE data about 2-quantum axis (C)

- index2** **Projection or 3D plane index selected (P)**
- Description: Stores whether a projection or 3D plane index is selected. It shows the current status only and cannot be used to select a plane or projection. This parameter is also displayed in the Status window below “Index.”
- Values: 0 indicates a projection is selected.
- 1 to the half the Fourier number of the normal axis indicates a 3D plane is selected; the number is the index of the 3D plane.
- See also: *NMR Spectroscopy User Guide*
- Related: `dplane` Display a 3D plane (M)
`dproj` Display a 3D plane projection (M)
`nextpl` Display the next 3D plane (M)
`prevpl` Display the previous 3D plane (M)
`select` Select a spectrum or 2D plane without displaying it (C)
- inept** **Set up parameters for INEPT pulse sequence (M)**
- Description: Sets up parameters for the INEPT (Insensitive Nuclei Enhanced by Polarization Transfer) experiment.
- See also: *NMR Spectroscopy User Guide*
- Related: `ppcal` Proton decoupler pulse calibration (M)
- initialize_iterate** **Set iterate string to contain relevant parameters (M)**
- Description: Takes the current spin system (contained in `spinsys`) and derives from it relevant parameters. This can be used to control which parameters are iterated during a spin simulation iteration (e.g., for an ABC spin system, `iterate` is set to 'A,JAB,JAC,B,JBC,C').
- See also: *NMR Spectroscopy User Guide*
- Related: `iterate` Parameters to be iterated (P)
- input** **Receive input from keyboard (C)**
- Syntax: `input(<prompt><,delimiter>):var1,var2,...`
- Description: Receives fields of characters from the keyboard and stores them into one or more variables.
- Arguments: `prompt` is a string displayed on the command line.
- `delimiter` is a character separating input fields. The default is a comma.
- `var1,var2,...` are return values. `input` stores the values into as many of these arguments as given and ignores the rest of the input line.
- Examples: `input:$b`
`input('Enter pulse width:'):pw`
`input('x and y coordinates'):cr,cr1`
`input('Enter lastname:firstname',':'):$last,$first`
- See also: *User Programming*
- Related: `string` Create a string variable (C)
- ins** **Integral normalization scale (P)**
- Description: Sets the integral value, independent of `is` and `vs`. Reported integral values are scaled by `fn`; that is, the reported integral of a given region is independent of

fn. The **insref** parameter is also used to determine a reference integral value. The **setint** macro sets integral value.

See also: *NMR Spectroscopy User Guide*

Related:	dlni	Display list of normalized integrals (M)
	fn	Fourier number in directly detected dimension (P)
	is	Integral scale (P)
	insref	Fourier number scaled value of an integral (P)
	mark	Determine intensity of spectrum at a point (C)
	setint	Set value of an integral (M)
	vs	Vertical scale (P)

ins2 **2D volume value (P)**

Description: Adjusts the 2D volume value, independent of **is** and **vs**. The volume is scaled by Fourier numbers for the two dimensions.

See also: *NMR Spectroscopy User Guide*

Related:	is	Integral scale (P)
	ins2ref	Fourier number scaled volume of a peak (P)
	ll2d	Automatic and interactive 2D peak peaking (C)
	vs	Vertical scale (P)

insref **Fourier number scaled value of an integral (P)**

Description: Set to the Fourier number scaled value of a selected integral. The reported integral values will be $(\text{integral value}) * \text{ins} / \text{insref} / \text{fn}$. If **insref** is “not used”, the sum of all integrals will be **ins**. The “not used” mode is the equivalent of the normalized integral mode. If **insref** is zero or not defined, the reported integrals will be $(\text{integral value}) * \text{ins} / \text{fn}$.

See also: *NMR Spectroscopy User Guide*

Related:	fn	Fourier number in directly detected dimension (P)
	ins	Integral normalization scale (P)
	liamp	Amplitudes of integral reset points (P)
	setint	Set value of an integral (M)

ins2ref **Fourier number scaled volume of a peak (P)**

Description: Set to the Fourier number scaled volume of the selected peak. The reported volume is $\text{volume} * \text{ins2} / \text{ins2ref} / \text{fn} / \text{fn1}$. If **ins2ref** is “not used”, sum of all volumes is **ins2**. The “not used” mode is equivalent to a normalized volume mode. If **ins2ref** is zero or not defined, the reported volume is $\text{volume} * \text{ins2} / \text{fn} / \text{fn1}$.

See also: *NMR Spectroscopy User Guide*

Related:	fn	Fourier number in directly detected dimension (P)
	fn1	Fourier number in first indirectly detected dimension (P)
	ins2	2D volume value (P)
	ll2d	Automation and interactive 2D peak picking (C)

insert **Insert sample (M)**

Description: Turns off the eject air, waits for the sample to slowly drop, and then turns off the slow drop air. The macro **i** is identical in function to **insert**.

See also: *NMR Spectroscopy User Guide*

Related: **e** Eject sample (M)
eject Eject sample (M)
i Insert sample (M)

inset Display an inset spectrum (C)

Description: Displays the part of the spectrum between the two cursors as an inset. Before entering **inset**, run the **ds** command and display two cursors. The vertical position is shifted up about one-quarter of the height of the whole display canvas. The old spectrum remains on the screen, but the parameters shown at the bottom are relevant to the new display. If present, the integral trace is duplicated. The scale is also duplicated if it is present. After running **inset**, you can shift the displayed spectrum, expand it, or even contract it with the left and right mouse buttons.

See also: *NMR Spectroscopy User Guide*

Related: **ds** Display a spectrum FID (C)

integ Find largest integral in a specified region (C)

Syntax: `integ<(highfield,lowfield)><:size,value>`

Description: Finds the largest absolute-value integral in the specified region, or the total integral if no reset points are present between the specified limits.

Arguments: **highfield** and **lowfield** are the limits of the region. The default values are the parameters **sp** and **sp+wp**, respectively.

size is a return value with the size of the largest integral. The size depends on the value of the parameter **is** and can be positive or negative.

value is a return argument with the value of the largest integral. This value depends on **ins**, **insref**, and **fn**, and is independent of **is**.

Examples: `integ:r1,r2`
`integ(500,1000):$height`
`integ(100+sp,300+sp):$ht,$val`

See also: *User Programming*

Related: **fn** Fourier number in directly detected dimension (P)
ins Integral normalization scale (P)
insref Fourier number scaled value of an integral (P)
is Integral scale (P)
rp Zero-order phase in directly detected dimension (P)
sp Start of plot in directly detected dimension (P)
wp Width of plot in directly detected dimension (P)

integrate Automatically integrate 1D spectrum (M)

Description: A universal macro for selecting integral regions and adjusting the integrals in size and offset. Only if regions are not already selected, and if **intmod** is set to 'partial', will **integrate** call **region** to select integral regions. For proton spectra, the selection is done through the **hregions** macro; for ¹⁹F and ³¹P spectra (for wide spectral windows, multiplet spectra), **region** is called with optimized arguments, and for other nuclei (mostly decoupled, single-line spectra) other optimized parameters are used with **region**, such that lines consisting of a few data points only are recognized.

See also: *NMR Spectroscopy User Guide*

Related: **hregions** Select integral regions in proton spectrum (M)
intmod Integral display mode (P)
isadj Adjust integral scale (M)
region Automatically select integral regions (C)

intmod Integral display mode (P)

Description: Controls display and plotting of the spectral integral.

Values: 'off' indicates that no integrals are displayed or plotted.
 'full' indicates that all integral regions are displayed or plotted.
 'partial' indicates that every other integral region is plotted (typically used to display integrals of only peaks and not of the baseline region).

See also: *NMR Spectroscopy User Guide*

Related: **plc** Plot carbon spectrum (M)
plh Plot proton spectrum (M)
plp Plot phosphorus spectrum (M)

intvast Produces a text file of integral regions (M)

Applicability: Systems with VAST accessory.

Syntax: `intvast (last)`

Description: `intvast` produces a text file, `integ.out` in the current experiment, containing the integrals of the partial regions of each spectra from wells 0 to `last`.

Arguments: `last` is the number last sample well. The default is 96.

See also: *NMR Spectroscopy User Guide*

Related: **pintvast** Plot the integrals (M)

io Integral offset (P)

Description: Offset of the integral with respect to the spectrum.

Values: 0 to 200, in mm.

See also: *NMR Spectroscopy User Guide*

is Integral scale (P)

Description: Multiplier that adjusts height of the displayed integral trace. Note that the **ins** parameter controls integral value, and that **is** has no effect on integral value.

Values: 1 to 1e9

See also: *NMR Spectroscopy User Guide*

Related: **ins** Integral normalization scale (P)
ins2 2D volume value (P)
insref Fourier number scaled value of an integral (P)
integ Find largest integral in a specified region (C)

isadj Automatic integral scale adjustment (M)

Syntax: `isadj<(height<,neg_height>)>`

Description: Adjusts the height of the integrals in a display to make the tallest integral fit the paper. Optionally, the height of the maximum integral can be specified by an

argument. Negative integrals, if present, are given a limit of 10 mm if parameter `io` is less than 10; otherwise, they are set so they end 5 mm above the spectrum. Negative integrals can also be given a height. Whichever part of the integrals (positive or negative) runs into the given limit will be used to scale `is`.

Arguments: `height` is the size, in mm, of the maximum integral on display. The default is the height that makes the tallest integral fit the paper.

`neg_height` is the desired height, in mm, of the largest negative integral. If `io` is less than 10, the default is 10; otherwise, the default height is 5 mm above the spectrum.

Examples: `isadj`
`isadj(100)`
`isadj(100,100)`

See also: *NMR Spectroscopy User Guide*

Related: `io` Integral offset (P)
`is` Integral scale (P)
`isadj2` Automatic integral scale adjustment by powers of two (M)

`isadj2` Automatic integral scale adjustment by powers of two (M)

Syntax: `isadj2<(height<,neg_height>)>:scaling_factor`

Description: Functionally the same as `isadj` except that `isadj2` adjusts the integral height by powers of two and returns the scaling factor to the calling macro.

Arguments: `height` is the size, in mm, of the maximum integral on display.

`neg_height` is the desired height, in mm, of the maximum negative integral on display.

`scaling_factor` is a return value giving the ratio of the new integral size to the old value (`new_is/old_is`).

Examples: `isadj2`
`isadj2(100)`
`isadj2(100,100)`
`isadj2(50):r1`

See also: *NMR Spectroscopy User Guide*

Related: `is` Integral scale (P)
`isadj` Automatic integral scale adjustment (M)

`isreal` Utility macro to determine a parameter type (M)

Syntax: `isreal(paramname<,tree>)`

Description: Returns 1 if and only if `paramname` is a real type. It returns 0 if `paramname` is a string type. If there is an error, the error is reported and the macro also returns 0. The value of `tree` is 'current', 'global', 'processed' or 'systemglobal' and the default is 'current'.

There is some unfortunate ambiguity and vagueness in regard to `vnmr` parameters and their types. The meaning of `real` and `string` vary slightly depending upon context. There are seven types altogether. The macro `gettype` returns a unique integer value when operating on the parameter. Of the seven types, two can be broadly categorized as string, and five can be broadly categorized as real. Since one of the string category types is 'string' and one of the real category types is 'real', this is where the ambiguity arises. The return values for `gettype` are:

<i>category</i>	<i>type</i>	<i>gettype returns</i>
string	'string'	2
	'flag'	4
real	'real'	1
	'delay'	3
	'frequency'	5
	'pulse'	6
	'integer'	7

The `isreal` function returns 0 for the string category and 1 for the real category. This function is consistent with the `typeof()` operator. The `typeof()` operator is primarily intended to ascertain the type of the input argument to a macro, so using it for other purposes is not recommended. Also, it does not take a tree argument. Note that `typeof()` returns 0 for reals and 1 for strings, the opposite of this macro, but it should be clear from the name what is intended. A sister macro `isstring` returns the same value as `typeof()`.

Related: `isstring` Utility macro to determine a parameter type (M)
`typeof` Return identifier for argument type (O)

`isstring` Utility macro to determine a parameter type (M)

Syntax: `isstring(paramname<,tree>)`

Description: Returns 1 if and only if `paramname` is a string type. It returns 0 if `paramname` is a real type. If there is an error, the error is reported and the macro also returns 0. The value of `tree` is 'current', 'global', 'processed' or 'systemglobal' and the default is 'current'.

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	'flag'	4
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	'delay'	3
	'frequency'	5
	'pulse'	6
	'integer'	7

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for strings, the opposite of this macro, but it should be clear from the name what is intended. A sister macro `isstring` returns the same value as `typeof()`.

Related: `isreal` Utility macro to determine a parameter type (M)
`typeof` Return identifier for argument type (O)

iterate Parameters to be iterated (P)

Description: Contains parameters to be iterated during iterative spin simulations. If the Set Params button is used in setting up spin simulation parameters, `iterate` is initialized to a string containing all parameters appropriate to the current spin system.

Values: List of parameters, separated by commas (e.g., `iterate='A,B,JAB'`).

See also: *NMR Spectroscopy User Guide*

Related: `initialize_iterate` Set `iterate` string to contain relevant parameters (M)

J

<code>jcurwin</code>	Work space numbers of all viewports (P)
<code>jdesign</code>	Start Plot Designer Program (M)
<code>jexp</code>	Join existing experiment (C)
<code>jexp1-jexp9999</code>	Join existing experiment and display new parameters (M)
<code>jplot</code>	Plot from Plot Designer program (C)
<code>jplotscale</code>	Scale plot parameters (M)
<code>jplotunscale</code>	Restore current experiment parameters (M)
<code>jprint</code>	Prints the selected images to a printer or file (M)
<code>jumpret</code>	Set up parameters for JUMPRET pulse sequence (M)
<code>jviewport</code>	Work space numbers of the current viewports (P)
<code>jviewportlabel</code>	Work space labels for all viewport buttons (P)
<code>jviewports</code>	Viewport layout (P)
<code>jwin</code>	Activate and record activity in current window (M)

`jcurwin` **Work space numbers of all viewports (P)**

Description: An arrayed global parameter, set to the work space numbers used by all viewports.

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related:	<code>curwin</code>	Current window (P)
	<code>jviewport</code>	Work space numbers of the current viewports (P)
	<code>jviewportlabel</code>	Work space labels for all viewport buttons (P)

`jdesign` **Start Plot Designer Program (M)**

Syntax: `jdesign`

Description: Opens the Plot Designer program, which provides mechanisms for positioning spectra, parameters, axes, and other plot output on a page. Text annotation and drawing features are available.

See also: *NMR Spectroscopy User Guide*

Related:	<code>jplot</code>	Plot from Plot Designer program (C)

`jexp` **Join existing experiment (C)**

Syntax: (1) `jexp (exp_number)`
(2) `jexp:$current_exp_number,$current_exp_name`

Description: Joins an existing experiment (syntax 1) or returns the current experiment number and experiment name (syntax 2). After entering this command, until another “join experiment” command or macro is entered, all actions (including changes of parameters, acquisition of data, and display of data) apply to the parameters and data of the experiment joined.

The `jexp` command does not refresh the display or display new experiment parameters. Use one of the macros `jexp1`, `jexp2`, etc. to join an experiment and have the screen refreshed and new parameters displayed.

Arguments: `exp_number` is a number from 1 to 9999 for existing experiment to be joined.
`$current_exp_number` is a return value with the current experiment number.
`$current_exp_name` is a return value with the current experiment name.

Examples: `jexp(3)`
`jexp:$expp`
`jexp:r1,n1`

See also: *NMR Spectroscopy User Guide; VnmrJ Walkup*

Related: `cexp` Create an experiment (M)
`delexp` Delete an experiment (M)
`jexp1-jexp9` Join existing experiment and display new parameters (M)
`unlock` Remove inactive lock and join experiment (C)

jexp1-jexp9999 Join existing experiment and display new parameters (M)

Syntax: `jexp1, jexp2, jexp3, ..., jexp9999`

Description: Joins an existing experiment, refreshes the screen, and displays the main menu and the new experiment parameters. After entering this macro, until another “join experiment” command or macro is entered, all actions (including changes of parameters, acquisition of data, and display of data) apply to the parameters and data of the experiment joined.

To join an experiment without refreshing the screen and displaying new parameters, use the `jexp` command.

Examples: `jexp8`
`jexp354`

See also: *NMR Spectroscopy User Guide*

Related: `cexp` Create an experiment (M)
`delexp` Delete an experiment (M)
`jexp` Join existing experiment (C)
`unlock` Remove inactive lock and join experiment (C)

jplot Plot from Plot Designer program (C)

Syntax: `jplot(<' -setup'><, template>)`

Description: Starts plotting from the Plot Designer program to the current plotter.

Arguments: `' -setup'` is a keyword to start `jdesign`, the Plot Designer program, to allow interactive design and plotting.
`template` is the name of a file that will be used to make a plot of the current experiment. The default is a saved file chosen by the user.

Examples: `jplot`
`jplot('t1')`

See also: *NMR Spectroscopy User Guide*

Related: `jdesign` Start Plot Designer program (M)
`jplotscale` Scale plot parameters (M)
`jplotunscale` Restore current experiment parameters (M)

jplotscale Scale plot parameters (M)

Applicability: Plot Designer program

Description: Scales parameters of plotting area and an imported plot. When a region is drawn in Plot Designer, `jplot` automatically changes the plotting area parameters `wcmax` and `wc2max`. The parameters `io`, `is`, `vs`, `wc`, and `wc2` of a plot imported into a region are adjusted according to `wcmax` and `wc2max`.

See also: *NMR Spectroscopy User Guide*

Related: `jplot` Plot from Plot Designer program (C)
`jplotunscale` Restore current experiment parameters (M)

jplotunscale Restore current experiment parameters (M)

Applicability: Plot Designer program

Description: Restores the current experiment parameters (`io`, `is`, `vs`, `wc`, and `wc2`) to a plot within a region that was created in Plot Designer. For example, entering `jplotunscale jexp2 jplot` restores the parameters of experiment 2 to a plot and then `jplot` applies the adjusted parameters to the plot.

See also: *NMR Spectroscopy User Guide*

Related: `jplot` Plot from Plot Designer program (C)
`jplotscale` Scale plot parameters (M)

jprint Prints the selected images to a printer or file (M)

Description: The `jprint` macro takes the value of the parameters `printregion`, `printsend`, `printfile`, `printlayout`, `printformat`, `printsize`.

jumpret Set up parameters for JUMPRET pulse sequence (M)

Description: Sets up parameters for a jump-and-return water suppression sequence.

See also: *NMR Spectroscopy User Guide*

jviewport Work space numbers of the current viewports (P)

Description: A global parameter, set to the work space number that the current viewport is joined to. The parameter is set when the viewport starts. Each viewport may be joined to a different work space.

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related: `curwin` Current window (P)
`jcurwin` Work space numbers of all viewports (P)
`jviewports` Viewport layout (P)
`jviewportlabel` Work space labels for all viewport buttons (P)

jviewportlabel Work space labels for all viewport buttons (P)

Description: An arrayed global parameter, set to the labels on the toolbar buttons used to switch viewports. It is used by the viewport editor under **Edit -> Viewports**.

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related: `jviewport` Work space numbers of the current viewports (P)
`jviewports` Viewport layout (P)
`vpaction` Set initial state for multiple viewports (M)

J

jviewports Viewport layout (P)

Description: An arrayed global parameter, used to keep track of the viewport layout. It is used by the viewport editor under **Edit -> Viewports** to change the viewport layout.

Related:	jcurwin	Work space numbers of all viewports (P)
	jviewport	Work space numbers of the current viewports (P)
	jviewportlabel	Work space labels for all viewport buttons (P)
	vpaction	Set initial state for multiple viewports (M)
	vpset3def	Set the viewport state to three default viewports (M)
	vpsetup	Set new viewports (M)

jwin Activate and record activity in current window (M)

Syntax: jwin (pane_number)

Description: Activates and records the activity in a specific window pane, created by **setgrid**, in the VnmrJ graphics window. jwin is executed when you double-click the left mouse button in a multiple-paned graphics window.

Arguments: pane_number is the number of the pane to join.

Examples: jwin (2)

See also: *NMR Spectroscopy User Guide*

Related:	curwin	Current window (P)
	fontselect	Open FontSelect window (C)
	mapwin	List of experiment numbers (P)
	setgrid	Activate selected window (M)
	setwin	Activate selected window (C)

K

<code>killft3d</code>	Terminate any ft3d process started in an experiment (M,U)
<code>killplot</code>	Stop plot jobs and remove from plot queue (M)
<code>killprint</code>	Stop print jobs and remove from print queue (M)
<code>kind</code>	Kinetics analysis, decreasing intensity (M)
<code>kinds</code>	Kinetics analysis, decreasing intensity, short form (M)
<code>kini</code>	Kinetics analysis, increasing intensity (M)
<code>kinis</code>	Kinetics analysis, increasing intensity, short form (M)

killft3d Terminate any ft3d process started in an experiment (M,U)

Syntax: `killft3d(exp_number)`

Description: Terminates any `ft3d` program that has been started in the specified VnmrJ experiment. `killft3d` can be executed from any experiment. For each `ft3d` process terminated, the relevant 3D data subdirectory is also deleted. Remote `ft3d` processes, denoted by the call name `ft3d` in the process table (displayed by the UNIX command `ps -aux`), are not directly terminated by `killft3d` but die of their own accord due to the deletion of the 3D data subdirectory.

The `killft3d` command can also be run as a shellscript from UNIX. Its function is analogous to the associated VnmrJ macro.

Arguments: `exp_number` is a number from 1 to 9 that identifies the experiment that started the `ft3d` program.

Examples: `killft3d(4)`

See also: *NMR Spectroscopy User Guide*

Related: `ft3d` Perform a 3D Fourier transform (M,U)

killplot Stop plot jobs and remove from plot queue (M)

Description: Kills all current plot jobs in the plot queue for the active plotter in VnmrJ, then removes the jobs from the plot queue. Unless the user executing `killplot` is `root`, only that user's plot jobs are deleted from the plot queue. To kill a plot that is in progress (i.e., a plot in which you have not entered `page`), use the `page('clear')` command.

The plotter may have to be reinitialized after `killplot` is executed. To reinitialize the plotter, turn it off and then back on after a few seconds. Hewlett-Packard (HP) pen plotters appear to be more susceptible to this problem than the other HP output devices supported by VnmrJ.

If one port is configured to be both a printer and a plotter, `killplot` can cause both plot *and* print jobs to that port to be deleted. For example, if `printer='LaserJet_300'`, `plotter='LaserJet_300R'`, and a plot command `pl pscale page` is followed by a print command `ptext(vnmruser+'/psglib/noesy.c')`, entering `killplot` deletes both jobs.

K

See also: *NMR Spectroscopy User Guide*

Related:	<code>killprint</code>	Stop print jobs and remove from print queue (M)
	<code>page</code>	Move plotter forward one or more pages (C)
	<code>pl</code>	Plot spectra (C)
	<code>pscale</code>	Plot scale below spectrum or FID (C)
	<code>ptext</code>	Print out a text file (M)
	<code>showplotq</code>	Display plot jobs in plot queue (M)

killprint Stop print jobs and remove from print queue (M)

Description: Kills all current print jobs in the print queue for the active printer in VnmrJ, then removes the jobs from the print queue. Unless the user executing `killprint` is `root`, only that user's print job is deleted from the print queue. It is slightly possible that the printer may have to be reinitialized after the execution of this macro. To reinitialize the printer, turn it off, wait a few seconds, and then turn it back on.

If one port is configured to be both a printer and a plotter, `killprint` can cause both print *and* plot jobs to that port to be deleted. For example, if `printer='LaserJet_300'`, `plotter='LaserJet_300R'`, and a plot command `pl pscale page` is followed by a print command `ptext (vnmruser+'/psglib/noesy.c')`, entering `killprint` deletes both jobs.

See also: *NMR Spectroscopy User Guide*

Related:	<code>killplot</code>	Stop plot jobs and remove from plot queue (M)
	<code>ptext</code>	Print out a text file (M)
	<code>showprintq</code>	Display print jobs in print queue (M)

kind Kinetics analysis, decreasing intensity (M)

Description: If the signal decreases exponentially toward a limit, the output is matched by $I = A1 * EXP(-T/TAU) + A3$. This macro supplies the necessary keywords to the `analyze` command, which uses the output of `fp` (i.e., the file `fp.out`) as input. The results can be displayed with `expl`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>analyze</code>	Generalized curve fitting (C)
	<code>expl</code>	Display exponential/polynomial curves (C)
	<code>fp</code>	Find peak heights (C)
	<code>kinds</code>	Kinetic analysis, decreasing intensity, short form (M)
	<code>kini</code>	Kinetics analysis, increasing intensity (M)
	<code>kinis</code>	Kinetic analysis, increasing intensity, short form (M)

kinds Kinetics analysis, decreasing intensity, short form (M)

Description: Produces a summary of the results from `kind`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>kind</code>	Kinetics analysis, decreasing intensity (M)

kini Kinetics analysis, increasing intensity (M)

Description: If the signal increases exponentially toward a limit, the output is matched by $I = -A1 * EXP(-T/TAU) + A3 - A1$. This macro supplies the necessary keywords to the `analyze` command, which uses the output of `fp` (i.e., the file `fp.out`) as input. The results can be displayed with `expl`.

See also: *NMR Spectroscopy User Guide*

Related: [kind](#) Kinetics analysis, decreasing intensity (M)
[kinis](#) Kinetic analysis, increasing intensity, short form (M)

kinis **Kinetics analysis, increasing intensity, short form (M)**

Description: Produces a summary of the results from [kini](#).

See also: *NMR Spectroscopy User Guide*

Related: [kind](#) Kinetics analysis, decreasing intensity (M)
[kini](#) Kinetics analysis, increasing intensity (M)

L

<code>lastlk</code>	Last lock solvent used (P)
<code>lastmenu</code>	Menu to display when Return button is selected (P)
<code>latch</code>	Frequency synthesizer latching (P)
<code>lb</code>	Line broadening in directly detected dimension (P)
<code>lb1</code>	Line broadening in 1st indirectly detected dimension (P)
<code>lb2</code>	Line broadening in 2nd indirectly detected dimension (P)
<code>lcld</code>	Pulse sequence for LC-NMR (M)
<code>lcpar2d</code>	Create 2D LC-NMR acquisition parameters (M)
<code>lcpeak</code>	Peak number (P)
<code>lcplot</code>	Plot LC-NMR data (M)
<code>lcpsgset</code>	Set up parameters for various LC-NMR pulse sequences (M)
<code>lcset2d</code>	General setup for 2D LC-NMR experiments (M)
<code>left</code>	Set display limits to left half of screen (C)
<code>legrelay</code>	Independent control of magnet leg relay (P)
<code>length</code>	Determine length of a string (C)
<code>lf</code>	List files in directory (C)
<code>liamp</code>	Amplitudes of integral reset points (P)
<code>lifrq</code>	Frequencies of integral reset points (P)
<code>liqbear</code>	Liquids Bearing Air Level (P)
<code>listenoff</code>	Disable receipt of messages from send2Vnmr (M)
<code>listenon</code>	Enable receipt of messages from send2Vnmr (M)
<code>lkof</code>	Track changes in lock frequency (P)
<code>ll2d</code>	Automatic and interactive 2D peak picking (C)
<code>ll2dbackup</code>	Copy current ll2d peak file to another file (M)
<code>ll2dmode</code>	Control display of peaks picked by ll2d (P)
<code>llamp</code>	List of line amplitudes (P)
<code>llfrq</code>	List of line frequencies (P)
<code>ln</code>	Find natural logarithm of a number (C)
<code>load</code>	Load status of displayed shims (P)
<code>loadcolors</code>	Load colors for graphics window and plotters (M)
<code>loc</code>	Location of sample in tray (P)
<code>locaction</code>	Locator action (M)
<code>lock</code>	Submit an Autolock experiment to acquisition (C)
<code>lockacqtc</code>	Lock loop time constant during acquisition (P)
<code>lockfreq</code>	Lock frequency (P)
<code>lockgain</code>	Lock gain (P)
<code>lockphase</code>	Lock phase (P)
<code>lockpower</code>	Lock power (P)
<code>locktc</code>	Lock time constant (P)
<code>logate</code>	Transmitter local oscillator gate (P)
<code>lookup</code>	Look up words and lines from a text file (C)
<code>locprotoexec</code>	Execute a protocol from the locator (M)
<code>lp</code>	First-order phase in directly detected dimension (P)

L

<code>lp1</code>	First-order phase in 1st indirectly detected dimension (P)
<code>lp2</code>	First-order phase in 2nd indirectly detected dimension (P)
<code>lpalg</code>	LP algorithm in np dimension (P)
<code>lpalg1</code>	LP algorithm in ni dimension (P)
<code>lpalg2</code>	LP algorithm in ni2 dimension (P)
<code>lpext</code>	LP data extension in np dimension (P)
<code>lpext1</code>	LP data extension in ni dimension (P)
<code>lpext2</code>	LP data extension in ni2 dimension (P)
<code>lpfilt</code>	LP coefficients to calculate in np dimension (P)
<code>lpfilt1</code>	LP coefficients to calculate in ni dimension (P)
<code>lpfilt2</code>	LP coefficients to calculate in ni2 dimension (P)
<code>lpnupts</code>	LP number of data points in np dimension (P)
<code>lpnupts1</code>	LP number of data points in ni dimension (P)
<code>lpnupts2</code>	LP number of data points in ni2 dimension (P)
<code>lpopt</code>	LP algorithm data extension in np dimension (P)
<code>lpopt1</code>	LP algorithm data extension in ni dimension (P)
<code>lpopt2</code>	LP algorithm data extension in ni2 dimension (P)
<code>lpprint</code>	LP print output for np dimension (P)
<code>lpprint1</code>	LP print output for ni dimension (P)
<code>lpprint2</code>	LP print output for ni2 dimension (P)
<code>lptrace</code>	LP output spectrum in np dimension (P)
<code>lptrace1</code>	LP output spectrum in ni dimension (P)
<code>lptrace2</code>	LP output spectrum in ni2 dimension (P)
<code>ls</code>	List files in directory (C)
<code>lsfid</code>	Number of complex points to left-shift the np FID (P)
<code>lsfid1</code>	Number of complex points to left-shift ni interferogram (P)
<code>lsfid2</code>	Number of complex points to left-shift ni2 interferogram (P)
<code>lsfrq</code>	Frequency shift of the fn spectrum (P)
<code>lsfrq1</code>	Frequency shift of the fn1 spectrum (P)
<code>lsfrq2</code>	Frequency shift of the fn2 spectrum (P)
<code>lvl</code>	Zero-order baseline correction (P)
<code>lvl1tlt</code>	Control sensitivity of lvl and tlt adjustments (P)

lastlk **Last lock solvent used (P)**

Description: Contains the name of the last lock solvent. Intended for use with the optional sample changer, this parameter is a user global variable (stored in the user's `global` file) and is not accessible to multiple users simultaneously. On a multiuser automation run, you should preferably access the last lock solvent from the file `/vnmr/acqqueue/lastlk`.

Values: String containing the name of the solvent.

See also: *NMR Spectroscopy User Guide*

Related: `solvent` Lock solvent (P)

lastmenu **Menu to display when Return button is selected (P)**

Description: Contains the name of the menu to display when the Return button is clicked on certain menus. For example, if the Phase F2 button in the 2D Processing menu (controlled by the file `process_2D`) is clicked, `lastmenu` is set to `'process_2D'`, the `ft` and `aph` commands are executed, the `ds` window is opened, and the Interactive 1D Spectrum Display menu (`ds_1` file) is displayed. Appearing in this menu is a Return button. Because `lastmenu` is still set to `'process_2D'`, clicking on the Return button redisplay the 2D Processing menu. `lastmenu` is stored in the `$vnmrsys/global` file.

Values: String containing the name of a menu (e.g., `'process_2D'`).

See also: *User Programming*

Related: `menu` Change status of menu system (C)
`newmenu` Select a menu without immediate activation (C)

latch **Frequency synthesizer latching (P)**

Description: Configuration parameter for whether the PTS frequency synthesizer has latching capabilities (all digits of the frequency value are sent to the synthesizer at once). The value for each channel is by the Latching label in the Spectrometer Configuration window.

Values: `'n'` indicates the synthesizers do not have latching capabilities (Not Present choice from the Spectrometer Configuration window).
`'y'` indicates the synthesizers have latching capabilities (Present choice from the Spectrometer Configuration window).

See also: *VnmrJ Installation and Administration*

Related: `config` Display current configuration and possibly change it (M)

1b **Line broadening in directly detected dimension (P)**

Description: Sets line broadening and exponential weighting along the directly detected dimension. This dimension is often referred to as the f_2 dimension in 2D data sets, the f_3 dimension in 3D data sets, etc.

Values: A positive value gives the desired line broadening, in Hz, which is then used to calculate a decaying exponential function of the form `exp(-t* $\pi$ *1b)`.

A negative value gives a resolution enhancement function (increasing exponential) of the form `exp(-t* $\pi$ *1b)`.

`'n'` turns off line broadening and exponential weighting.

See also: *NMR Spectroscopy User Guide*

Related: `exp` Find exponential value of a number (C)
`1b1` Line broadening in 1st indirectly detected dimension (P)
`1b2` Line broadening in 2nd indirectly detected dimension (P)

1b1 **Line broadening in 1st indirectly detected dimension (P)**

Description: Sets line broadening and exponential weighting along the first indirectly detected dimension. This dimension is often referred to as the f_1 dimension in multidimensional data sets. `1b1` works analogously to the parameter `1b`. The “conventional” parameters (`1b`, `gf`, etc.) operate on the detected FIDs, while this “2D” parameter is used during processing of the interferograms.

Values: A positive value gives the desired line broadening, in Hz, which is then used to calculate a decaying exponential function of the form `exp(-t* $\pi$ *lb1)`. A typical value is between 0.0001 to 1000 Hz.

A negative value gives a resolution enhancement function (increasing exponential) of the form `exp(-t* $\pi$ *lb1)`.

'n' turns off line broadening and exponential weighting.

See also: *NMR Spectroscopy User Guide*

Related:	<code>exp</code>	Find exponential value of a number (C)
	<code>lb</code>	Line broadening in directly detected dimension (P)
	<code>lb2</code>	Line broadening in 2nd indirectly detected dimension (P)

1b2 Line broadening in 2nd indirectly detected dimension (P)

Description: Sets line broadening and exponential weighting along the second indirectly detected dimension. This dimension is often referred to as the f_2 dimension in multidimensional data sets. 1b2 works analogously to the parameter `lb`. 1b2 can be set with `wti` on the 2D interferogram data.

Values: A positive value gives the desired line broadening, in Hz, which is then used to calculate a decaying exponential function of the form `exp(-t* $\pi$ *lb2)`.

A negative value gives a resolution enhancement function (increasing exponential) of the form `exp(-t* $\pi$ *lb2)`.

'n' turns off line broadening and exponential weighting.

See also: *NMR Spectroscopy User Guide*

Related:	<code>exp</code>	Find exponential value of a number (C)
	<code>lb</code>	Line broadening in directly detected dimension (P)
	<code>wti</code>	Interactive weighting (C)

1c1d Pulse sequence for LC-NMR (M)

Applicability: Systems with LC-NMR accessory.

Description: Creates parameters to set up a pulse sequence that can be used to start an LC-NMR run, including triggering the injection of a sample, and can be used also to obtain multiple solvent-suppressed spectra using multi frequency Shifted Laminar Pulses (SLP) and gradients. The sequence is coded without a `d2` variable, thus allowing `ni` to be used to obtain a series of spectra without resulting in any delay in the sequence being incremented.

The sequence requires a phase table, 1c1d, to be found in the `tablib` directory. Phases of the selective pulses, the observe pulse, and the receiver and separately controlled by phase variables.

Note that the 1c1d sequence uses power scaling of shaped pulses, which is supported starting in VnmrJ 5.2. Because of this feature, this sequence *will not run* in earlier versions of VnmrJ.

1cpar2d Create 2D LC-NMR acquisition parameters (M)

Applicability: Systems with LC-NMR accessory.

Description: Creates the acquisition parameters `ni`, `sw1`, and `phase`, which can be used to acquire a 2D LC-NMR data set. 1cpar2d is functionally the same as `addpar('2d')`.

Related:	<code>addpar</code>	Add selected parameters to current experiment (M)
	<code>lcset2d</code>	General setup for 2D LC-NMR experiments (M)

- lcpeak** **Peak number (P)**
 Applicability: Systems with LC-NMR accessory.
 Description: Contains the number of the peak being sensed or the loop being flushed.
- lcplot** **Plot LC-NMR data (M)**
 Applicability: Systems with LC-NMR accessory.
 Syntax: `lcplot`
 Description: Plots LC-NMR data. This macro is executed with the Plot LC-NMR button on the Spare pane when LC-NMR is active.
- lcpsgset** **Set up parameters for various LC-NMR pulse sequences (M)**
 Applicability: Systems with LC-NMR accessory.
 Syntax: `lcpsgset (file,parameter1,parameter2,...,parameterN)`
 Description: Sets up parameters for various LC-NMR pulse sequences using information in a `parlib` file. Rather than returning the entire parameter file, `lcpsgset` returns the parameters listed. `lcpsgset`, in general, is never entered from the keyboard but is used as part of experiment setup macros.
 Arguments: `file` is the file from the user or system `parlib` that provides information on setting up parameters listed. The parameters `seqfil` and `pslabel` are set to the supplied file name.
 `parameter1,parameter1,...,parameterN` are 1 to 11 parameters to be returned from the `parlib` file.
 Examples: `lcpsgset ('lccosy','ds','ap','ss','d1','axis','phase')`
- lcset2d** **General setup for 2D LC-NMR experiments (M)**
 Applicability: Systems with LC-NMR accessory.
 Syntax: `lcset2d (experiment<,F2_dig_res<,F1_dig_res>>)`
 Description: Runs the macro `lcpa2d` to create new parameters needed for 2D LC-NMR experiments, then selects starting values for a number of parameters. The `lcset2d` macro is “internal” and not normally entered directly by the user.
 Arguments: `experiment` is the name of a 2D LC-NMR experiment.
 `F2_dig_res` is the f_2 digital resolution desired, in Hz/pt.
 `F1_dig_res` is the f_1 digital resolution desired, in Hz/pt.
 Examples: `lcset2d ('lcnoesy')`
- left** **Set display limits to left half of screen (C)**
 Description: Sets the horizontal control parameters `sc` and `wc` to produce a display (and subsequent plot) in the left half of a screen (and page). For 2D data, space is left for the scales.
- Related: `center` Set display limits for center of screen (C)
 `full` Set display limits for a full screen (C)
 `fullt` Set display limits for full screen with room for traces (C)
 `right` Set display limits for right half of screen (C)

L

legrelay **Independent control of magnet leg relay (P)**

Description: Gives override capability over the magnetic leg high and low (broad) band rf signal routing. This parameter does not normally exist but can be created by the user with the command `create('legrelay','string')`.

The `legrelay` override is operational only on standard systems shipped starting in November 1990 and on certain special systems shipped before that date. A system includes the override capability if it uses N-type connectors instead by BNC connectors on the magnet leg.

Values: 'n' indicates normal logic is used to set the leg relay.

'h' indicates the leg relay is set to the high band.

'l' indicates the leg relay is set to the low (broad) band.

Any other value results in an error message and an abort of pulse sequence generation.

See also: *User Programming*

Related: `create` Create new parameter in a parameter tree (C)

length **Determine length of a string (C)**

Syntax: `length(string):$string_length`

Description: Returns the length in characters of a specified string.

Arguments: `string` is zero or more characters enclosed in single quotes.

`string_length` is the number of characters (a real number) in `string`.

Examples: `length('abc'):r1`
`length(solvent):$len`

See also: *User Programming*

Related: `substr` Select a substring from a string (C)

lf **List files in directory (C)**

Syntax: `lf<(directory)>`

Description: Lists the files in a directory, with output on the text output window. Directories are suffixed by "/", executable files by "*", and links by "@".

Arguments: `directory` is the name of a directory. The default is the current working directory. `lf` is equivalent to the UNIX command `ls -F` and uses the same options (e.g., `-l` for a long listing such as `lf('-l *.fid')`).

Examples: `lf`
`lf('data')`
`lf('-l *.fid')`

See also: *NMR Spectroscopy User Guide*

Related: `dir` List files in directory (C)
`ls` List files in directory (C)

liamp **Amplitudes of integral reset points (P)**

Description: Stores the integral amplitudes at the integral reset points for a list of integrals. To display the values of `liamp`, enter `display('liamp')`. Values of `liamp` can also be accessed in MAGICAL macros using, for example, `liamp[$i]`. Values are stored as absolute numbers (summations of data point values) and, as such, are a function of the parameter `fn`. The values displayed

by the `dli`, `pir`, and `dpir` programs are related to `liamp` values by the relationship:

$$\text{Displayed or plotted integral} = \text{liamp}[i] * \text{is} / (\text{fn}/128) * \text{ins}$$

See also: *NMR Spectroscopy User Guide*

Related:	<code>display</code>	Display parameters and their attributes (C)
	<code>dli</code>	Display list of integrals (C)
	<code>dpir</code>	Display integral amplitudes below spectrum (C)
	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>lifrq</code>	Frequencies of integral reset points (P)
	<code>pir</code>	Plot integral amplitudes below spectrum (C)

lifrq **Frequencies of integral reset points (P)**

Description: Stores the frequencies of integral reset points for a list of integrals. The frequencies are stored in Hz and are *not* adjusted by the reference parameters `rfl` and `rfp`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>liamp</code>	Amplitudes of integral reset points (P)
	<code>rfl</code>	Ref. peak position in directly detected dimension (P)
	<code>rfp</code>	Ref. peak frequency in directly detected dimension (P)

liqbear **Liquids Bearing Air Level (P)**

Description: This global parameter is the DAC value used when the liquids spinner bearing air is turned on. If the parameter does not exist the value defaults to 0xc000.

To create the parameter:

```
create('liqbear','integer','global')
setlimit('liqbear',65535,0,1,'global')
```

Values: 0 - 65535

listenoff **Disable receipt of messages from send2Vnmr (M)**

Description: Deletes the file `$vnmruser/.talk`, thereby disallowing `send2Vnmr` to send commands to `VnmrJ`

See also: *User Programming*

Related:	<code>listenon</code>	Enable receipt of messages from <code>send2Vnmr</code> (M)
	<code>send2vnmr</code>	Send a command to <code>VnmrJ</code> (U)

listenon **Enable receipt of messages from send2Vnmr (M)**

Description: Writes files with the `VnmrJ` port number that `/vnmr/bin/send2Vnmr` needs to talk to `VnmrJ`. The command then to send commands to `VnmrJ` is `/vnmr/bin/send2Vnmr $vnmruser/.talk` command.

See also: *User Programming*

Related:	<code>listenoff</code>	Disable receipt of messages from <code>send2Vnmr</code> (M)
	<code>send2vnmr</code>	Send a command to <code>VnmrJ</code> (U)

lkof **Track changes in lock frequency (P)**

Description: Tracks changes in the lock frequency resulting from changes in the solvent, and minor changes caused by the magnet drifting. The frequency units for `lkof` are in Hz, analogous to `sfrq` and `tof`, or `dfrq` and `dof`. `lkof` affects two

components of the system: autolock on the console and `acqi` on the host computer. If `lkof` exists, it offsets the current value of the `lockfreq` parameter.

See also: *NMR Spectroscopy User Guide*

Related: `lockfreq` Lock frequency (P)

112d Automatic and interactive 2D peak picking (C)

Syntax: (1) `112d<(options)><:$num>`
 (2) `112d('info'<,$#>):$peak_number,$f1,$f2,$amplitude,$volume,$label,$comment,$FWHH1,$FWHH2,$f1_min,$f1_max,$f2_min,$f2_max`

Description: Automatically finds and integrates peaks that are above the threshold `th` in a 2D spectrum or a 2D plane of a 3D spectrum, and writes the peak location, volume, full-width at half-height (FWHH), volume, and the boundaries of the integrated region to a file in the `112d` subdirectory of the current experiment directory. For 2D spectra, the file name is `peaks.bin`, and for 2D planes of 3D spectra, the file name is `peaks_f#f#_#.bin`, where `f#f#` gives the plane direction (e.g., `f1f3`) and the final `#` gives the number of the plane. For easy import and export of peak data, `112d` also allows insertion and deletion of peaks interactively as well as reading and writing of text peak files.

Two-dimensional volumes are scaled in a manner analogous to 1D integrals, using the parameters `ins2` and `ins2ref`. The `ins2ref` parameter is the Fourier number scaled value of a selected volume. The reported value of a peak volume is $(\text{unscaled volume}) \times \text{ins2} / \text{ins2ref} / \text{fn} / \text{fn1}$. The unscaled volume of a peak can be obtained from the command `112d('info',peak#).ins2ref` can be set to the unscaled value divided by `fn` and `fn1`. The report volume for that peak is then the value of `ins2`.

Arguments: `options` (syntax 1) are any of the following (`dconi` is not necessarily active):

- `'adjust'` is a keyword to adjust the bounds of all peaks in the displayed area so that no boundaries overlap, and then to recalculate peak volumes.
- `'draw'` is a keyword to draw the peaks, boxes, numbers, and labels on the spectrum based on the value of the parameter `112dmode`.
- `'info', 'total'` displays the total number of peaks in the current peak table. If a single return value is requested, printing is suppressed and the total number of peaks is returned.
- `'peaks'` is a keyword to find all peaks in the displayed area above a threshold `th`. If `dconi` is active and in the box mode, `112d` finds peaks only in the area defined by the cursors. The `'peaks'` option is the default if no arguments are entered.
- `'pos'` or `'neg'` keywords can be used in addition to `'peak'`, `'volume'`, or `'clear'` to operate only on positive or negative peaks.
- `'read'<,file>` reads in a binary peak file, where `file` is the name of the peak file. If a full path is not specified, the file is searched for first in the current working directory and then in the `112d` subdirectory of the current experiment directory.
- `'readtext'<,file>` reads in a text peak file, where `file` is the name of the peak file. If a full path is not specified, the file is searched for first in the current working directory and then in the `112d` subdirectory of the current experiment directory.

- 'reset' is a keyword to delete all peaks in the peak table.
- 'volume' is a keyword to find the bounds of each peak in the displayed area and integrate this area.
- 'writetext' <, file> writes a peak file to a text file, where file is the name of the text file written. If a full path is not specified, the file is written in the current working directory.

options (syntax 1) can also be any of the following (dconi must be active):

- 'clear' is a keyword to delete all peaks in the displayed region if in the dconi cursor mode, or to delete all peaks within the cursors if in the dconi box mode.
- 'combine' is a keyword to combine all peaks within the area defined by the cursors into a single peak (in dconi box mode only). The center of the new peak is at the average of all combined peaks' centers, and the bounds of this peak contains the maximum extents of the combined peaks' bounds. If all combined peaks have the same label, this label is assigned to the new peak. **CAUTION: All individual peaks to be combined are deleted prior to the creation of the new combination peak, and there is no automatic way to restore the original peaks. Therefore, it is recommended that you make a backup copy of the peak file prior to using this option.**
- 'comment' is a keyword to prompt for an 80-character comment. The comment is assigned to the nearest peak in the dconi cursor mode or to all peaks within the cursors in the dconi box mode.
- 'comment', text executes the 'comment' option using the string entered for text instead of prompting for a comment.
- 'label' is a keyword to prompt for a 15-character label. The label is assigned to the nearest peak in dconi cursor mode or assigned to all peaks within the cursors in dconi box mode. To erase an existing label, enter a label consisting of one or more spaces.
- 'label', text executes the 'label' option using the string entered for text instead of prompting for a label.
- 'mark' is a keyword to insert a peak at the current cursor position if in the dconi cursor mode. If in the dconi box mode, 'mark' is a keyword to integrate the area within the cursors and assign that area to all peaks within the cursors that do not have their bounds already defined. If there are no peaks within the area defined by the cursors, using 'mark' finds the highest point within this area, marks that as a peak, integrates the area within the cursors, and assigns that area to the peak. The displayed values of the volume integrals are scaled by ins2 and ins2ref and the Fourier number of the 2D experiment.
- 'unmark' is a keyword to delete the nearest peak if in dconi cursor mode. If in the dconi box mode, 'unmark' deletes all peak bounds that are completely within the area defined by the cursors. Peaks are not deleted in the box mode.

options (syntax 1) also can be any of the following (dconi does not have to be active because l12d is executed on a peak number):

- 'combine', #1, #2, ... executes the 'combine' option on the list of peak numbers that follow the 'combine' keyword. If a single return value is requested, the peak number of the new combination peak is returned.

- 'comment', text, # executes the 'comment' option on peak # using the string entered for text instead of prompting for a comment.
- 'label', text, # executes the 'label' option on peak # using the string entered for text instead of prompting for a label.
- 'unmark', # deletes peak number #.

\$num (syntax 1) is a return value set to the total number of peaks that have been picked unless the arguments 'combine', #1, #2, ... are used, in which case \$num is the number of the newly created combination peak.

Syntax 2 arguments are the following:

- 'info' <, #> displays information in the text window about peak number #. If no peak number is included, **dcon**i must be active and the default is the peak nearest to the cursor. If return values are requested, the display is suppressed.
- \$peak_number is a return value set to the number of the peak, either the second argument # or, if no value is given for #, the peak nearest to the cursor in **dcon**i.
- \$f1 and \$f2 are return values set to the peak frequencies in f_1 and f_2 of peak \$peak_number.
- \$amp is a return value set to the amplitude of peak \$peak_number.
- \$vol is a return value set to the unscaled volume of \$peak_number peak. This value can be used to set the **ins2ref** parameter.
- \$label is a return value set to the label of peak \$peak_number.
- \$comment is a return value set to the comment about \$peak_number.
- \$FWHH1 and \$FWHH2 are return values set to full-width at half-height of \$peak_number.
- \$f1_min, \$f1_max, \$f2_min, \$f2_max are return values set to the bounds of \$peak_number.

```
Examples: 112d
112d:$npeaks
112d('volume')
112d('read','peaklist.inp')
112d('mark')
112d('label','Peak 1')
112d('info','total'):$npeaks
112d('combine',3,4,5,6):$cpn
112d('info',3):$num,$f1,$f2,$amp,$vol,$label
```

See also: *NMR Spectroscopy User Guide*

Related:	dcon i	Interactive 2D contour display (C)
	ins2	2D volume value (P)
	ins2ref	Fourier number scaled volume of a peak (P)
	112dbackup	Copy current 112d peak file to another file (M)
	112dmode	Control display of peaks picked by 112d (P)
	par112d	Create parameters for 2D peak picking (M)
	p112d	Plot results of 2D peak picking (C)
	th	Threshold (P)
	th2d	Threshold for integrating peaks in 2D spectra (P)
	xdiag	Threshold for excluding diagonal peaks when peak picking (P)

l12dbackup Copy current l12d peak file to another file (M)

Syntax: `l12dbackup< (file) >`

Description: Backs up the current **l12d** peak file by copying it to a file with a different file name. The default **l12d** peak file is `peaks.bin` for 2D data.

Arguments: `file` is the name to be given to the backup file. If a full path is not specified, the file is written to the current working directory. If no argument is provided, the system prompts for a file name. If no file name is specified at the prompt, the default **l12d** peak file name with `.bck` appended is used.

See also: *NMR Spectroscopy User Guide*

Related: **l12d** Automatic and interactive 2D peak picking (C)

l12dmode Control display of peaks picked by l12d (P)

Description: Sets the display attributes of peaks picked by the **l12d** command

Values: A string variable composed of 4 characters, with each character taking the value 'y' (display the peak attribute) or 'n' (do not display the attribute). The first character determines if a "+" is drawn on the screen in **dcon**i displays to mark peaks, the second character controls the drawing of the peak number, the third character controls drawing of the peak bounds box, and the last character controls drawing of the peak label.

See also: *NMR Spectroscopy User Guide*

Related: **l12d** Automatic and interactive 2D peak picking (C)

l1amp List of line amplitudes (P)

Description: Stores a list of line amplitudes above the threshold set by **th**.

See also: *NMR Spectroscopy User Guide*

Related: **d11** Display listed line frequencies and intensities (C)
l1frq List of line frequencies (P)
th Threshold (P)

l1frq List of line frequencies (P)

Description: Stores a list of line frequencies above the threshold set by **th**. Frequencies are stored in Hz and are *not* adjusted by reference parameters **rfl** and **rfp**.

See also: *NMR Spectroscopy User Guide*

Related: **l1amp** List of line amplitudes (P)
rfl Ref. peak position in directly detected dimension (P)
rfp Ref. peak frequency in directly detected dimension (P)
th Threshold (P)

ln Find natural logarithm of a number (C)

Syntax: `ln (value) <:n>`

Description: Finds the natural logarithm (base e) of a number. To convert the value to base 10, use $\log_{10}x = 0.43429 \cdot \ln(x)$.

Arguments: `value` is a number.

`n` is the return value giving the logarithm of `value`. The default is to display the logarithmic value in the status window.

L

Examples: `ln(.5)`
`ln(val):ln_val`

See also: *User Programming*

Related: `atan` Find arc tangent of a number (C)
`cos` Find cosine value of an angle (C)
`exp` Find exponential value of a number (C)
`sin` Find sine value of an angle (C)
`tan` Find tangent value of an angle (C)

load Load status of displayed shims (P)

Description: Sets whether shim values are used. `load` is automatically set to 'y' by the `rts` and is automatically set to 'n' by `su`, `go`, `au`, and `shim`. Shim DAC values are automatically loaded after the console is rebooted (the last values returned before the console was rebooted).

Values: 'y' begins any noninteractive shimming process or data acquisition after loading the shim DACs with the shim values from the current experiment. It also prevents `acqi` from delivering shim values to that experiment.

'n' begins any noninteractive shimming process or data acquisition with the current values stored in the shim DACs. Shim values in the current experiment are ignored.

See also: *NMR Spectroscopy User Guide*

Related: `acqi` Interactive acquisition display process (C)
`au` Submit experiment to acquisition and process data (C)
`go` Submit experiment to acquisition (C)
`rts` Retrieve shim coil settings (C)
`shim` Submit an autoshim experiment to acquisition (C)
`su` Submit a setup experiment to acquisition (M)

loadcolors Load colors for graphics window and plotters (M)

Syntax: `loadcolors<(color_file)>`

Description: Loads the color table for VnmrJ graphics window and plotters. `loadcolors` is generated by the `color` program and includes a series of `setcolor` commands. On bootup, the `bootup` macro calls `loadcolors` to set the graphics and plotter colors.

The `loadcolors` macro checks the value of `maxpen` to decide if the plotter supports colors. If `maxpen` is greater than 1, a color printer is configured.

Arguments: `color_file` is the name of the file to load. `loadcolors` first searches for this file in the directory `$vnmruser/templates/` directory. If not found there, `loadcolors` then searches the `user_templates/vnmr` directory. The default is a color table with the same name as the value of the plotter parameter that `loadcolors` searches for in the same two directories.

Examples: `loadcolors`
`loadcolors('mycolortable')`

See also: *VnmrJ Imaging NMR*

Related: `bootup` Macro executed automatically when VnmrJ activated (M)
`color` Select plotting colors from a graphic interface (M)
`maxpen` Maximum number of pens to use (P)
`setcolor` Set colors for graphics window and for plotters (C)

loc Location of sample in tray (P)

Description: Indicates whether a sample changer is present and enabled, present but disabled, or not present. If the changer is present and enabled, the value of `loc` sets the location in the tray of the sample in use or to be used. The `loc` parameter is stored in the global tree. When an acquisition is started, certain global parameters, including `loc`, are saved with the experiment parameters. The `saveglobal` parameter specifies which global parameters are saved.

The `auto_au` macro controls most of the automation features, including setting the value of `loc`.

Values: A number between 1 and `traymax` indicates the sample location.
0 indicates the changer is not present or disabled.

See also: *NMR Spectroscopy User Guide; VnmrJ Walkup*

Related:

<code>auto_au</code>	Controlling macro for automation (M)
<code>saveglobal</code>	Save selected parameters from global tree (P)
<code>traymax</code>	Sample changer tray size (P)

location Locator action (M)

Description: Perform an action on an object in the locator database. The action depends on the type of object selected, the action performed, and the target selected for the action.

Related:

<code>dndfid</code>	Retrieve and process fid data from the locator (M)
<code>dndjoin</code>	Join a work space from the locator (M)
<code>dndpar</code>	Retrieve a parameter set from the locator (M)
<code>dndshims</code>	Retrieve a shimset set from the locator (M)
<code>locprotoexec</code>	Execute a protocol from the locator (M)
<code>xmmakenode</code>	Make a new study queue node (M)

lock Submit an Autolock experiment to acquisition (C)

Description: Performs an automatic locking operation using the acquisition computer, optimizing lock power, phase, and gain. If necessary, `lock` obtains lock through a software-controlled search. `lock` is the only method to automatically adjust lock phase (usually needed only after probe change or lock channel tuning). `lock` also sets the rf frequencies, decoupler status, and temperature.

See also: *NMR Spectroscopy User Guide*

Related:

<code>au</code>	Submit experiment to acquisition and process data (C)
<code>change</code>	Submit a change sample experiment to acquisition (M)
<code>ga</code>	Submit experiment to acquisition and FT the result (C)
<code>go</code>	Submit experiment to acquisition (C)
<code>sample</code>	Submit change sample, autoshim experiment to acquisition (M)
<code>shim</code>	Submit an Autoshim experiment to acquisition (C)
<code>spin</code>	Submit a spin setup experiment to acquisition (C)
<code>su</code>	Submit a setup experiment to acquisition (M)

lockacqtc Lock loop time constant during acquisition (P)

Description: Controls time constant of lock loop during acquisition (i.e., time constant by which the lock feedback corrects disturbances of the magnetic field).

Values: 1, 2, 3, or 4 (where 1 sets 1.2 seconds, 2 sets 4.7 seconds, 3 sets 12 seconds, and 4 sets 48 seconds).

If `lockacqtc` does not exist, it is set to 48 seconds. All systems are designed to work well with the default settings, and there should rarely be a reason to alter the lock time constant. However, to experiment with other values, create `lockacqtc` and set a new value:

```
create('lockacqtc','integer','global')
setlimit('lockacqtc',4,1,1,'global') lockacqtc=n
```

where n is the new value.

See also: *NMR Spectroscopy User Guide*

Related: `create` Create new parameter in a parameter tree (C)
`locktc` Lock time constant (P)
`setlimit` Set limits of a parameter in a tree (C)

lockfreq Lock frequency (P)

Description: Sets system lock frequency. The value is entered using the Lock Frequency label in Spectrometer Configuration window. **The value of lockfreq must be set correctly in order to observe NMR signals.**

`lockfreq` can find the lock signal or resonance. Traditionally, Varian spectrometers have used the parameter `z0` for this purpose; however, using `lockfreq` can require less shimming when switching solvents and less adjustment to the lock phase. To use `lockfreq`, set `z0='n'`.

Values: 1 to 160 (in MHz), 'n'

Use the true ^2H frequency. Typical values of `lockfreq` are shown in the chart below.

^1H Frequency		
200	30.710	30.6976
300	46.044	46.0625
400	61.395	61.471
500	76.729	...
600	92.095	...
750	115.250	...

Refer to the manual *VnmrJ Installation and Administration* for details on finding the correct lock frequency.

The commands; `go`, `lock`, `shim`, and `su` reset the lock frequency in the console to the current value of `lockfreq`. Lock frequency in the console can be set with the `sethw` command.

`lockfreq` is offset by the value of `lkof`, if that parameter exists, but `sethw` directly uses its numeric argument, without any offset by `lkof`.

See also: *VnmrJ Installation and Administration; NMR Spectroscopy User Guide*

Related: `config` Display current configuration and possibly change it (M)
`go` Submit experiment to acquisition (M)
`lkof` Track changes in lock frequency (P)
`lock` Submit an Autolock experiment to acquisition (C)
`sethw` Set values for hardware in acquisition system (C)
`setlockfreq` Set lock frequency (C)
`shim` Submit an Autoshim experiment to acquisition (C)
`su` Submit a setup experiment to acquisition (M)
`z0` Z0 field position (P)

lockgain Lock gain (P)

Description: Contains the current lock gain value as set by computer control. The value is stored in `vnmrsys/global` and can be examined by typing `lockgain?`.

Values: 0 to 48 dB, in 1-dB steps.

See also: *NMR Spectroscopy User Guide*

lockphase Lock phase (P)

Description: Contains the current lock phase. The value is stored in `vnmrsys/global` and can be examined by typing `lockphase?`.

Values: 0 to 360, in degrees, in 1.4-degree steps.

See also: *NMR Spectroscopy User Guide*

lockpower Lock power (P)

Description: Contains the current lock power value as set by computer control. The value is stored in `vnmrsys/global` and can be examined by typing `lockpower?`.

Values: 0 to 68 dB, in 1-dB steps, 68 is full power.

See also: *NMR Spectroscopy User Guide*

locktc Lock time constant (P)

Description: Controls lock loop time constant when system is not performing acquisition (idle, lock display, shim display, FID display, autoshim, autolock, etc.).

Values: 1, 2, 3, or 4 (where 1 corresponds to 1.2 seconds, 2 to 4.7 seconds, 3 to 12 seconds, and 4 to 48 seconds). If `locktc` does not exist, the system uses a value of 1, the fastest value. To experiment with other value, create `locktc` and set a value (e.g., `create('locktc','integer','global')`
`setlimit('locktc',4,1,'global') locktc=2`).

See also: *NMR Spectroscopy User Guide*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>lockacqtc</code>	Lock acquisition time constant (P)
	<code>setlimit</code>	Set limits of a parameter in a tree (C)

logate Transmitter local oscillator gate (P)

Description: Specifies whether the transmitter local oscillator (L.O.) is gated with the transmitter rf output or with the transmitter I.F. (intermediate frequency).

The `logate` parameter does not exist in most parameter sets; the system internally sets it to '1'. To use the value 's', create `logate` and change the value by entering: `create('logate','string')`
`setenumerals('logate',2,'1','s') logate='s'`.

Values: '1' makes the transmitter L.O. gate with the rf output, producing better signal-to-noise, usually most important in liquids NMR.

's' makes the transmitter L.O. gate with the I.F. signal, producing sharper pulses, especially important in solid-state NMR.

See also: *User Guide: Solid-State NMR*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>setenumerals</code>	Set values of a string variable in a tree (C)

lookup Look up words and lines from a text file (C)

Applicability: VnmrJ

Syntax: `lookup('codeword', argument<, 'codeword',
argument<, ...>>) : $n1<$n2<, ...>>`

Description: Search a text file or files for a word or any string of characters delimited by white space characters (space character, a tab, a new line, a carriage return, or a comma) or codeword and return to the user subsequent words or lines.

The white space characters may be specified. Punctuation marks, unless they are defined as white space as the comma is by default, also form words or are part of a word. A line is any string of characters from the current word to the next carriage return. A line will include all "white space" characters except the carriage return. Depending on the codeword, word searches and word counts can be case insensitive or case sensitive.

The codewords `mfile` and `filekey` implement multiple text file lookup and `lookup` reads the contents of the specified files.

The `mfile` and `file` keywords are used together to keep track of various locations within a single file to restart the search from that location.

The first time a file is selected, or the search is restarted at the beginning of the file, use the name of the file instead of the `filekey`. Subsequent calls to `lookup` on this file use the value returned by the `filekey` codeword as the argument following the `mfile` codeword. The `mfile` codeword resets the white space to the default values.

Arguments: Default white space characters: space character, tab, new line, carriage return, or comma.

`file` codeword specifies that the next supplied argument is the name of the active text file. This codeword must be the first argument and the file name must be the second argument passed to `lookup`. The search through a text file is a top to bottom search. The `file` codeword resets the search to start from the top of the text file. Subsequent searches through a previously accessed text file will continue from where the previous search stopped provided the `file` codeword is not used. The `file` codeword resets the white space characters to their default values.

`mfile` codeword specifies that the next supplied argument is the `filekey` to select one of multiple text files to access. This codeword must be first argument and the `filekey` must be the second argument passed to `lookup` if `mfile` is used.

`seek` this codeword causes the `lookup` program to search the text file for words which match those supplied as arguments following the `seek` codeword. An implicit `seek` is initially assumed for each call to `lookup`. The `lookup` program maintains a pointer to the word following the last successful `seek`. The first argument following an explicit `seek` codeword is interpreted as a word to search for and not a codeword. The second or later argument following an explicit `seek` is interpreted as a codeword if it matches one of the nine cases. Therefore, for example, one can search for the word `file` without having it interpreted as a codeword by having it immediately follow the `seek` codeword in the argument list. This `seek` is case insensitive.

`seekcs` this codeword is the case sensitive equivalent to the `seek` codeword and follows the same rules as `seek`. Alternate case sensitive and case insensitive searches are allowed.

`skip` increments the word pointer to the next word in the text file. This codeword may optionally be followed by a number which will specify how many words to skip.

`read` returns to the user the word currently being pointed to and increments the pointer to the next word in the text file. This codeword may optionally be followed by a number which will specify how many words to return to the user.

`readline` returns to the user the word currently being pointed to and all following words until the end of the current line. The pointer is moves to the first word of the next line in the text file. This codeword may optionally be followed by a number which will specify how many lines to return to the user.

`count` returns to the user the number of times words in the text file match the subsequent argument. The `count` starts at the current word pointer and proceeds to the end of the text file. The word `count` is not case sensitive.

`countcs` this codeword is the case sensitive equivalent to the `count` codeword. In all other respects, it is the same as `count`.

`delimiter` this codeword specifies that the next supplied argument is a list of characters which are used to identify the white space used to identify words.

Characters are specified by the following:

```
\n — new line
\t — tab
\r — carriage return
\\ — backslash
\' — single quote.
```

The two arguments `delimiter, ' \t\n\r'`, reselect the default white space. The `file` codeword will also reselect the default white space. The distinction is that the `file` codeword restarts the search from the beginning of the file while the `delimiter` codeword continues from the current search position. An implicit `seek` is applied following the '`delimiter`' codeword and argument.

`filekey` returns the current location within the file being accessed.

Combined with the `mfile` codeword, a subsequent call to `lookup` starts the search at the location within the file specified by the value of `filekey`. The `filekey` serves both as a pointer to the file and as the character offset within that file.

Examples: `lookup('file',systemdir + '/manual/lookup')`
Select this file for the search.

```
lookup('user','skip',2,'read',2,'readline'):$n1,$n2,
$n3,$ret
```

Seek is assumed with the call to `lookup`. Finding the word `user` the next instruction, '`skip`', 2, causes the pointer to jump two words. The codeword `read` causes the word to be put into `$n1`. The argument 2 specifies two words to be read into `$n2`. The word pointer now points to the next. The codeword `readline` causes the remaining characters up to the next carriage return to be placed in `$n3`. The pointer now points to the first word in the next line. The variable `$ret` is set to the number of arguments successfully returned from the text file and is used to determine if the end of the text file has been reached.

```
lookup('skip',8,'read','skip',3,'read',2,'seek','comma'):$n3,$n4,$n5
```

'`skip`', 8 causes the pointer to jump eight words. The '`read`' sets `$n3` equal to word where the pointer is now located. '`skip`', 3 jumps the next three words. '`Read`', 2 reads two consecutive words and sets `$n4` to the first word and `$n5` equal the second word. The `seek` argument searches for the word '`comma`'. If the word '`comma`' is at the end of a sentence it will not be found because the period is treated (by default) as part of the word. Define the period as a white space and occurrences comma at the end of sentences are also found. The word pointer now points to the next word.

```
lookup('delimiter',' ,\'.\n\t"', 'seek','file',
'skip',6,'read'):n6
```

The `delimiter` with the argument `' , \ ' . \n\t "'` sets white space to space, comma, single quote, period, new line, tab, and double quote. Setting single quotes to white space causes the explicit `seek` to select the next argument `file` as a search word not a codeword. The search for the word must matches both `MUST` and `must` because `seek` is not case sensitive. `'Skip'`, 6 jumps six words. `Read` sets `$n6` equal to word found between the next set of single quotes because single quotes are defined as white space.

`lookup('seekcs','Test','read'):$n7`
`seekcs` is the case sensitive form of `seek` and searches for the word that is an exact match to the case of `Test` (the argument following the codeword `seekcs`). Finding the word `'Test'`, `read` sets `$n7` to `search`. Any occurrence of the word `test` is skipped.

See also: *User Programming*

Related: `dialog` Display a dialog box from a macro (C)
`systemdir` VnmrJ system directory (P)

locprotoexec Execute a protocol from the locator (M)

Description: When a protocol is dragged from the locator and dropped onto the graphics canvas, this macro adds the protocol to the end of the study queue, and executes the macro associated with the protocol.

Related: `dndfid` Retrieve and process fid data from the locator (M)
`dndjoin` Join a work space from the locator (M)
`dndpar` Retrieve a parameter set from the locator (M)
`dndshims` Retrieve a shimset set from the locator (M)
`locaction` Locator action (M)
`xmmakenode` Make a new study queue node (M)

lp First-order phase in directly detected dimension (P)

Description: Specifies the first-order phase-correction angles along the directly detected dimension according to the formula

$$\text{absorption spectrum}(\omega) = \text{real channel}(\omega) * \sin \theta + \text{imaginary channel}(\omega) * \cos \theta$$

where the phase angle θ is a function of frequency, i.e.

$$\theta = \text{rp} + (\omega - \omega_0) * \text{lp}$$

ω_0 is defined to be the right end of the spectrum (i.e., `lp` has zero effect at the right edge of the spectrum and a linearly increasing effect going to the left). In multidimensional data sets, `lp` controls the phase of the directly detected dimension: f_2 dimension in 2D data sets, f_3 dimension in 3D data sets, etc.

Values: -3600 to +3600, in degrees. Typical values are between 0 and -180.

See also: *NMR Spectroscopy User Guide*

Related: `aph` Automatic phase adjustment of spectra (C)
`lp1` First-order phase in 1st indirectly detected dimension (P)
`lp2` First-order phase in 2nd indirectly detected dimension (P)
`rp` Zero-order phase in directly detected dimension (P)
`setlp0` Set parameters for zero linear phase (M)

lp1 First-order phase in 1st indirectly detected dimension (P)

Description: Controls the first-order phase constant along the first indirectly detected dimension during the process of phase-sensitive 2D transformation. The first

indirectly detected dimension is often referred to as the f_1 dimension of a multidimensional data set.

See also: *NMR Spectroscopy User Guide*

Related: **lp** First-order phase in directly detected dimension (P)
lp2 First-order phase in 2nd indirectly detected dimension (P)
rp1 Zero-order phase in 1st indirectly detected dimension (P)

lp2 First-order phase in 2nd indirectly detected dimension (P)

Description: Controls the first-order phase constant along the second indirectly detected dimension during a **ds**, **dconi**, or equivalent display operation on the 2D data or a 1D trace therein. The second indirectly detected dimension is often referred to as the f_2 dimension of a 3D (or higher dimensionality) data set.

See also: *NMR Spectroscopy User Guide*

Related: **dconi** Interactive 2D contour display (C)
ds Display a spectrum (C)
lp First-order phase in directly detected dimension (P)
rp2 Zero-order phase in 2nd indirectly detected dimension (P)

lpalg LP algorithm in np dimension (P)

Description: Specifies the linear prediction (LP) algorithm to use in the **np** dimension. The resulting LP coefficients are used to appropriately extend the complex time-domain data prior to a normal Fourier transform. The LP algorithms work both on complex t_2 FIDs and on hypercomplex or complex t_1 interferograms. Enter **addpar** ('lp') to create **lpalg** and other **np** dimension LP parameters in the current experiment

Values: 'lpfft' does a least-squares calculation of **lpfilt** complex LP coefficients using **lpnupts** complex time-domain data points. Eigenvalue decomposition of the least-squares matrix is done using Householder tridiagonalization followed by the QL method with implicit shifts.

'lpparfft' does a non-least-squares calculation of **lpfilt** complex LP coefficients using (**lpfilt**+1) complex, autoregressive (AR) matrix elements. These AR matrix elements are calculated from the raw, complex time-domain data using **lpnupts** points.

Note that the 'lpfft' algorithm is preferred by far. While 'lpparfft' can model broad lines and can extend data sets when mostly noise exists, it cannot model narrow lines.

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg1 LP algorithm in n_1 dimension (P)
lpalg2 LP algorithm in n_1^2 dimension (P)
lpext LP data extension in **np** dimension (P)
lpfilt LP coefficients to calculate in **np** dimension (P)
lpnupts LP number of data points in **np** dimension (P)
lpopt LP algorithm data extension in **np** dimension (P)
lpprint LP print output in **np** dimension (P)
lptrace LP output spectrum in **np** dimension (P)
np Number of data points (P)
proc Type of processing on **np** FID (P)
strtlp Starting point for LP calculation in **np** dimension (P)
strtext Starting point for LP data extension in **np** dimension (P)

L

lpalg1 LP algorithm in ni dimension (P)

Description: Specifies the LP (linear prediction) algorithm to use in the **ni** dimension. **lpalg1** functions analogously to **lpalg**. Enter **addpar** ('lp' , 1) to create **lpalg1** and other **ni** dimension LP parameters in the current experiment.

Values: 'lpfft' or 'lparfft'

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg LP algorithm in np dimension (P)
ni Number of increments in 1st indirectly detected dimension (P)

lpalg2 LP algorithm in ni2 dimension (P)

Description: Specifies the LP (linear prediction) algorithm to use in the **ni2** dimension. **lpalg2** functions analogously to **lpalg**. Enter **addpar** ('lp' , 2) to create **lpalg2** and other **ni2** dimension LP parameters in the current experiment.

Values: 'lpfft' or 'lparfft'

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg LP algorithm in np dimension (P)
ni2 Number of increments in 2nd indirectly detected dimension (P)

lpext LP data extension in np dimension (P)

Description: Specifies number of complex time-domain data points for LP (linear prediction) in the **np** dimension by which the original data is to be extended (or altered) in either the forward or backward direction. **lpext** is constrained by $(\text{strtext} - \text{lpext}) \geq 0$ for **lpopt** = 'b' and by $(\text{strtext} + \text{lpext} - 1) \leq \text{fn}/2$ for **lpopt** = 'f'. In the **np** direction, if $(\text{strtext} - \text{lpext}) = 0$ and **lpopt** = 'b' (backwards linear prediction with calculation of the first point), **fpmult** defaults to the theoretical value of 0.5 instead of 1.0. Enter **addpar** ('lp') to create **lpext** and other **np** dimension LP parameters in the current experiment.

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg LP algorithm in np dimension (P)
lpext1 LP data extension in ni dimension (P)
lpext2 LP data extension in ni2 dimension (P)
lpopt LP algorithm data extension in np dimension (P)
np Number of data points (P)
strtext Starting point for LP data extension in np dimension (P)

lpext1 LP data extension in ni dimension (P)

Description: Specifies number of complex time-domain data points for LP (linear prediction) in the **ni** dimension by which the original data is to be extended (or altered) in either the forward or backward direction. **lpext1** functions analogously to **lpext**. Enter **addpar** ('lp' , 1) to create **lpext1** and other **ni** dimension LP parameters in the current experiment.

Related: **addpar** Add selected parameters to the current experiment (M)
lpext LP data extension in np dimension (P)
ni Number of increments in 1st indirectly detected dimension (P)

lpext2 LP data extension in ni2 dimension (P)

Description: Specifies number of complex time-domain data points for LP (linear prediction) in the **ni2** dimension by which the original data is to be extended (or altered) in either the forward or backward direction. **lpext2** functions analogously to **lpext**. Enter **addpar** ('lp' , 2) to create **lpext2** and other **ni2** dimension LP parameters in the current experiment.

Related: **addpar** Add selected parameters to the current experiment (M)
lpext LP data extension in np dimension (P)
ni2 Number of increments in 2nd indirectly detected dimension (P)

lpfilt LP coefficients to calculate in np dimension (P)

Description: Specifies number of complex LP (linear prediction) coefficients in the **np** dimension to be calculated from a specified region of the time-domain data. **lpfilt** should be greater than **nsignals**, where **nsignals** is the number of sinusoidal signals contained in that FID (or interferogram). Enter **addpar** ('lp') to create **lpfilt** and other **np** dimension LP parameters in the current experiment.

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg LP algorithm in np dimension (P)
lpfilt1 LP coefficients to calculate in ni dimension (P)
lpfilt2 LP coefficients to calculate in ni2 dimension (P)
np Number of data points (P)

lpfilt1 LP coefficients to calculate in ni dimension (P)

Description: Specifies number of complex LP (linear prediction) coefficients in the **ni** dimension to be calculated from a specified region of the time-domain data. **lpfilt1** functions analogously to **lpfilt**. Enter **addpar** ('lp' , 1) to create **lpfilt1** and other **ni** dimension LP parameters in the current experiment.

Related: **addpar** Add selected parameters to the current experiment (M)
lpfilt LP coefficients to calculate in np dimension (P)
ni Number of increments in 1st indirectly detected dimension (P)

lpfilt2 LP coefficients to calculate in ni2 dimension (P)

Description: Specifies number of complex LP (linear prediction) coefficients in the **ni2** dimension to be calculated from a specified region of the time-domain data. **lpfilt2** functions analogously to **lpfilt**. Enter **addpar** ('lp' , 2) to create **lpfilt1** and other **ni2** dimension LP parameters in the current experiment.

Related: **addpar** Add selected parameters to the current experiment (M)
lpfilt LP coefficients to calculate in np dimension (P)
ni Number of increments in 1st indirectly detected dimension (P)

lpnupts LP number of data points in np dimension (P)

Description: Specifies number of complex time-domain data points in the **np** dimension to be used in constructing the autoregressive (**lpalg**= 'lparfft') or least-

squares (`lpalg='lpnefft'`) matrix from which the complex LP (linear prediction) coefficients are calculated. Note that `lpnupts` greater than or equal to `2*lpfilt` is required for both algorithms. Enter `addpar('lp')` to create `lpnupts` and other `np` dimension LP parameters in the current experiment.

Related: `addpar` Add selected parameters to the current experiment (M)
`lpalg` LP algorithm in `np` dimension (P)
`lpfilt` LP coefficients to calculate in `np` dimension (P)
`lpnupts1` LP number of data points in `ni` dimension (P)
`lpnupts2` LP number of data points in `ni2` dimension (P)
`np` Number of data points (P)

lpnupts1 LP number of data points in ni dimension (P)

Description: Specifies number of complex time-domain data points in the `ni` dimension to be used in constructing the autoregressive (`lpalg1='lparfft'`) or least-squares (`lpalg1='lpnefft'`) matrix from which the complex LP (linear prediction) coefficients are calculated. `lpnupts1` functions analogously to `lpnupts`. Enter `addpar('lp',1)` to create `lpnupts1` and other `ni` dimension LP parameters in the current experiment.

Related: `addpar` Add selected parameters to the current experiment (M)
`lpalg1` LP algorithm in `ni` dimension (P)
`lpnupts` LP number of data points in `np` dimension (P)
`ni` Number of increments in 1st indirectly detected dimension (P)

lpnupts2 LP number of data points in ni2 dimension (P)

Description: Specifies number of complex time-domain data points in the `ni2` dimension to be used in constructing the autoregressive (`lpalg2='lparfft'`) or least-squares (`lpalg2='lpnefft'`) matrix from which the complex LP (linear prediction) coefficients are calculated. `lpnupts2` functions analogously to `lpnupts`. Enter `addpar('lp',2)` to create `lpnupts2` and other `ni2` dimension LP parameters in the current experiment.

Related: `addpar` Add selected parameters to the current experiment (M)
`lpalg2` LP algorithm in `ni2` dimension (P)
`lpnupts` LP number of data points in `np` dimension (P)
`ni2` Number of increments in 2nd indirectly detected dimension (P)

lpopt LP algorithm data extension in np dimension (P)

Description: Specifies how the specific LP (linear prediction) algorithm is to extend (or alter) forward or backward the time-domain data in the `np` dimension. Enter `addpar('lp')` to create `lpopt` and other `np` dimension LP parameters in the current experiment.

Multiple LP operations, extended forward or backward, can be performed on each FID or interferogram. This is accomplished by arraying the LP processing parameters (e.g., `lpopt='b','f','b'`). The number of LP operations is determined by the LP processing parameter with the largest array size. LP parameters having a smaller array size are padded out with their last value. The most common use for this capability is to back-calculate the first 1 to 2 points in an FID or interferogram and subsequently to extend the length of the time-domain data by LP.

A printout can be obtained for each LP operation on an individually definable FID or interferogram. For example, if `lpprint=30,30` and `lptrace=1,2`, the text file `lpanalyz.out.1` contains the LP printout for the first LP operation on FID 1 and `lpanalyz.out.2` contains the LP printout for the second LP operation on FID 2.

Values: 'b' indicates the LP coefficients are to be used in the back-calculation of a specified number of time-domain data points.

'f' indicates the LP coefficients are to be used in the forward extension of the time-domain data by a specified number of points. The characteristic polynomial in z space, derived from the complex LP coefficients, is set up and rooted. Any root found to lie outside the unit circle is reflected back into the unit circle. New complex LP coefficients are then calculated from these adjusted complex roots.

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>lpalg</code>	LP algorithm in np dimension (P)
	<code>lpopt1</code>	LP algorithm data extension for ni dimension (P)
	<code>lpopt2</code>	LP algorithm data extension for ni2 dimension (P)
	<code>lpprint</code>	LP print output for np dimension (P)
	<code>lptrace</code>	LP output spectrum for np dimension (P)
	<code>np</code>	Number of data points (P)

lpopt1 LP algorithm data extension in ni dimension (P)

Description: Specifies how the specific LP (linear prediction) algorithm is to extend (or alter) forward or backward the time-domain data in the `ni` dimension. `lpopt1` functions analogously to `lpopt`. Enter `addpar('lp',1)` to create `lpopt1` and other `ni` dimension LP parameters in the current experiment.

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>lpopt</code>	LP algorithm data extension for np dimension (P)
	<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)

lpopt2 LP algorithm data extension in ni2 dimension (P)

Description: Specifies how the specific LP (linear prediction) algorithm is to extend (or alter) forward or backward the time-domain data in the `ni2` dimension. `lpopt2` functions analogously to `lpopt`. Enter `addpar('lp',2)` to create `lpopt2` and other `ni2` dimension LP parameters in the current experiment.

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>lpopt</code>	LP algorithm data extension for np dimension (P)
	<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)

lpprint LP print output for np dimension (P)

Description: Controls LP (linear prediction) print output for the `np` dimension and creates an output file in the current experiment directory (`curexp`) with the name `lpanalyz.out.1`. Enter `addpar('lp')` to create `lpprint` and other `np` dimension LP parameters in the current experiment.

Values: Comprised of sum of decimal values of the following bit fields, in which each bit field controls an independent output option:

- Bit 0 (decimal value 1) writes out the LP matrix and Y vector from which the LP coefficients are calculated.

- Bit 1 (decimal value 2) writes out the LP coefficients that have been obtained using either of the two supported algorithms.
- Bit 2 (decimal value 4) writes out the LP roots obtained from the characteristic polynomial derived from the LP coefficients; this only applies for `lpalg='lpfft'` and `lpopt='f'`.
- Bit 3 (decimal value 8) writes out the original and recalculated values for each LP extended (or altered) complex time-domain data point.
- Bit 4 (decimal value 16) writes out the internal LP parameter structure.

For example, `lpprint=12` and `lptrace=1` yields the following information in the file `curexp/lpanalyz.out.1` for spectrum 1 along f_2 : the values for all `lpfilt` complex LP coefficients and the original and recalculated values for each of the `lpext` LP extended (or altered) complex time-domain data points.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>curexp</code>	Current experiment directory (P)
	<code>lpalg</code>	LP algorithm in <code>np</code> dimension (P)
	<code>lpext</code>	LP data extension in <code>np</code> dimension (P)
	<code>lpfilt</code>	LP coefficients to calculate in <code>np</code> dimension (P)
	<code>lpopt</code>	LP algorithm data extension for <code>np</code> dimension (P)
	<code>lpprint1</code>	LP print output for <code>ni</code> dimension (P)
	<code>lpprint2</code>	LP print output for <code>ni2</code> dimension (P)
	<code>lptrace</code>	LP output spectrum in <code>np</code> dimension (P)
	<code>np</code>	Number of data points (P)

lpprint1 LP print output for ni dimension (P)

Description: Controls LP (linear prediction) print output for the `ni` dimension and creates an output file in the current experiment directory (`curexp`) with the name `lpanalyz1.out.1`. `lpprint1` functions analogously to `lpprint`. Enter `addpar('lp',1)` to create `lpprint1` and other `ni` dimension LP parameters in the current experiment.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>lpprint</code>	LP print output for <code>np</code> dimension (P)
	<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)

lpprint2 LP print output for ni2 dimension (P)

Description: Controls LP (linear prediction) print output for the `ni2` dimension and creates an output file in the current experiment directory (`curexp`) with the name `lpanalyz2.out.1`. `lpprint2` functions analogously to `lpprint`. Enter `addpar('lp',2)` to create `lpprint2` and other `ni2` dimension LP parameters in the current experiment.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>lpprint</code>	LP print output for <code>np</code> dimension (P)
	<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)

lptrace LP output spectrum in np dimension (P)

Description: Specifies for which spectrum LP (linear prediction) output in the **np** dimension is produced in accordance with the parameter **lpprint**. Enter **addpar('lp')** to create **lptrace** and other **np** dimension LP parameters in the current experiment.

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg LP algorithm in np dimension (P)
lpprint LP print output in np dimension (P)
lptrace1 LP output spectrum in ni dimension (P)
lptrace2 LP output spectrum in ni2 dimension (P)
np Number of data points (P)

lptrace1 LP output spectrum in ni dimension (P)

Description: Specifies for which spectrum or trace LP (linear prediction) output in the **ni** dimension is produced in accordance with the parameter **lpprint1**. **lptrace1** functions analogously to **lptrace**. Enter **addpar('lp',1)** to create **lpprint2** and other **ni** dimension LP parameters in the current experiment.

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpprint1 LP print output in ni dimension (P)
lptrace LP output spectrum in np dimension (P)
ni Number of increments in 1st indirectly detected dimension (P)

lptrace2 LP output spectrum in ni2 dimension (P)

Description: Specifies for which spectrum or trace LP (linear prediction) output in the **ni2** dimension is produced in accordance with the parameter **lpprint2**. **lptrace2** functions analogously to **lptrace**. Enter **addpar('lp',2)** to create **lptrace2** and other **ni2** dimension LP parameters in the current experiment.

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpprint2 LP print output in ni2 dimension (P)
lptrace LP output spectrum in np dimension (P)
ni2 Number of increments in 2nd indirectly detected dimension (P)

ls List files in directory (C)

Syntax: **ls<(directory)>**

Description: Lists the names of files in a directory on the text output window. **ls** is identical to **dir** and **lf**.

Arguments: **directory** is the name of a directory. The default is the current working directory. **ls** is equivalent to the UNIX command **ls** and uses the same options (e.g., **-l** for a long listing such as **ls('-l *.fid')**).

Examples: **ls**
ls('data')
ls('-l *.fid')

Related: `dir` List files in directory (C)
`lf` List files in directory (C)

lsfid Number of complex points to left-shift the np FID (P)

Description: Specifies number of complex points (not real points) that the `np` FID is to be either left-shifted (`lsfid`>0) or right-shifted (`lsfid`<0). A right shift adds zeros to the front of the FID. `lsfid` (and related parameters `phfid` and `lsfrq`) operate on complex `np` FID data, referred to as the t_2 dimension in a 2D experiment or as the t_3 dimension in a 3D experiment. `lsfid` is in the processing group and is properly handled by a `wti` operation (display).

Values: $-\text{fn}/2$ to $\text{np}/2$ (or $-\text{fn}/2$ to $\text{fn}/2$ if $\text{fn}<\text{np}$), 'n'

Related: `dfid` Display a single FID (C)
`ds` Display a spectrum FID (C)
`fn` Fourier number in directly detected dimension (P)
`ft` Fourier transform 1D data (C)
`ft1d` Fourier transform along f_2 dimension (C)
`ft2d` Fourier transform 2D data (C)
`lsfid1` Number of complex points to left-shift n_i interferogram(P)
`lsfid2` Number of complex points to left-shift n_{i2} interferogram (P)
`lsfrq` Frequency shift of the `fn` spectrum in Hz (P)
`np` Number of data points (P)
`phfid` Zero-order phasing constant for the `np` FID (P)
`wft` Weight and Fourier transform 1D data (C)
`wft1d` Weight and Fourier transform f_2 of 2D data (C)
`wft2d` Weight and Fourier transform 2D data (C)
`wti` Interactive weighting (C)

lsfid1 Number of complex points to left-shift n_i interferogram (P)

Description: Specifies number of hypercomplex (for hypercomplex interferogram data) or complex (for complex interferogram data) points that the n_i interferogram is to be either left-shifted (`lsfid1`>0) or right-shifted (`lsfid1`<0). A right shift adds zeros to the front of the FID. `lsfid1` (and related parameters `phfid1` and `lsfrq1`) operate on n_i interferogram data, both hypercomplex and complex. n_i interferogram data are referred to as the t_1 dimension in both a 2D and a 3D experiment. `lsfid1` is in the processing group and is properly handled by a `wti` operation (display); that is, a `wti` operation on an n_i interferogram applies the parameters `phfid1`, `lsfid1`, and `lsfrq1`, if selected, to the time-domain data prior to the Fourier transformation.

Values: $-\text{fn1}/2$ to n_i (or $-\text{fn1}/2$ to $\text{fn1}/2$ if $\text{fn1}<2*n_i$), 'n'

Related: `fn1` Fourier number in 1st indirectly detected dimension (P)
`lsfid` Number of complex points to left-shift `np` FID (P)
`lsfid2` Number of complex points to left-shift n_{i2} interferogram (P)
`lsfrq1` Frequency shift of the `fn1` spectrum in Hz (P)
`ni` Number of increments in 1st indirectly detected dimension (P)
`phfid1` Zero-order phasing constant for n_i interferogram (P)
`wti` Interactive weighting (C)

lsfid2 **Number of complex points to left-shift ni2 interferogram (P)**

Description: Specifies the number of hypercomplex (for hypercomplex interferogram data) or complex (for complex interferogram data) points that the **ni2** interferogram is to be either left-shifted (**lsfid2**>0) or right-shifted (**lsfid2**<0). A right shift adds zeros to the front of the FID. **lsfid2** (and related parameters **phfid2** and **lsfrq2**) operate on **ni2** interferogram data, both hypercomplex and complex. **ni2** interferogram data are referred to as the t_2 dimension in a 3D experiment. **lsfid2** is in the processing group and is properly handled by a **wti** operation (display).

Values: $-\text{fn2}/2$ to **ni2** (or $-\text{fn2}/2$ to $\text{fn2}/2$ if $\text{fn2} < 2 * \text{ni2}$), 'n'

Related:	fn2	Fourier number in 2nd indirectly detected dimension (P)
	lsfid	Number of complex points to left-shift np FID (P)
	lsfid1	Number of complex points to left-shift ni interferogram(P)
	lsfrq2	Frequency shift of the fn2 spectrum in Hz (P)
	ni2	Number of increments in 2nd indirectly detected dimension (P)
	phfid2	Zero-order phasing constant for ni2 interferogram (P)
	wti	Interactive weighting (C)

lsfrq **Frequency shift of the fn spectrum (P)**

Description: Sets a frequency shift of spectral data, in Hz. **lsfrq** is the time-domain equivalent of **lp** within VnmrJ. **lsfrq** (and related parameters **phfid** and **lsfid**) operate on complex np FID data, referred to as the t_2 dimension in a 2D experiment or as the t_3 dimension in a 3D experiment. **lsfrq** is in the processing group and is properly handled by a **wti** operation (display).

Values: A positive value results in peaks being shifted downfield (to the left).
A negative value results in peaks being shifted upfield (to the right).

Related:	dfid	Display a single FID (C)
	ds	Display a spectrum FID (C)
	fn	Fourier number in directly detected dimension (P)
	ft	Fourier transform 1D data (C)
	ft1d	Fourier transform along f_2 dimension (C)
	ft2d	Fourier transform 2D data (C)
	lp	First-order phase in directly detected dimension (P)
	lsfid	Number of complex points to left-shift np FID (P)
	lsfrq1	Frequency shift of the fn1 spectrum in Hz (P)
	lsfrq2	Frequency shift of the fn2 spectrum in Hz (P)
	phfid	Zero-order phasing constant for np FID (P)
	wft	Weight and Fourier transform 1D data (C)
	wft1d	Weight and Fourier transform f_2 of 2D data (C)
	wft2d	Weight and Fourier transform 2D data (C)
	wti	Interactive weighting (C)

lsfrq1 **Frequency shift of the fn1 spectrum (P)**

Description: Sets a frequency shift of spectral data, in Hz. **lsfrq1** is the time-domain equivalent of **lp1** within VnmrJ. **lsfrq1** (and related parameters **phfid1** and **lsfid1**) operate on **ni** interferogram data, both hypercomplex and complex. **ni** interferogram data are referred to as the t_1 dimension in both a 2D and a 3D experiment. **lsfrq1** is in the processing group and is properly handled by a **wti** operation (display); that is, a **wti** operation on an **ni**

interferogram applies the parameters `phfid1`, `lsfid1`, and `lsfrq1`, if selected, to the time-domain data prior to the Fourier transformation.

Values: A positive value results in peaks being shifted downfield (to the left).
A negative value results in peaks being shifted upfield (to the right).

Related: `fn1` Fourier number in 1st indirectly detected dimension (P)
`lp1` First-order phase in 1st indirectly detected dimension (P)
`lsfid1` Number of complex points to left-shift `ni` interferogram (P)
`lsfrq` Frequency shift of the `fn` spectrum in Hz (P)
`lsfrq2` Frequency shift of the `fn2` spectrum in Hz (P)
`ni` Number of increments in 1st indirectly detected dimension (P)
`phfid1` Zero-order phasing constant for `ni` interferogram (P)
`wti` Interactive weighting (C)

lsfrq2 Frequency shift of the fn2 spectrum (P)

Description: Sets a frequency shift of spectral data in Hz. `lsfrq2` is the time-domain equivalent of `lp2` within VnmrJ. `lsfrq2` (and related parameters `phfid2` and `lsfid2`) operate on `ni2` interferogram data, both hypercomplex and complex. `ni2` interferogram data is referred to as the t_2 dimension in a 3D experiment. `lsfrq2` is in the processing group and is properly handled by a `wti` operation (display).

Values: A positive value results in peaks being shifted downfield (to the left).
A negative value results in peaks being shifted upfield (to the right).

Related: `fn2` Fourier number in 2nd indirectly detected dimension (P)
`lp2` First-order phase in 2nd indirectly detected dimension (P)
`lsfid1` Number of complex points to left-shift `ni` interferogram (P)
`lsfid2` Number of complex points to left-shift `ni2` interferogram (P)
`lsfrq` Frequency shift of the `fn` spectrum in Hz (P)
`ni2` Number of increments in 2nd indirectly detected dimension (P)
`phfid2` Zero-order phasing constant for `ni2` interferogram (P)
`wti` Interactive weighting (C)

lv1 Zero-order baseline correction (P)

Description: When spectral display is active, the command `cdc` turns on a linear drift correction (baseline correction). The result of this operation includes calculating a zero-order baseline correction parameter `lv1`. This is done by averaging of a small number of points at either end of the display and drawing a straight line baseline between them.

Related: `cdc` Cancel drift correction (C)
`lv1tlt` Control sensitivity of `lv1` and `tlt` adjustments (P)
`tlt` First-order baseline correction (P)

lv1tlt Control sensitivity of lv1 and tlt adjustments (P)

Description: Controls the sensitivity of the interactive `lv1` and `tlt` adjustments. `lv1tlt` is in the “current” parameter set and is basically a multiplier for the sensitivity. If this parameter does not exist, it can be created by commands `create('lv1tlt')` `setgroup('lv1tlt', 'display')`.

Values: The default value is 1.0. Larger values make the adjustments larger. Smaller values make the adjustments smaller.

Related: `create` Create new parameter in a parameter tree (C)
`ds` Display a spectrum (C)
`lvl` Zero-order baseline correction (P)

L

M

<code>macro</code>	Macro name (P)
<code>macrocat</code>	Display a user macro file in text window (C)
<code>macrocp</code>	Copy a user macro file (C)
<code>macrodir</code>	List user macro files (C)
<code>macroedit</code>	Edit a macro with user-selectable editor (M)
<code>macrold</code>	Load a macro into memory (C)
<code>macrorm</code>	Remove a user macro (C)
<code>macrosyscat</code>	Display a system macro file in text window (C)
<code>macrosyscp</code>	Copy a system macro to become a user macro (C)
<code>macrosysdir</code>	List system macros (C)
<code>macrosysrm</code>	Remove a system macro (C)
<code>macrovi</code>	Edit a user macro with the vi text editor (M)
<code>make3dcoef</code>	Make a 3D coefficients file from 2D coefficients (M)
<code>makedosyparams</code>	Create parameters for DOSY processing (M)
<code>makefid</code>	Make a FID element using numeric text input (C)
<code>makeeccglobals</code>	Create global parameters for ECC control (M)
<code>makeslice</code>	Synthesize 2D projection of 3D DOSY experiment (C)
<code>man</code>	Display online description of command or macro (M)
<code>managedb</code>	Update user files (U)
<code>manualpath</code>	Path to user's manual directory (P)
<code>manvi</code>	Edit online description of a command or macro (M)
<code>mapwin</code>	List of experiment numbers (P)
<code>mark</code>	Determine intensity of spectrum at a point (C)
<code>masvt</code>	Type of variable temperature system (P)
<code>maxattench1-4</code>	Maximum limit for attenuator setting for rf channel 1-4 (P)
<code>maxpen</code>	Maximum number of pens to use (P)
<code>md</code>	Move display parameters between experiments (C)
<code>menu</code>	Change status of menu system (C)
<code>menuvi</code>	Edit a menu with vi text editor (M)
<code>method</code>	Autoshim method (P)
<code>mf</code>	Move FIDs between experiments (C)
<code>mfblk</code>	Copy FID block (C)
<code>mfclose</code>	Close memory map FID (C)
<code>mfdata</code>	Move FID data (C)
<code>mfopen</code>	Memory map open FID file (C)
<code>mftrace</code>	Move FID trace (C)
<code>minsw</code>	Reduce spectral width to minimum required (M)
<code>mkdir</code>	Create new directory (C)
<code>mlabel</code>	Menu label (P)
<code>move</code>	Move to an absolute location to start a line (C)
<code>movedssw</code>	Set down sampling parameters for selected spectral region (M)
<code>moveossw</code>	Set over sampling parameters for selected spectral region (M)
<code>movesw</code>	Move spectral window according to cursors (M)

M

<code>movetof</code>	Move transmitter offset (M)
<code>mp</code>	Move parameters between experiments (C)
<code>mqcosy</code>	Set up parameters for MQCOSY pulse sequence (M)
<code>mrev8</code>	Set up parameters for MREV8 pulse sequence (M)
<code>mrfb</code>	Set the filter bandwidths for multiple receivers (P)
<code>mref</code>	Set referencing based on a existing spectrum of the sample (M)
<code>mrgain</code>	Set the gain for multiple receivers (P)
<code>mstat</code>	Display memory usage statistics (C)
<code>mstring</code>	Menu string (P)
<code>mtune</code>	Tune probe using swept-tune graphical display (M)
<code>mv</code>	Move and/or rename a file (C)
<code>mxconst</code>	Maximum scaling constant (P)

macro **Macro name (P)**

Description: A string parameter, available in each experiment, similar to the `n1`, `n2`, and `n3` parameters. Certain macros, such as `h1p`, need to know which macro invoked them. This parameter is used to pass that information.

See also: *User Programming*

Related: `h1p` Process simple proton spectra from h1 macro (M)
`n1, n2, n3` Name storage for macros (P)

macrocat **Display a user macro file in text window (C)**

Syntax: `macrocat (file1<, file2>< , ...>)`

Description: Displays one or more user macro files in the text window.

Arguments: `file1`, `file2`, ... are the names of macros in the user macro library.

Examples: `macrocat ('build')`
`macrocat ('dan', 'george')`

See also: *User Programming*

Related: `macrodir` List user macros (C)
`macrosyscat` Display a system macro file in text window (C)

macrocp **Copy a user macro file (C)**

Syntax: `macrocp (from_file, to_file)`

Description: Makes a copy of the existing user macro file and places the copy in the user's macro library. Using `macrocp` to make a backup copy is the recommended procedure to modify a macro but still be able to revert to the previous version if you are unsure about the modification. `macrocp` can also be useful for writing a new macro that is very similar to an existing macro.

Arguments: `from_file` is the name of an existing user macro file to be copied. The file must be in the user's macro library.
`to_file` is the file name to be given to the copy. This name must be different from the name of the original macro.

Examples: `macrocp ('dan', 'dan.old')`

See also: *User Programming*

Related: **macrocat** Display a user macro file in text window (C)
macrodir List user macros (C)
macrosyscp Copy a system macro to become a user macro (C)

macrodir List user macro files (C)

Description: Lists the names of user macro files in the user's macro library.

See also: *User Programming*

Related: **macrosysdir** Lists system macros (C)

macroedit Edit a macro with user-selectable editor (M)

Syntax: `macroedit (file)`

Description: Opens a MAGICAL macro file from a user's personal macro library for editing (if you want to edit a system macro, copy it to a personal library and then use `macroedit`).

The default editor is `vi`. To select another editor, first set UNIX environmental variable `vnmreditor` to the name of the editor; that is, in the `.login` file, change the line

```
setenv vnmreditor old_ed
```

to become

```
setenv vnmreditor new_ed (e.g., setenv vnmreditor emacs).
```

Second, make sure a script with the prefix `vnmr_` followed by the name of the editor is placed in the `bin` subdirectory of the VnmrJ system directory (e.g., `vnmr_emacs`).

The script file makes adjustments for the type of graphic interface in use. Scripts provided in the software include `vnmr_vi` and `vnmr_textedit`. To create other scripts, refer to the `vnmr_vi` script for non-window editor interfaces or refer to `vnmr_textedit` for window-based editor interfaces.

Arguments: `file` is the name of the macro file you wish to edit.

Examples: `macroedit ('pa')`

See also: *User Programming*

Related: **paramedit** Edit a parameter and its attributes with user-selected editor (C)
paramvi Edit a parameter and its attributes with `vi` editor (M)
edit Edit a file with user-selectable editor (C)
macrovi Edit a user macro with `vi` editor (M)
menuvi Edit a menu with the `vi` editor (M)
textvi Edit text file of current experiment with `vi` editor (M)

macrold Load a macro into memory (C)

Syntax: `macrold (file) <:dummy>`

Description: Loads a macro, user or system, into memory. If the macro already exists in memory, it is overwritten by the new macro. Loading a macro into memory increases the execution speed of the macro. The trade-off is that the macro uses memory. The **mstat** command displays macros that have been loaded into memory. One or more individual macros, or all the macros loaded in memory, can be removed from memory with the **purge** command.

If a macro already loaded into memory is edited using **macrovi** or **macroedit**, the changed macro automatically is loaded by those macros. This

overwrites the previous macro. However, if a macro is edited or created some other way (with `macrocp` perhaps), the changed version is not automatically loaded. If the macro already exists in memory, the previous version executes unless the user runs `macrold`.

Arguments: `file` is the name of the macro file to be loaded into memory. For loading macros, the same search path is used as when deciding which macro to execute. That is, the user's private `maclib` directory is searched first and finally the system `maclib`. If an absolute path is supplied as the `file` argument, that macro is loaded. This allows macros not in a `maclib` to be loaded and executed from VnmrJ.

`dummy` is any throwaway variable. Requesting a return value suppresses the message in the status window (line 3) that the macro is loaded.

Examples: `macrold('pa')`
`macrold('_sw'):$noline3`

See also: *User Programming*

Related:	<code>macrocp</code>	Copy a user macro file (C)
	<code>macroedit</code>	Edit a macro with user-selectable editor (M)
	<code>macrovi</code>	Edit a user macro with the vi text editor (M)
	<code>mstat</code>	Display memory usage statistics (C)
	<code>purge</code>	Remove macros from memory (C)

macrorm Remove a user macro (C)

Syntax: `macrorm(file)`

Description: Removes a user macro from the user's macro directory. If the macro has already been loaded in memory, it remains in memory until a new macro of the same name is loaded or the program exits.

Arguments: `file` is the name of the user macro to be removed.

Examples: `macrorm('pa')`

See also: *User Programming*

Related:	<code>delcom</code>	Delete a user macro (M)
	<code>macrodir</code>	List user macros (C)
	<code>macrosysrm</code>	Remove a system macro (C)
	<code>purge</code>	Remove all macros from memory (C)

macrosyscat Display a system macro file in text window (C)

Syntax: `macrosyscat(file1<,file2><,...>)`

Description: Displays one or more system macro files in the text window.

Arguments: `file1`, `file2`, ... are names of macros in the system macro library.

Examples: `macrosyscat('build')`
`macrosyscat('dan','george')`

See also: *User Programming*

Related:	<code>macrocat</code>	Display a user macro file in text window (C)
	<code>macrosysdir</code>	Lists system macros (C)

macrosyscp Copy a system macro to become a user macro (C)

Syntax: `macrosyscp(from_file,to_file)`

Description: Makes a copy of the existing system macro file and places the copy in the user's macro library. This is the recommended way to modify a system macro for personal use.

Arguments: `from_file` is the name of an existing system macro file to be copied. The file must be in the system macro library.

`to_file` is the file name to be given to the copy. In this case, the name of the copied macro can be the same as the original macro. In many cases, it is the same, allowing the user to have a personal macro of the same name as the system macro but which will override the system macro.

Examples: `macroscopy('pa', 'pa')`
`macroscopy('pa', 'mypa')`

See also: *User Programming*

Related: `macrocp` Copy a user macro file (C)
`macroscopycat` Display a system macro file in text window (C)
`macroscopydir` Lists system macros (C)

macroscopydir List system macros (C)

Description: Lists the names of system macros in the system macro library.

See also: *User Programming*

Related: `macrodir` List user macros (C)

macroscopyrm Remove a system macro (C)

Syntax: `macroscopyrm(file)`

Description: Removes a system macro file from the system macro directory. If the macro has already been loaded in memory, it remains in memory until a new macro of the same name is loaded or the program exits.

Arguments: `file` is the name of the system macro file to be removed.

Examples: `macroscopyrm('pa')`

See also: *User Programming*

Related: `macrocopyrm` Remove a user macro (C)
`macroscopydir` Lists system macros (C)
`purge` Remove all macros from memory (C)

macrovi Edit a user macro with the vi text editor (M)

Syntax: `macrovi(file)`

Description: Initiates creating a new user macro or modifying an existing user macro using the UNIX `vi` text editor. On the Sun workstation, a pop-up window contains the edit. On the GraphOn, the edit is done on the entire terminal. To edit a system macro, first copy the macro to a personal library and then edit it using `macroedit` or `macrovi`.

Arguments: `file` is the name of an existing user's macro to be edited or the name of a new user's macro to be created.

Examples: `macrovi('pa')`

See also: *User Programming*

Related: `macroedit` Edit a macro with a user-selectable editor (C)
`vi` Edit text file with `vi` text editor (C)

M

make3dcoef **Make a 3D coefficients file from 2D coefficients (M)**

Syntax: `make3dcoef<('t1t2' | 't2t1')>`

Description: Makes a 3D coefficients file from 2D coefficients and writes the file in the path stored by `curexp`. 2D coefficients are supplied as strings in the parameters `f2coef` and `f1coef`. This macro is capable of handling 3D data collected with any number of data sets (e.g., TPPI, Hypercomplex, Rance SE, Kay SE, and phase-sensitive gradient in one or both dimensions). `make3dcoef` is called by the `ft3d` macro.

The 2D coefficients are supplied as strings in `f1coef` and `f2coef`. These coefficients are the same as found by processing with `wft2d(2dcoefs)`. Note that `wft2da` (for States-Hypercomplex method) is equivalent to `wft2d(1, 0, 0, 0, 0, 0, -1, 0)`, and that `wft2d` (for absolute-value mode) is equivalent to `wft2d(1, 0, 0, -1)`.

Coefficients are separated by spaces and not commas. For example, if a 3D data set collected by the States-Hypercomplex method in both `ni` and `ni2` dimensions, `f1coef`='1 0 0 0 0 -1 0' and `f2coef`='1 0 0 0 0 -1 0'. And if a 3D data set collected in absolute-value mode in both `ni` and `ni2` dimensions, `f1coef`='1 0 0 -1' and `f2coef`='1 0 0 -1'.

The `f1coef` and `f2coef` parameters are created by the `par3d` macro. Execution of `make3dcoef` when `f1coef` and `f2coef` have no value or inconsistent values causes the macro to abort, which enables the user to enter these values and reexecute the macro. For example, the value of `f1coef` when the F1 dimension can be processed with `wft2da` is '1 0 0 0 0 -1 0'. The value of `f2coef` when the F2 dimension can be processed with `wft2d(1, 0, 1, 0, 0, -1, 0, 1)` is '1 0 1 0 0 -1 0 1'.

The parameters `f1coef` and `f2coef` must be 2D coefficients that give proper `ni` and `ni2` first planes with the same `rp` (assuming `lp` is 0 by using `calfa`) values. For example, processing the phase-sensitive gradient dimension should not be done with 1 0 0 1 0 1 1 0 and applying 45° phase shifts to `rp`, but with 1 0 1 0 0 1 0 -1, or its variant, that gives the same `rp` value as the other dimension. This also applies to Rance-type or Kay-type sensitivity-enhanced dimensions.

Note that sensitivity-enhanced sequences (gradient or otherwise) can be processed two different ways to give “orthogonal” data sets. The coefficients must be picked so that they have the same `rp` as the other dimension.

This macro can also handle coefficients that are not 1s or 0s. For example, if processing requires that a data set contributes to the interferogram after a 30° phase shift, `cos(30)` and `sin(30)` can be selected as the real and imaginary contributions, respectively, during the construction of the interferogram.

Arguments: 't1t2' means `array`='phase, phase2' in simple hypercomplex data sets. It means `array`='t1related', 't2related' with multiple sets in general.

't2t1' means `array`='phase2, phase' in simple hypercomplex data sets. It means `array`='t2related', 't1related' with multiple sets in general.

If no argument is used and if `array`='phase, phase2' or `array`='phase2, phase', the macro automatically decides on 't1t2' or 't2t1', respectively.

See also: *NMR Spectroscopy User Guide*

Related:	<code>array</code>	Parameter order and precedence (P)
	<code>calfa</code>	Recalculate alfa so that first-order phase is zero (M)
	<code>curexp</code>	Current experiment directory (P)
	<code>f1coef</code>	Coefficient to construct F1 interferogram (P)
	<code>f2coef</code>	Coefficient to construct F2 interferogram (P)

<code>ft3d</code>	Perform a 3D Fourier transform on a 3D FID data set (M)
<code>lp</code>	First-order phase in directly detected dimension (P)
<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)
<code>ntype3d</code>	Specify whether f_1 or f_2 display expected to be N-type (P)
<code>rp</code>	Zero-order phase in directly detected dimension (P)
<code>wft2d</code>	Weight and Fourier transform 2D data (C)
<code>wft2da</code>	Weight and Fourier transform phase-sensitive data (M)

makedosyparams Create parameters for DOSY processing (M)

Syntax: `makedosyparams (dosytimecubed, dosyfrq)`

Description: This macro is automatically called by the `Dbppste`, `DgcsteSL`, `Doneshot`, `Dbppsteinept`, `Dgcstecosy`, and `Dgcstehmqc` sequences to create the parameters `dosyfrq`, `dosygamma`, and `dosytimecubed`, which are necessary for the `dosy` analysis. Do not manually run `makedosyparams`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dosy</code>	Process DOSY experiments (M)
	<code>dosyfrq</code>	Larmor frequency of phase encoded nucleus in DOSY (P)
	<code>dosygamma</code>	Gyromagnetic constant of phase encoded nucleus in DOSY (P)
	<code>dosytimecubed</code>	Gyromagnetic constant of phase encoded nucleus in DOSY (P)

makefid Make a FID element using numeric text input (C)

Syntax: `makefid (file<, element_number<, format>)`

Description: Creates FID files that can be used to introduce computed data into an experiment. The number of points comes from the number of numeric values read from the input file. If the current experiment already contains a FID, you will not be able to change either the format or the number of points from that present in the FID file. Use `rm (curexp+ '/acqfil/fid')` to remove the FID.

The `makefid` command does not look at parameter values when establishing the format of the data or the number of points in an element. Thus, if the FID file is not present, it is possible for `makefid` to write a FID file with a header that does not match the value of `dp` or `np`. Because the active value is in the processed tree, you need to use the `setvalue` command if any changes are required.

Arguments: `file` is the name of the input file. It contains numeric values, two per line. The first value is assigned to the X (or real) channel; the second value on the line is assigned to the Y (or imaginary) channel.

`element_number` is the number of the element or FID and is any integer larger than 0. The default is the first element or FID. If the FID element already exists in the FID file, the program overwrites the old data.

`format` is a character string with the precision of the resulting FID file and can be specified by one of the following strings:

<code>'dp=n'</code>	single-precision (16-bit) data
<code>'dp=y'</code>	double-precision (32-bit) data
<code>'16-bit'</code>	single-precision (16-bit) data
<code>'32-bit'</code>	double-precision (32-bit) data

If an FID file exists, `makefid` uses the same `format` string for precision; otherwise, the default is double-precision (32-bit) data.

M

element_number and format arguments can be entered in any order.

Examples: `makfid('fid.in', 2, '32-bit')`

See also: *NMR Spectroscopy User Guide; User Programming*

Related:

<code>cp</code>	Copy a file (C)
<code>curexp</code>	Current experiment directory
<code>dp</code>	Double precision (P)
<code>mv</code>	Move and/or rename a file (C)
<code>np</code>	Number of data points (P)
<code>rm</code>	Delete file (C)
<code>setvalue</code>	Set value of any parameter in a tree (C)
<code>writefid</code>	Write numeric text file using a FID element (C)

makeeccglobals Create global parameters for ECC control (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Creates the following nine global parameters required for ECC control by PSG: `tc1z`, `tc2z`, `tc3z`, `tc4z`, `amp1z`, `amp2z`, `amp3z`, `amp4z`, and `chiliConf`

Related: `chiliConf`

makeslice Synthesize 2D projection of 3D DOSY experiment (C)

Syntax: `makeslice(<option>, lowerlimit, upperlimit)`

Arguments: `option` is either 'i' or 's'.

'i' includes the “tails” of diffusion peaks that lie outside the range between `lowerlimit` and `upperlimit`. The default is 'i'.

's' only includes the integration peaks whose diffusion coefficient lies between the specified limits.

`lowerlimit` is the lower diffusion limit (in units of $10^{-10} \text{ m}^2/\text{s}$) to be displayed.

`upperlimit` is the upper diffusion limit (in units of $10^{-10} \text{ m}^2/\text{s}$) to be displayed.

Description: Synthesizes an integral projection between specified diffusion limits of a 3D DOSY spectrum onto the frequency-frequency plane. `makeslice` requires the first 2D increment of the 3D DOSY data to have been transformed.

See also: *NMR Spectroscopy User Guide*

Related:

<code>dosy</code>	Process DOSY experiments (M)
<code>showoriginal</code>	Restore first 2D spectrum in 3D DOSY spectrum (M)

man Display online description of command or macro (M)

Syntax: `man('file')<:$return>`

Displays a description of commands and macros from files in the applications directory. The manual file is displayed in the text window when it is retrieved by the `man` macro. The `man` macro aborts if a name is not supplied as an argument.

Arguments: `file` — name of a command or macro in one of the applications directories.
`:$res` — supply a return argument to suppress messages if the manual page does not exist.

Examples: `man('mark')`

`man('notAcommand'):$res`

See also: *NMR Spectroscopy User Guide; User Programming*

Related: `manvi` Edit online description of a command or macro (M)
`manualpath` Path to user's manual directory (P)

managedb Update user files (U)

Syntax: `managedb update`

Description: Updates VnmrJ database for the Locator.

See also: *NMR Spectroscopy User Guide*

manualpath Path to user's manual directory (P)

Description: Contains the absolute path to a user's directory of VnmrJ manual entries. If `manualpath` exists for a user, it must be defined in the user's global parameter file. Enter `create('manualpath','string','global')` to create the `manualpath` parameter.

See also: *User Programming*

Related: `man` Display online description of a command or macro (M)

manvi Edit online description of a command or macro (M)

Syntax: `manvi('file')`

Description: Enables editing or creating an online description of commands and macros stored in any of the applications directories for to which the user has write permission.

Arguments: `file` is the name of a command macro.

Examples: `manvi('mark')`

See also: *User Programming*

Related: `man` Display online description of command or macro (M)

mapwin List of experiment numbers (P)

Description: Arrayed global parameter that maintains a list of experiment numbers for the window panes in the VnmrJ graphics window.

Related: `curwin` Current window (P)
`fontselect` Open FontSelect window (C)
`jwin` Activate current window (M)
`setgrid` Activate selected window (M)
`setwin` Activate selected window (C)

mark Determine intensity of spectrum at a point (C)

Syntax: (1) `mark<(f1_position)><:intensity>`
(2) `mark<(left_edge,region_width)><:intensity, integral>`
(3) `mark<(f1_position,f2_position)><:intensity>`
(4) `mark<(f1_start,f1_end,f2_start,f2_end)><:intensity,integral,c1,c2>`

```
(5) mark<('trace', <options>) ><:intensity, integral,
    c1, c2>
```

```
(6) mark('reset')
```

Description: Find the intensity of a spectrum at a point. Either 1D or 2D operations can be performed in the cursor or box mode for a total of four separate functions: 1D operations in cursor mode (syntax 1), 1D operations in box mode (syntax 2), 2D operations in cursor mode (syntax 3) and 2D operations in box mode (syntax 4).

In the *cursor mode*, the intensity at a particular point is found. In the *box mode*, the integral over a region is calculated. The displayed integral is scaled in the same way as output from `dli` is scaled; that is, by the `ins` and `insref` parameters. For 2D operations, this is the volume integral and the volume is scaled by `ins2` and `ins2ref`. In addition, the `mark` command in the box mode finds the maximum intensity and the coordinate(s) of the maximum intensity.

The `mark` command requires that transformed data be present in the current experiment. If required, it recomputes the phase file from the complex data (i.e., it rephases the data if required); however, the `mark` command requires parameters from the command line if no data is displayed (i.e., if `ds` or `dcon` has not been executed).

Note that 2D operations require that 2D data be present. This not only means that `ni` must be larger than 1, but also that the data was transformed using `ft1d`, `ft2d` or an equivalent (and not `ft` or its equivalents).

The `mark` command, as well as the MARK button of `ds`, writes output to a file in the current experiment. For 1D operations, the file is named `mark1d.out`; for 2D operations, it is `mark2d.out`. If this file already exists, VnmrJ appends output from the current `mark` operation to the end of the file. (Older versions of VnmrJ used `ds.out` and `dcon.out` as files for output from the MARK button). Either file can be read by other programs at any time between operations.

The following criteria establish the exact function. The command checks them in the following order until it determines the exact function:

1. Number of numeric parameters.
2. Number of return values called out.
3. Which display command (`ds` or `dcon`) was last used.
4. Nature of the data in the experiment.

The first two criteria only serve to distinguish between box mode and cursor mode. The nature of the data in the experiment and the last display command entered determines whether a 1D or a 2D operation is selected.

Arguments: `f1_position` defines the position, in Hz, along the f_1 axis in the 1D and 2D cursor modes. The default is `cr` (1D) or `cr1` (2D).

`left_edge` defines the position of the left edge of the region, in Hz, to be integrated in 1D box mode. The default is `cr`.

`region_width` defines the width, in Hz, of the region, which extends to the right of `left_edge`, in 1D box mode. The default is `delta`.

`f2_position` defines the position, in Hz, along the f_2 axis in the 2D cursor mode. The default is `delta1`.

`f1_start` and `f1_end` define region along the f_1 axis in the 2D box mode.

`f2_start` and `f2_end` define region along the f_2 axis in the 2D box mode.

`'trace'` is a keyword to select a 1D operation if 2D data is present. It must be either the first or the last argument (e.g., `mark('trace', 400)` determines the intensity at 400 Hz in the current trace).

c1, c2 are return values set to the coordinates where the maximum intensity was found in 2D mode. c1 and c2 are not returned in the cursor mode.

<code>mark(cr)</code>	cursor mode for 1D data
<code>mark(cr,delta)</code>	box mode for 1D data

<code>mark (cr1, cr)</code>	cursor mode for 2D data
<code>mark (cr1, delta1, cr, delta)</code>	box mode for 2D data

<code>mark('trace',cr)</code>	cursor mode for selected 2D trace
<code>mark('trace',cr1,delta1)</code>	box mode for selected 2D trace

See also: *NMR Spectroscopy User Guide; User Programming*

Related:	<code>cr</code>	Cursor position in directly detected dimension (P)
	<code>cr1</code>	Cursor position in 1st indirectly detected dimension (P)
	<code>curexp</code>	Current experiment directory (P)
	<code>dconi</code>	Interactive 2D contour display (C)
	<code>delta</code>	Difference of two frequency cursors (P)
	<code>dli</code>	Display list of integrals (C)
	<code>ds</code>	Display a spectrum (C)
	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>ft2d</code>	Fourier transform 2D data (C)
	<code>ins</code>	Integral normalization scale (P)
	<code>ins2</code>	2D volume value (P)
	<code>insref</code>	Fourier number scaled value of an integral (P)
	<code>ins2ref</code>	Fourier number scaled volume of a peak (P)
	<code>mv</code>	Move and/or rename a file (C)
	<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)

Description: Identifies the type of VT system in use: the standard Oxford VT controller or the Oxford-Sorenson or solids VT controller system (used with the Varian VT CP/MAS probe). `masvt` is a global parameter that is active on all of each user's experiments on a per user account basis. The current value of the parameter can be displayed by typing `masvt ?`.

Note that the VT Controller option displayed by `config` must be set to Present for either VT controller system to be active. If `masvt` does not exist, it can be created with the command `create('masvt','string','global')`.

The new Highland VT controller is autosensing, making `masvt` superfluous for systems with this controller.

Values: 'y' indicates the solids VT system is in use.

'n', any other value but 'n' and 'y', or if `masvt` does not exist, indicate that the Oxford Varian VT controller, if present, is in use.

See also: *VnmrJ Installation and Administration*

Related:	<code>config</code>	Display current configuration and possibly change values (M)
	<code>create</code>	Create a new parameter in a parameter tree (C)
	<code>vttype</code>	Variable temperature controller present (P)

maxattach1-4 Maximum limit for attenuator setting for rf channel 1-4 (P)

Description: `maxattach1`, `maxattach2`, `maxattach3`, and `maxattach4`, are optional global parameters for the limiting the maximum attenuator settings for rf channel 1, channel 2, channel 3, and channel 4 (respectively) from pulse sequence statements and through `tpwr/dpwr/...` settings on `go` command. If `maxattach2` is present, the attenuator setting check will be carried out by SpinCAD and C psg. If the attenuator setting exceeds the limit set in `maxattach2`, psg aborts with error message. This command is only applicable for check during the `go` command.

See also: *SpinCAD*

maxpen Maximum number of pens to use (P)

Description: Controls the maximum number of pens that will be used.

Values: 1 to the number of pens in the system plotter. If `maxpen=x` and the software attempts to use pen `x+y`, it uses pen `y` instead.

See also: *NMR Spectroscopy User Guide*

Related:	<code>pen</code>	Select a pen or color for drawing (C)
	<code>setpen</code>	Set maximum number of HP plotter pens (M)

md Move display parameters between experiments (C)

Syntax: `md(<from_exp,>to_exp)`

Description: Moves the saved display parameters from one experiment to another. These parameters must have been saved with the `s` command (e.g., `s2`).

Arguments: `from_exp` specifies the number of the experiment, 1 through 9, from which the parameters are to be taken. The default is that the parameters are moved from the currently active experiment.

`to_exp` specifies to which experiment the parameters are to be moved.

Examples: `md(4)`
`md(2,3)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>mf</code>	Move FIDs between experiments (C)
	<code>mp</code>	Move parameters between experiments (C)
	<code>s</code>	Save display parameters as a set (M)

menu **Change status of menu system (C)**

Syntax: (1) `menu(menu_name)`
 (2) `menu<('off')>`

Description: The VNMR menu system allows up to eight buttons to be active at a time, enabling the user to perform most actions with the mouse rather than typing in commands. All menus are stored in the library `menulib` in the system directory or in the user's `menulib`. See [menuvi](#) to change these menus.

If the menu system becomes deactivated for some reason, select the Menu On button in the Permanent Menu to reactivate it. Entering `menu('main')` also works.

Arguments: `menu_name` is the name of the file controlling the menu (e.g., 'main'). Including this argument activates the menu system and displays the menu controlled by `menu_name`.

'off' is a keyword to turn off the menu system.

Examples: `menu`
`menu('fitspec')`
`menu('off')`

See also: *User Programming*

Related: [menuvi](#) Edit a menu with the `vi` text editor (M)
[mlabel](#) Menu label (P)
[newmenu](#) Select a menu without immediate activation (C)

menuvi **Edit a menu with vi text editor (M)**

Syntax: `menuvi(menu)`

Description: Edits a Classic VNMR menu file using the UNIX `vi` text editor. On the Sun workstation, a pop-up window contains the edit. On the GraphOn, the edit is done on the entire terminal.

Arguments: `menu` is the name of file controlling a menu.

Examples: `menuvi('display_1D')`

See also: *User Programming*

Related: [menu](#) Change status of menu system (C)
[newmenu](#) Select a menu without immediate activation (C)
[vi](#) Edit text file with `vi` text editor (C)

method **Autoshim method (P)**

Description: Selects the method for automatic shimming. Refer to the manual *NMR Spectroscopy User Guide* for information on how to write or alter methods.

Values: Name of file in the `/vnmr/shimmethods` library for one of the defined shim methods in the system. To display all available methods, enter `ls('/vnmr/shimmethods')`. Standard methods include 'z1z2' (selects shimming of the Z1 and Z2 gradients) and 'allzs' (selects shimming all spinning gradients, Z1 to Z4 or Z5, depending on the magnet type). Shim methods can also be stored in a user's `shimmethods` directory (e.g., `/home/vnmr1/vnmrsys/shimmethods`).

See also: *NMR Spectroscopy User Guide*

Related: [ls](#) List files in current directory (C)
[newshm](#) Interactively create a shim method with options (M)
[stdshm](#) Interactively create a shim method (M)

M

mf Move FIDs between experiments (C)

Syntax: `mf(<from_exp,>to_exp)`

Description: Moves the last acquired FID, as well as its associated parameters, from one experiment to another. The text, the processed acquisition parameters and the current display and processing parameters are also moved to the specified experiment.

Arguments: `from_exp` specifies number of the experiment from which the FID is to be taken. The default is the FID is moved from the currently active experiment.
`to_exp` specifies to which experiment the FID is to be moved.

Examples: `mf(4)`
`mf(3,2)`

See also: *NMR Spectroscopy User Guide*

Related: `md` Move display parameters between experiments (C)
`mp` Move parameters between experiments (C)

mfblk Copy FID block (C)

Syntax: `mfblk(<src_expno,>src_blk_no,dest_expno,dest_blk_no)`

Description: Copies data from a source FID block specified by `src_blk_no` to a destination FID block specified by `dest_expno` and `dest_blk_no`, using memory-mapped input and output.

`mfblk` searches for the source and destination FID file in the directory `$vnmruser/expN/acqfil`, where N is the requested experiment number or the current experiment number. If the FID file is not open, `mfblk` opens the file, copies the data, and closes the file. If a number of blocks need to be copied, explicitly opening and closing the files with the commands `mfopen` and `mfclose` can significantly speed up the data reformatting process.

`mfblk` can also be used to append blocks of data to a FID file by specifying that the `dest_blk_no` is greater than the number of blocks in a file.

Be aware that `mfblk` can modify data returned to an experiment with the `rt` command. To avoid modification, enter the following sequence of VnmrJ commands before running `mfblk`:

```
cp(curexp+'/acqfil/fid',curexp+'/acqfil/fidtmp')
rm(curexp+'/acqfil/fid')
mv(curexp+'/acqfil/fidtmp',curexp+'/acqfil/fid')
```

Arguments: `src_expno` specifies the experiment number of the source FID file. The default is the FID file of the current experiment.

`src_blk_no` specifies the source block of data to be copied. Block numbers start at 1 and run from 1 to the number of blocks in a file.

`dest_expno` specifies the experiment number of the destination FID file.

`dest_blk_no` specifies the destination block to send the copied data.

Examples: `mfblk(1,2,1)` copies current experiment, block 1 to exp 2, block 1.
`mfblk(3,2,6,2)` copies exp 2, block 2 to exp 6, block 2.

See also: *User Programming*

Related: `mfclose` Memory map close FID file (C)
`mfdata` Move FID data (C)
`mfopen` Memory map open FID file (C)
`mftrace` Move FID trace (C)

mfclose Close memory map FID (C)

Description: Closes experiment source and destination FID files that have been explicitly opened with **mfopen**.

See also: *User Programming*

Related: **mfblk** Move FID block (C)
mfdata Move FID data (C)
mfopen Memory map open FID file (C)
mftrace Move FID trace (C)
rfbk Reverse FID block (C)
rfddata Reverse FID data (C)
rftrace Reverse FID trace (C)

mfdata Move FID data (C)

Syntax: `mfdata(<src_expno,>src_blk_no,src_start_loc, \`
`dest_expno,dest_blk_no,dest_start_loc,num_points)`

Description: Copies data specified by `src_start_loc` from a FID block specified by `src_blk_no` to a destination location specified by `dest_expno`, `dest_blk_no`, and `dest_start_lo`, using memory-mapped input and output. The data point locations and the `num_points` to be copied are specified by data points corresponding to the **np** parameter, not bytes or complex points.

mfdata searches for the source and destination FID file in the directory `$vnmruser/expN/acqfil`, where `N` is the requested experiment number or the current experiment number. If the FID file is not open, **mfdata** opens the file, copies the data, and closes the file. If a number of blocks need to be copied, explicitly opening and closing the files with the commands **mfopen** and **mfclose** can significantly speed up the data reformatting process.

Be aware that **mfdata** can modify data returned to an experiment with the **rt** command. To avoid modification, enter the following sequence of VnmrJ commands before running **mfdata**:

```
cp(curexp+' /acqfil/fid', curexp+' /acqfil/fidtmp')
rm(curexp+' /acqfil/fid')
mv(curexp+' /acqfil/fidtmp', curexp+' /acqfil/fid')
```

Arguments: `src_expno` specifies the experiment number of the source FID file. The default is the FID file of the current experiment.

`src_blk_no` specifies the source block of data to be copied. Block numbers start at 1 and run from 1 to the number of blocks in a file.

`src_start_loc` specifies the starting data location within the specified block to copy the data. Data locations start from 0 and are specified as data points corresponding to the **np** parameter.

`dest_expno` specifies the experiment number of the destination FID file.

`dest_blk_no` specifies the destination block to send the copied data.

`dest_start_loc` specifies the starting data destination location within the specified block to send the copied data.

Examples: `mfdata(1,0,2,1,(nv-1)*np,np)` copies `np` points of data from the starting location 0 of block 1 of the current experiment to the data location `(nv-1)*np` of block 1 of experiment 2.

See also: *User Programming*

Related: **mfblk** Move FID block (C)
mfclose Memory map close FID file (C)
mfdata Move FID data (C)

<code>mfopen</code>	Memory map open FID file (C)
<code>mftrace</code>	Move FID trace (C)
<code>rfblk</code>	Reverse FID block (C)
<code>rftrace</code>	Reverse FID trace (C)

mfopen Memory map open FID file (C)

Syntax: `mfopen(<src_expno,>dest_expno) >`

Description: Explicitly opens experiment source and destination FID files for using memory-mapped input and output. Opening a file explicitly can significantly speed up the data reformatting process.

`mfopen` searches for the FID file to be opened in the directory `$vnmruser/expN/acqfil`, where N is the requested experiment number or the current experiment number. Without arguments, `mfopen` assumes the source and destination files are the same and are in the current experiment.

After a file is open, the data reformatting commands `mfblk`, `mfdata`, `mftrace`, `rfblk`, `rfdata`, and `rftrace` can be used for moving around data. The `mfclose` must be used to close the file when data reformatting has been completed.

Arguments: `src_expno` specifies the experiment number of the source FID file. The default is the FID file of the current experiment.

`dest_expno` specifies the experiment number of the destination FID file. The default is the FID file of the current experiment.

If only one argument is provided, `mfopen` uses that as the experiment number of the destination FID file and assumes the source is the FID file of the current experiment.

Examples: `mfopen`
`mfopen(3)`
`mfopen(1,2)`

See also: *User Programming*

Related:	<code>mfblk</code>	Move FID block (C)
	<code>mfclose</code>	Memory map close FID file (C)
	<code>mfdata</code>	Move FID data (C)
	<code>mftrace</code>	Move FID trace (C)
	<code>rfblk</code>	Reverse FID block (C)
	<code>rfdata</code>	Reverse FID data (C)
	<code>rftrace</code>	Reverse FID trace (C)

mftrace Move FID trace (C)

Syntax: `mftrace(<src_expno,>src_blk_no,src_trace_no, \`
`dest_expno,dest_blk_no,dest_trace_no)`

Description: Copies FID traces specified by `src_trace_no` from a FID block specified by `src_blk_no` to a destination location specified by `dest_expno`, `dest_blk_no`, and `dest_trace_no`, using memory-mapped input and output. If a number of blocks need to be copied, explicitly opening and closing the files with the commands `mfopen` and `mfclose` can significantly speed up the data reformatting process.

`mftrace` searches for the source and destination FID file in the directory `$vnmruser/expN/acqfil`, where N is the requested experiment number or the current experiment number. If the FID file is not open, `mftrace` opens the file, copies the data, and closes the file.

`mftrace` cannot be used to append data to a FID file. Its purpose is for moving around data.

Be aware that `mftrace` can modify data returned to an experiment with the `rt` command. To avoid modification, enter the following sequence of VnmrJ commands before running `mftrace`:

```
cp(curexp+' /acqfil/fid', curexp+' /acqfil/fidtmp')
rm(curexp+' /acqfil/fid')
mv(curexp+' /acqfil/fidtmp', curexp+' /acqfil/fid')
```

Arguments: `src_expno` specifies the experiment number of the source FID file. The default is the FID file of the current experiment.

`src_blk_no` specifies the source block of data to be copied. Block numbers start at 1 and run to the number of blocks in a file.

`src_trace_no` specifies the source trace of data within the specified block to be copied. Trace numbers run from 1 to number of traces in a file.

`dest_expno` specifies the experiment number of the destination FID file.

`dest_blk_no` specifies the destination block to send the copied data.

`src_trace_no` specifies the destination trace of data within the specified block to be copied. Trace numbers run from 1 to the number of traces in a file.

Examples: `mftrace(1,1,2,1,nv)` copies trace 1 from block 1 of the current experiment to trace `nv` of block 1 of experiment 2.

See also: *User Programming*

Related:	<code>mfblk</code>	Move FID block (C)
	<code>mfclose</code>	Memory map close FID file (C)
	<code>mfdata</code>	Move FID data (C)
	<code>mfopen</code>	Memory map open FID file (C)
	<code>rftrace</code>	Reverse FID trace (C)
	<code>rfblk</code>	Reverse FID block (C)
	<code>rfdata</code>	Reverse FID data (C)

minsw **Reduce spectral width to minimum required (M)**

Description: Searches the spectrum for peaks, sets new limits accordingly, and then calls `movesw` to calculate a new transmitter offset `tof` and spectral width `sw`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>movesw</code>	Move spectral window according to cursors (M)
	<code>movetof</code>	Move transmitter offset (M)
	<code>sw</code>	Spectral width in directly detected dimension (P)
	<code>tof</code>	Frequency offset for transmitter offset (P)

mkdir **Create new directory (C)**

Syntax: `mkdir(directory)`

Description: Creates a new UNIX directory. The function of the VnmrJ `mkdir` command is similar to the UNIX `mkdir` command.

Arguments: `directory` is the name of the new directory to be created.

Examples: `mkdir('tests')`
`mkdir('/home/george')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>rmdir</code>	Remove directory (C)

M

mlabel **Menu label (P)**

Description: Stores the label for a menu button. Usually this parameter is arrayed, with one label for each button in the menu. This parameter is stored in a user's global file and is set whenever a menu is called.

See also: *User Programming*

Related: **menu** Change status of menu system (C)
mstring Menu string (P)

move **Move to an absolute location to start a line (C)**

Syntax: `move (<'graphics' | 'plotter'>, x, y)`

Description: Moves the start of a line to an absolute location with the coordinates given as an argument. **move** is part of a line drawing capability that includes the **pen** and **draw** commands. **pen** selects the pen number of the plotter ('pen1', 'pen2', etc.) or the color ('red', 'green', 'blue', etc.). **move** sets the point from which to start drawing the line. **draw** draws a line from that point to the point given by the **draw** arguments. Refer to the description of the **draw** command for examples of using the line drawing capability.

Arguments: 'graphics' and 'plotter' are keywords selecting output to the graphics window or a plotter device. The default is 'plotter'. The output selected is passed to subsequent **pen**, **move**, or **draw** commands, remaining unchanged until different output is specified.

x, y are the absolute coordinates, in mm, of a point to move to. The range of *x* is 0 at the left edge of the chart and **wcmax** at the right edge of the chart. The range of *y* is -20 at the bottom of the chart and **wc2max** at the top.

See also: *NMR Spectroscopy User Guide*

Related: **draw** Draw line from current location to another location (C)
gin Return current mouse position and button values (C)
pen Select a pen or color for drawing (C)
wcmax Maximum width of chart (P)
wc2max Maximum width of chart in second direction (P)

movedssw **Set downsampling parameters for selected spectral region (M)**

Description: Sets the parameters **ds** and **dsfsfrq** to appropriate values for digital filtering and downsampling in a cursor-selected spectral region. To accomplish this, Fourier transform an oversampled data set, and then run the **ds** program. In the resulting spectral display, enclose the desired region with the cursors, and then run **movedssw**.

See also: *NMR Spectroscopy User Guide*

Related: **downsamp** Downsampling factor applied after digital filtering (P)
ds Display a spectrum (C)
dsfsfrq Bandpass filter offset for downsampling (P)

moveossw **Set oversampling parameters for selected spectral region (M)**

Description: Sets the parameters **osfsfrq** and **sw** to appropriate values for oversampling and digital filtering in a cursor-selected spectral region. To accomplish this, acquire a data set without digital filtering, and then run the **ds** program. In the resulting spectral display, enclose the desired region with the cursors, and then run **moveossw**. The value of **oversamp** is manually set.

See also: *NMR Spectroscopy User Guide*

Related:	ds	Display a spectrum (C)
	oslsfrq	Bandpass filter offset for oversampling (P)
	oversamp	Oversampling factor for acquisition (P)
	sw	Spectral width in directly detected dimension (P)

movesw **Move spectral window according to cursors (M)**

Syntax: `movesw<(width)>`

Description: Uses the parameters **cr** and **delta** to calculate a new transmitter offset **tof** and a new spectral width **sw**. If referencing was used, it is also adjusted. The `movesw` macro also sets **sp** and **wp** to display the spectral window.

Arguments: `width` specifies the spectral width **sw**. The default is to use a value calculated from the parameter **delta**.

Examples: `movesw`
`movesw(5000)`

See also: *NMR Spectroscopy User Guide*

Related:	cr	Cursor position in directly detected dimension (P)
	delta	Cursor difference in directly detected dimension (P)
	minsw	Reduce spectral width to minimum required (M)
	movetof	Move transmitter offset (M)
	sp	Start of plot (P)
	sw	Spectral width in directly detected dimension (P)
	tof	Frequency offset for observe transmitter (P)
	wp	Width of plot (P)

movetof **Move transmitter offset (M)**

Syntax: `movetof<(frequency)>`

Description: Moves the transmitter offset parameter **tof** so that the current cursor position, defined by **cr**, becomes the center of the spectrum. If referencing was used, `movetof` maintains the referencing.

Arguments: `frequency` specifies the transmitter frequency rather than using the cursor position to define the frequency. This provides a convenient method of moving the transmitter frequency outside the current spectral window.

See also: *NMR Spectroscopy User Guide*

Related:	cr	Cursor position in directly detected dimension (P)
	minsw	Reduce spectral width to minimum required (M)
	movesw	Move spectral window according to cursors (M)
	tof	Frequency offset for observe transmitter (P)

mp **Move parameters between experiments (C)**

Syntax: `mp(<from_exp,>to_exp)`

Description: Moves text and the current display, processing, and acquisition parameters from one experiment to another. No FID is transferred.

Arguments: `from_exp` specifies the number of the experiment from which the parameters are to be taken; default is the parameters are moved from the currently active experiment.

`to_exp` specifies to which experiment the parameters are to be moved.

M

Examples: `mp(4)`
`mp(2,3)`

See also: *NMR Spectroscopy User Guide*

Related: `md` Move display parameters between experiments (C)
`mf` Move FIDs between experiments (C)

mqcosy Set up parameters for MQCOSY pulse sequence (M)

Syntax: `mqcosy<(level)>`

Description: Sets up a multiple-quantum filtered COSY experiment.

Arguments: `level` is the desired quantum level of filtration.

Examples: `mqcosy`
`mqcosy(3)`

See also: *NMR Spectroscopy User Guide*

mref Set referencing based on a existing spectrum of the sample (M)

Syntax: `mref(<source_exp,>target_exp)<:$ret>`
`mref(source_fid)<:$ret>`

Description: Use a primary referenced spectrum to reference a secondary spectrum acquired in another work space (or experiment) at the same temperature, using the same lock sample, and either a different or the same nucleus without adding a secondary reference sample. The primary spectrum must be properly referenced using the IUPAC recommended Ξ values. Ξ is the normalized frequency such that the ^1H signal from TMS is 100.00 MHz.

Begin with a `source_exp` spectrum (typically a ^1H spectrum) and reference it using an internal reference (such as TMS, see the IUPAC recommendations).

Join a different experiment and acquire a `target_exp` spectrum on a different (or same) nucleus. Enter `mref(<source_exp,>target_exp)`.

Referencing of 2D data sets using `mref` only applies to the directly detected dimension. The indirect dimensions is referenced using `reff1` and `reff2` (after using `mref` or after manual referencing of the observe dimension). The reference frequency for the secondary spectrum, `reffrq_b`, is calculated as follows:

$$\text{reffrq\_b} = (\text{reffrq\_a} / \Xi_a) * \Xi_b$$

`mref` also corrects for possible changes in the lock frequency:

$$\text{reffrq\_b} = (\text{reffrq\_a} / \text{lockfreq\_a}) * \text{lockfreq\_b}$$

`mref` works if the lock frequency changed between the two acquisitions, if the two spectra were acquired on different instruments, or at different field strengths.

`mref` calculates `rfl` and `rfp` after calculating `reffrq`:

$$\text{rfp} = 0$$

$$\text{rfl} = \text{sw}/2 - (\text{sfrq} - \text{reffrq}) * 1e6$$

The `systemglobal` parameters `lockfreq` and `h1freq` must saved in the local parameters using the `saveglobal` mechanism when the `go` command is executed. The `mref` macro only tracks lock frequency changes if these `systemglobal` parameters are saved in the local parameters.

The `mref` macro works with earlier data if both data sets were:

- acquired at the same lock frequency (on the same instrument).

- the `lockfreq` (on a data station) and (on older instruments) `h1freq` parameters are set to the values used to acquire the data.

Referencing action from `mref` are reported the on line 3. Suppress the report by supplying a return argument, e.g.:

```
$ret= ' ' mref('myfid.fid'):$ret
```

The referencing message is captured in the return argument "\$ret" and the contents of this string variable can be used to label plots with the referencing information.

Limitations: the macro works with data recalled from an archive or acquired on an other system provided the data was acquired using VNMR6.1C or newer.

Setting the global (or local) flag `bioref='y'` enables Bio-NMR referencing (based on `nuctables/nuctabrefBio`) and disables standard IUPAC / organic chemistry referencing (based on `nuctables/nuctabref`).

See `/vnmr/nuctables/nuctabref`.

Arguments: `source_exp` — experiment containing the primary referenced spectrum or the full (or relative) path and fid file name containing the primary references spectrum.

`target_exp` — experiment contining spectra to be referenced based upon the primary experiment referencing.

`$ret` — return argument for output of `mref`.

Alternatively, the name of a FID file (with or without extension) can be given as a single argument; in this case, the data in the CURRENT experiment are referenced based on the referencing in the specified FID file.

Examples: `mref(3)` — uses the current experiment as the source and applies the reference to the specified experiment as the target.

`mref(1,2)` — experiment 1 is the source and experiment 2 is the target.

`mref('myfid')`

`mref('/data/fids/myfid.fid')`

Related	<code>setref</code>	Set Frequency Referencing Based on Lock Signal Shift (M)
	<code>setref1</code>	Set Frequency Referencing for f1 Evolution Dimension (M)
	<code>setref2</code>	Set Frequency Referencing for f2 Evolution Dimension (M)
	<code>reff1</code>	Reference f1 Indirect Dimension from Observe Dimension (M)
	<code>reff2</code>	Reference f2 Indirect Dimension from Observe Dimension (M)
	<code>bioref</code>	Flag for Bio-NMR Referencing (P)

mrev8 Set up parameters for MREV8 pulse sequence (M)

Applicability: Systems with a solids module.

Description: Converts FLIPFLOP, BR24, or S2PUL parameter set into the MREV8 multiple-pulse line narrowing sequence.

See also: *User Guide: Solid-State NMR*

Related:	<code>br24</code>	Set up parameters for BR24 pulse sequence (M)
	<code>cylmrev</code>	Set up parameters for cycled MREV8 pulse sequence (M)
	<code>flipflop</code>	Set up parameters for FLIPFLOP pulse sequence (M)
	<code>s2pul</code>	Set up parameters for standard two-pulse sequence (M)

mrfb Set the filter bandwidths for multiple receivers (P)

Applicability: Systems with multiple receivers

M

Description: An array of `fb` settings to apply to individual receivers in a multiple receiver system. The first element applies to the first receiver, the second to the second receiver, and so on. If `mrfb` exists and is active, these settings override the setting specified by the `fb` parameter; otherwise, `fb` is used as the filter bandwidth setting for all receivers. If there are fewer elements in `mrfb` than there are receivers, the remaining receivers are set to the `fb` value.

Note that some older multiple receiver systems do not have the hardware to provide individual receiver control. In that case, the filter setting for receiver 1 is used on receivers 1 and 2 and the setting for receiver 3 is used on receivers 3 and 4.

Also note that `mrfb` is not automatically set when `sw` is changed. Normally, you can leave `mrfb` inactive and let `fb` be used for all receivers.

Examples: `mrfb=fb/3, fb/2` sets the filter bandwidth of the first receiver to `fb/3`, the second to `fb/2`, and of the rest to `fb`.

Related: `fb` Filter bandwidth (P)

mrgain Set the gain for multiple receivers (P)

Applicability: Systems with multiple receivers

Description: An array of `'gain'` settings to apply to individual receivers in a multiple receiver system. If it exists and is active, these settings override the setting specified by the `'gain'` parameter; otherwise, `'gain'` is used as the gain setting for all receivers.

Note that not all multiple receiver systems have the hardware set up to provide individual receiver control. In that case, the gain setting for receiver 1 is used on receivers 1 and 2 and the setting for receiver 3 is used on receivers 3 and 4.

Examples: `mrgain=30, 40, 20` sets the gains of receiver 1 to 30, receiver 2 to 40 and receivers 3 and 4 to 20.

Related: `gain` Receiver gain (P)

mstat Display memory usage statistics (C)

Syntax: `mstat<(program_id)>`

Description: Displays statistics on memory usage by programs that use the procedures `allocateWithId` and `release`.

Arguments: `program_id` is the program ID, usually the same name as the program. The default is to display all program IDs and associated memory statistics.

Examples: `mstat`
`mstat('proc2d')`

See also: *User Programming*

mstring Menu string (P)

Description: Stores command strings to be executed when a VnmrJ menu button is clicked. Usually the `mstring` parameter is arrayed, with one string for each button in the menu. The string can be any string of commands that can otherwise appear in a macro or on the command line. This parameter is stored in a user's global file and is set whenever a menu is called.

See also: *User Programming*

Related: `menu` Change status of menu system (C)
`mlabel` Menu label (P)

mtune Tune probe using swept-tune graphical display (M)

Description: `mtune` replaces `qtune` on the Varian NMR System and/or Linux. `mtune` runs in the spectra screen and uses VnmrJ panels. Enter `mtune` to retrieve parameters and panels.

- all parameters changeable on-the-fly (exception: tune channel for the Varian NMR System).
- one or two markers are selectable to tune at the same time.
- vertical autoscale button.
- number of acquired points changeable for better resolution at large spectral widths (more points will update less often).
- quit button returns user to current experiment and returns `mtune` to the original frequencies.

See also: *NMR Spectroscopy User Guide*

Related: `tchan` RF channel number used for tuning (P)
`tugain` Amount of receiver gain used by `qtune` (P)
`tune` Assign frequencies (C)

mv Move and/or rename a file (C)

Syntax: `mv(from_file,to_file)`

Description: Renames and/or moves a file or directory. `mv` functions the same as the command `rename`.

Arguments: `from_file` is the name of the file to be moved and/or renamed.
`to_file` is the new name of the file and/or the new location. If the `from_file` argument has an extension such as `.fid` or `.par`, be sure the `to_file` argument has the same extension.

Examples: `mv('/home/vnmr1/vnmrsys/seqlib/d2pul',
'/vnmr/seqlib/d2pul')`

See also: *NMR Spectroscopy User Guide*

Related: `copy` Copy a file (C)
`cp` Copy a file (C)
`delete` Delete a file, parameter directory, or FID directory (C)
`rename` Move and/or rename a file (C)
`rm` Delete a file (C)

mxconst Maximum scaling constant (P)

Description: Before the start of data acquisition, noise is sampled to determine the number of bits of noise present. This number is used to set the maximum number of scaling operations on the data that can occur (essentially relevant only if `dp= 'n'`). `mxconst` is used to adjust this amount of scaling.

Increasing `mxconst` to 1, for example, permits additional scaling operations, allowing acquisition to proceed slightly longer in single-precision mode. Decreasing `mxconst` to -1 allows fewer scaling operations before reaching the message “maximum transients accumulated”.

One special case exists. If `mxconst` is set to less than -90 and single-precision acquisition is used (`dp='n'`), then scaling of the data is disabled. In this mode, reports of data overflowing the 16 bits is also disabled.

`mxconst` does not exist in standard parameter sets. If it does not exist, its value defaults to 0. To modify `mxconst`, first create it by entering `create('mxconst','integer')` and then enter the desired value.

CAUTION: Do not change `mxconst` unless you are fully aware of the consequences.

See also: *NMR Spectroscopy User Guide*

Related: `create` Create new parameter in a parameter tree (C)
`dp` Double precision (P)

N

<code>n1,n2,n3</code>	Name storage for macros (P)
<code>newmenu</code>	Select a menu without immediate activation (C)
<code>newshm</code>	Interactively create a shim method with options (M)
<code>nextpl</code>	Display the next 3D plane (M)
<code>nfni</code>	Number of increments in 1st indirectly detected dimension (P)
<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)
<code>ni3</code>	Number of increments in 3rd indirectly detected dimension (P)
<code>niter</code>	Number of iterations (P)
<code>nimax</code>	Maximum limit of <code>n.i</code> (P)
<code>nl</code>	Position cursor at the nearest line (C)
<code>nli</code>	Find integral values (C)
<code>nlivast</code>	Produces a text file of integral regions without a sum region (M)
<code>nlivast2</code>	Produces a text file with normalized integral regions (M)
<code>nlivast3</code>	Produces a text file with normalized integral regions (M)
<code>nll</code>	Find line frequencies and intensities (C)
<code>nm</code>	Select normalized intensity mode (C)
<code>nm2d</code>	Select Automatic 2D normalization (M)
<code>Noesy</code>	Convert the parameter to a NOESY experiment (M)
<code>Noesy1d</code>	Convert the parameter set to a Noesy1d experiment (M)
<code>noise</code>	Measure noise level of FID (C)
<code>noisemult</code>	Control noise multiplier for automatic 2D processing (M)
<code>noislm</code>	Limit noise in spectrum (M)
<code>notebook</code>	Notebook name (P)
<code>np</code>	Number of data points (P)
<code>npoint</code>	Number of points for fp peak search (P)
<code>nrecords</code>	Determine number of lines in a file (M)
<code>nt</code>	Number of transients (P)
<code>ntrig</code>	Number of trigger signals to wait before acquisition (P)
<code>ntype3d</code>	Specify whether f_1 or f_2 display expected to be N-type (P)
<code>nuctable</code>	Display VNMR style nucleus table for a given H1 frequency (M)
<code>numrcvrs</code>	Number of receivers in the system (P)
<code>numreg</code>	Return the number of regions in a spectrum (C)
<code>numrfch</code>	Number of rf channels (P)

n1,n2,n3 Name storage for macros (P)

Description: Stores arbitrary character strings for macros. Each experiment has these three string parameters available.

See also: *User Programming*

Related: `dgs` Display group of special/automation parameters (M)
`r1-r7` Real value storage for macros (P)

newmenu Select a menu without immediate activation (C)

Syntax: (1) `newmenu(menu_name)`
 (2) `newmenu:$current_menu`

Description: Selects a menu but does not activate it (syntax 1). This is most useful when picking which menu will be active when an interactive command exits. `newmenu` can also return the name of the currently active menu (syntax 2).

Arguments: `menu_name` is the name of the file controlling the menu selected. For example, the command string `newmenu('manipulate_1D')` `ds` causes the menu controlled by `manipulate_1D` to be displayed when the Return button in the `ds` menu is selected.

`$current_menu` returns the file name of the currently active menu.

Examples: `newmenu('display_1D')`
`newmenu:$name1`

See also: *User Programming*

Related: `menu` Change status of menu system (C)
`menuvi` Edit a menu with the vi text editor (M)

newshm Interactively create a shim method with options (M)

Syntax: `newshm`

Description: Interactively creates a *method* string to be used in autoshimming of the magnetic field homogeneity. The string may consist of a series of shimming operations. The command `dshim('method')` describes method strings. Any text editor may be used to make and modify the strings.

`newshm` provides for either lock shimming or FID shimming, permitting the user to choose whichever is best. Lock shimming is much faster, but FID shimming is frequently much more effective in improving the field. With FID shimming, the FID evaluation range limits are requested. The full range is 0 to 100. Sensitivity to higher order gradients is greatly increased by setting the finish limit to about 5 or 10 with the start limit at 0.

`newshm` begins by asking for the name of the user's new shim method. If the non-spin (transverse) controls are chosen for adjustment, the spinner is turned off; otherwise, it is turned on. If uncertain about the shim criteria, the "medium to medium" choice is suitable in most circumstances. The new method is found in `curexp+'.../shimmethods`.

To shim after running `newshm`, type `method='methodname'` and then enter `shim` or set the `wshim` parameter to shim before the start of acquisition. 'methodname' is the name supplied to `newshm`. For more information on shimming, see the manual *NMR Spectroscopy User Guide*.

Compared to `stdshm`, the `newshm` macro is more flexible and provides for a shimming time and FID evaluation limits supplied by the user. The primary difference between the macros is that `stdshm` provides for determining an estimated shimming time for the selected shim controls. When no time limit is supplied, autoshim continues until the exit criteria is met or the number of cycles reaches a limit.

See also: *NMR Spectroscopy User Guide*

Related: `curexp` Current experiment directory (P)
`dshim` Display a shim method string (M)
`method` Autoshim method (P)
`shim` Submit an Autoshim experiment to acquisition (C)
`stdshm` Interactively create a shim method (M)

`wshim` Conditions when shimming is performed (P)
`vi` Edit text file with `vi` text editor (C)

nextpl Display the next 3D plane (M)

Syntax: `nextpl`

Description: Displays the 2D color map of the next 3D plane in the set of planes defined by the parameters `plane` and `path3d`. If `nextpl` immediately follows the command `dproj`, `nextpl` results in the display of the first 3D plane within that specified set and is therefore equivalent to the command `dplane (1)`. For example, if `dplane (40)` has just been executed, `nextpl` results in the display of 3D plane 41 of that set. The `nextpl` macro is more efficient than `dplane` or `dproj` because the 3D parameter set (`procp3d`) is not loaded into VnmrJ—it is assumed to have already been loaded by `dplane` or `dproj`, for example.

See also: *NMR Spectroscopy User Guide*

Related: `dplane` Display a 3D plane (M)
`dproj` Display a 3D plane projection (M)
`dsplanes` Display a series of 3D planes (M)
`getplane` Extract planes from a 3D spectral data set (M)
`path3d` Path to currently displayed 2D planes from a 3D data set (P)
`plane` Currently displayed 3D plane type (P)
`plplanes` Plot a series of 3D planes (M)
`prevpl` Display the previous 3D plane (M)

nfni Number of increments in 1st indirectly detected dimension (P)

Description: Number of increments of the evolution time `d2`, and thus the number of FIDs that will comprise the first indirectly detected dimension of a multidimensional data set. To create parameters `ni`, `phase`, and `sw1` to acquire a 2D data set in the current experiment, enter `addpar ( '2d' )`.

Values: 8 is minimum; typical values range from 32 to 512. In microimaging, `ni` greater than 0 is the imaging mode and `ni` equal to 0 is the projection mode.

See also: *NMR Spectroscopy User Guide; VnmrJ Imaging NMR*

Related: `addpar` Add selected parameters to the current experiment (M)
`celem` Completed FID elements (P)
`d2` Incremented delay in 1st indirectly detected dimension (P)
`ni2` Number of increments in 2nd indirectly detected dimension (P)

ni2 Number of increments in 2nd indirectly detected dimension (P)

Description: Number of increments of the evolution time `d3`, and thus the number of FIDs that will comprise the second indirectly detected dimension of a multidimensional data set. To create parameters `d3`, `ni2`, `phase2`, and `sw2` to acquire a 3D data set in the current experiment, enter `addpar ( '3d' )`.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to the current experiment (M)
`d3` Incremented delay in 2nd indirectly detected dimension (P)
`ni` Number of increments in 1st indirectly detected dimension (P)
`par3d` Create 3D acquisition, processing, and display parameters (M)
`phase2` Phase selection for 3D acquisition (P)
`sw2` Spectral width in 2nd indirectly detected dimension (P)

N

ni3 Number of increments in 3rd indirectly detected dimension (P)

Description: Number of increments of the evolution time **d4**, and thus the number of FIDs that will comprise the third indirectly detected dimension of a multidimensional data set. To create parameters **d4**, **ni3**, **phase3**, and **sw3** to acquire a 4D data set in the current experiment, enter **addpar (' 4d ')**.

See also: *NMR Spectroscopy User Guide*

Related:	addpar	Add selected parameters to the current experiment (M)
	d4	Incremented delay in 3rd indirectly detected dimension (P)
	ni	Number of increments in 1st indirectly detected dimension (P)
	ni2	Number of increments in 2nd indirectly detected dimension (P)
	par4d	Create 4D acquisition parameters (M)
	phase3	Phase selection for 4D acquisition (P)
	sw3	Spectral width in 3rd indirectly detected dimension (P)

niter Number of iterations (P)

Description: Sets the maximum number of iterations in an iterative simulation.

Values: 1 to 9999. The value is initialized to 20 if the Set Params button is used in setting up spin simulation parameters.

See also: *NMR Spectroscopy User Guide*

nimax Maximum limit of ni (P)

Description: Maximum limit of **ni**. Used to prevent running an unrealistic number of Hadamard-encoded experiments.

Values: Any positive real integer.

See also: *NMR Spectroscopy User Guide*

Related:	sethtfrq1	Set a Hadamard frequency list from a line list (M)
	ni	Number of increments in 1st indirectly detected dimension (P)
	htfrq1	Hadamard frequency in ni (P)

n1 Position cursor at the nearest line (C)

Syntax: **n1<:height<, frequency>>**

Description: Moves the cursor to the nearest calculated line position.

Arguments: **height** is a return value set to the height of the line.

frequency is a return value set to the frequency of the line.

Examples: **n1**
n1:r1,r2

See also: *NMR Spectroscopy User Guide*

n1i Find integral values (C)

Description: Equivalent to the **d1i** command except that no screen display is produced. For a list of integrals, **n1i** stores the reset points in the parameter **lifrq** and stores the amplitudes in the parameter **liamp**.

See also: *NMR Spectroscopy User Guide*

Related:	cz	Clear integral reset points (C)
	d1i	Display list of integrals (C)
	dlni	Display list of normalized integrals (M)

<code>liamp</code>	Amplitudes of integral reset points (P)
<code>lifrq</code>	Frequencies of integral reset points (P)
<code>z</code>	Add integral reset point at cursor position (C)

nlivast Produces a text file of integral regions without a sum region (M)

Applicability: Systems with VAST accessory.

Syntax: `nlivast (last)`

Description: Using predefined integral regions from the spectra for each well, `nlivast` writes a text file, `integ.out`, containing the integrals of the regions. The file is written into the current experiment. Does not add an additional region that is the sum of all the defined regions for each well (see `dlivast`).

Arguments: `last` is the number of the last well. The default is 96.

See also: *NMR Spectroscopy User Guide*

nlivast2 Produces a text file with normalized integral regions (M)

Applicability: Systems with VAST accessory.

Syntax: `nlivast (well)`

Description: Using predefined integral regions from the spectra for each well, `nlivast2` writes a text file, `integ.out`, containing the integrals of the regions. The file is written into the current experiment. Integrals are normalized to the integral specified by the argument `well`. The macro `nlivast2` does not add an additional region that is the sum of all the defined regions for each well (see `dlivast`). All of the spectra are integrated.

Arguments: `well` is the number of the reference sample well. The default reference is well 96.

See also: *NMR Spectroscopy User Guide*

nlivast3 Produces a text file with normalized integral regions (M)

Applicability: Systems with VAST accessory.

Syntax: `nlivast (well)`

Description: Using predefined integral regions from the spectra for each well, `nlivast3` writes a text file, `integ.out`, containing the integrals of the regions. The file is written into the current experiment. Integrals are referenced to the integral specified by the argument `well`. The integral of spectrum from the sample specified by `well` is set to 1000. The macro `nlivast3` does not add an additional region that is the sum of all the defined regions for each well (see `dlivast`). All of the spectra are integrated.

Arguments: `well` is the number of the reference sample well. Reference integral set to 1000. The default reference is well 96.

See also: *NMR Spectroscopy User Guide*

nll Find line frequencies and intensities (C)

Syntax: `nll<('pos'<,noise_mult>)><:number_lines,scale>`

Description: Equivalent to the command `dll` except that the line listing is not displayed or printed. The results of this calculation are stored in `llfrq` and `llamp`. The frequencies are stored as Hz and are not referenced to `rfl` and `rfp`. Amplitudes are stored as the actual data point value; they are not scaled by `vs`.

Arguments: 'pos' is a keyword that causes only positive lines to be listed.

noise_mult is a numerical value that determines the number of noise peaks listed for broad, noisy peak. The default is 3. A smaller value results in more peaks, a larger value results in fewer peaks, and a value of 0.0 results in a line listing containing all peaks above the threshold **th**. Negative values of noise_mult are changed to 3.

number_lines is a return argument with the number of lines in the line list.

scale is a return argument with a scaling factor for line amplitudes. This scaling factor accounts for **vs** and whether the lines are listed in absolute intensity mode or normalized mode.

Examples: `nll:nl`
`nll('pos'):pn`
`nll(2.5),sc`

See also: *User Programming*

Related:	dll	Display listed line frequencies and intensities (C)
	llamp	List of line amplitudes (P)
	llfrq	List of line frequencies (P)

nm **Select normalized intensity mode (C)**

Description: Selects the normalized intensity mode in which spectra are scaled so that the largest peak in the spectrum is **vs** mm high. The alternative is the absolute intensity mode (selected by the **ai** command) in which the scale is kept constant from spectrum to spectrum to allow comparison of peak heights from one spectrum to another. The modes are mutually exclusive (i.e., the system is always in either nm or **ai** mode). Enter **aig?** to show which mode is currently active.

See also: *NMR Spectroscopy User Guide*

Related:	ai	Select absolute intensity mode (C)
	aig	Absolute intensity group (P)
	vs	Vertical scale (P)

nm2d **Select Automatic 2D normalization (M)**

Syntax: `nm2d<(noisemult)>`

Description: Sets up parameters **th** and **vs2d** automatically for a 2D contour plot and color map display. **nm2d** measures the highest signal in the spectrum and sets **vs2d** so that the highest signal is in the range of the highest color level. It then calculates the noise threshold so that the number of points above the noise threshold is between 10% and 30% of all the points. At the same time, the difference between the mean value of all the points above the threshold (peak points) and the mean value of all the points under the threshold (noise points) is maximized. This noise threshold is then multiplied by the noise multiplier.

nm2d works both with absolute-value and phase-sensitive spectra. **trace** can be set to 'f1' or 'f2'.

Arguments: **noisemult** specifies the noise multiplier number that multiplies the noise threshold:

- For ^1H , ^{19}F and ^{31}P (high dynamic range nuclei), and homonuclear spectra in general, the default value is 4.
- For HMQC/HSQC type spectra, the default value is also 4 but noise multipliers of 3 to 5 are often more adequate.
- For HETCOR and 2D-INADEQUATE spectra, the default value is 2.

- For “quick & dirty” COSY spectra with lots of t1 noise and other artifacts, a value of 8 and higher may be adequate for suppressing the artifacts.
- For 2D-INADEQUATE spectra, a value below 3 is appropriate to catch signals right above the noise level.
- If the multiplied noise threshold is below `th=1`, `vs2d` is scaled up; otherwise, `th` is increased to the desired level.
- Minimum value is 1.5 (if a lower value is entered, the value is set to 1.5).

Examples: `nm2d`
`nm2d (3)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dconi</code>	Interactive 2D contour display (C)
	<code>noisemult</code>	Control noise multiplier for automatic 2D processing (M)
	<code>proc2d</code>	Process 2D spectra (M)
	<code>th</code>	Threshold (P)
	<code>trace</code>	Mode for <i>n</i> -dimensional data display (P)
	<code>vs2d</code>	Vertical scale for 2D displays (P)

Noesy **Convert the parameter to a NOESY experiment (M)**

Description: Convert the parameter to a NOESY experiment.

See also: *NMR Spectroscopy User Guide*

Related: `foldt` Fold COSY-like spectrum along diagonal axis (C)

Noesy1d **Convert the parameter set to a Noesy1d experiment (M)**

Description: Convert the parameter set to a NOESY 1D experiment.

See also: *NMR Spectroscopy User Guide*

Related: `Proton` Set up parameters for ¹H experiment (M).
`sel1d` Selective 1D protocols to set up (M).

noise **Measure noise level of FID (C)**

Syntax: `noise<(excess_noise<,last_noise<,block_number>>)>`
`:r1,r2,r3,r4,r5,r6`

Description: Measures the noise level of a FID. By using `pw=0` so that no real signal is accumulated, one or more transients can be acquired. The value of `np` must be greater than 4096. `noise` then performs a statistical analysis of the noise, providing noise level, dc level, etc., for each channel. The noise level measurement can be repeated at various settings of `gain` and various settings of `fb`, etc., for a full system diagnosis.

Arguments: `excess_noise` is excess noise and is used to calculate the noise figure.
`last_noise` is the last measured mean square noise and is used to calculate the noise figure.
`block_number` is the block number. The default is 1.
`r1` returns the real dc offset.
`r2` returns the imaginary dc offset.
`r3` returns the real rms noise.
`r4` returns the imaginary rms noise.
`r5` returns the average rms noise.

r6 returns the percentage channel imbalance.

r7 returns the noise figure.

See also: *NMR Spectroscopy User Guide*

Related:	ddf	Display data file in current experiment (C)
	ddff	Display FID file in current experiment (C)
	ddfp	Display phase file in current experiment (C)
	fb	Filter bandwidth (P)
	gain	Receiver gain (P)
	np	Number of data points (P)
	pw	Pulse width (P)

noisemult **Control noise multiplier for automatic 2D processing (M)**

Syntax: `noisemult<(noise_multiplier)>`

Description: Predetermines the noise multiplier used by the **nm2d** macro when starting automatic 2D experiments. This multiplier determines the threshold level in 2D spectra.

Arguments: `noise_multiplier` is a noise multiplier, the same as used in the **nm2d** macro. The default is 8 for homonuclear 2D spectra or 4 for other spectra.

Examples: `noisemult`
`noisemult(10)`

See also: *NMR Spectroscopy User Guide*

Related:	nm2d	Automatic 2D normalization (M)
	proc2d	Process 2D spectra (M)

noislm **Limit noise in spectrum (M)**

Syntax: `noislm<(max_noise)>`

Description: Limits the noise present in a spectrum by reducing the vertical scale **vs**. If the noise is smaller than the noise limit, **vs** is left untouched. The noise limit is in single root-mean-square noise size; the peak-to-peak noise (width of the noise band) is about twice that value. The noise is determined by taking the smallest value from four 5% regions at the left end of the spectrum. Any filter cutoff at the end will decrease the apparent noise in the spectrum, and therefore increase the noise limit in the central part of the spectrum. Because of the particular algorithm used in this macro, signals at the left end of the spectrum should not affect the result of **noislm**.

Arguments: `max_noise` is the maximum root-mean-square size, in mm, of the noise. The default is 2.

Examples: `noislm`
`noislm(5)`

See also: *NMR Spectroscopy User Guide*

Related:	vs	Vertical scale (P)
	vsadj	Automatic vertical scale adjustment (M)
	vsadjc	Automatic vertical scale adjustment for ¹³ C spectra (M)
	vsadjh	Automatic vertical scale adjustment for ¹ H spectra (M)

notebook **Notebook name (P)**

Description: Specifies the notebook name of a sample, which is saved with a study.

Related:	<code>cqsavestudy</code>	Macro to save study queue parameters (M)
	<code>page</code>	Name of page (P)
	<code>samplename</code>	Sample name (P)
	<code>studypar</code>	Study parameters (P)

np **Number of data points (P)**

Description: Sets number of data points to be acquired. Generally, `np` is a *dependent* parameter and is calculated automatically when `sw` or `at` is changed. If a particular number of data points is desired, `np` can be entered, in which case `at` becomes the dependent parameter and is calculated based on `sw` and `np`.

Values: `np` is constrained to be a multiple of 2 (Acquisition Controller or Pulse Sequence Controller board) or a multiple of 64 (Output board). (See the `acquire` statement in the manual *User Programming* for a description of these boards.)

See also: *NMR Spectroscopy User Guide*

Related:	<code>at</code>	Acquisition time (P)
	<code>dp</code>	Double precision (P)
	<code>setlimit</code>	Set limits of a parameter in a tree (C)
	<code>sw</code>	Spectral width in directly detected dimension (P)

npoint **Number of points for fp peak search (P)**

Description: If `npoint` is defined in the current parameter set and has a value, it determines the range of data points over which the `fp` command searches for a maximum for each peak. To create `npoint` and give it a value other than the default, enter `create('npoint','integer') npoint=x`, where `x` is the new value.

Values: 1 to `fn/4`. The default is 2.

See also: *NMR Spectroscopy User Guide*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>fp</code>	Find peak heights (C)

nrecords **Determine number of lines in a file (M)**

Syntax: `nrecords(file):$number_lines`

Description: Returns the number of lines (or records) in a file.

Arguments: `file` is the name of the file.

`$number_lines` returns the number of lines in the named file.

Examples: `nrecords(userdir+'/mark1d.out'):$num`

See also: *User Programming*

nt **Number of transients (P)**

Description: Sets the number of transients to be acquired (i.e., the number of repetitions or scans performed to make up the experiment or FID).

Values: 1 to 1e9. For an indefinite acquisition, set `nt` to a very large number such as 1e9.

See also: *NMR Spectroscopy User Guide; VnmrJ Imaging NMR*

N

ntrig **Number of trigger signals to wait before acquisition (P)**

Applicability: Systems with LC-NMR accessory.

Description: Sets the number of trigger signals from the LC to wait for on the external gate line before beginning acquisition. If `ntrig` is 0 or the parameter does not exist, the external gate signal is ignored. If `ntrig` does not exist, the `parlc` macro can create it. `ntrig` is not normally entered by the user.

See also: *NMR Spectroscopy User Guide*

Related: `parlc` Create LC-NMR parameters (M)

ntype3d **Specify whether f_1 or f_2 display expected to be N-type (P)**

Description: Indicates whether the f_1 or f_2 display is expected to be N-type, that is, opposite to the sense of precession defined by f_3 , under normal 3D processing conditions.

Values: 'yn' specifies that f_1 is expected to have an N-type display under normal 3D processing conditions.

'ny' specifies that f_2 is expected to have an N-type display under normal 3D processing conditions.

'yy' specifies that both f_1 and f_2 are expected to have N-type displays under normal 3D processing conditions. Setting `ntype3d = 'yy'` changes the sense of precession in f_1 and f_2 by negating the imaginary portion of the t_1 and t_2 interferograms prior to Fourier transformation.

See also: *NMR Spectroscopy User Guide*

Related: `fiddc3d` 3D time-domain dc correction (P)
`ft3d` Perform a 3D Fourier transform on a 3D FID data set (M,U)
`ptspec3d` Region-selective 3D processing (P)
`specdc3d` 3D spectral drift correction (P)
`ssfilter` Full bandwidth of digital filter to yield a filtered FID (P)
`ssorder` Order of polynomial to fit digitally filtered FID (P)
`rftype` Type of rf generation

nuctable **Display VNMR style nucleus table for a given H1 frequency (M)**

Syntax: `nuctable<(h1_freq)>`

Description: The VnmrJ nucleus table is a single nucleus table, `/vnmr/nuctables/nuctable`, which is calculated based on a proton frequency of 1000.000 MHz. `nuctable` can be used to reconstruct a traditional nucleus table, e.g., based on a proton frequency of 200.057 MHz, or to calculate a nucleus table for any given proton frequency.

Arguments: `h1_freq` (optional): proton frequency on which the calculated / displayed nucleus table will be based. Without argument, `nuctable` prints a nucleus table based on the proton frequency for which the current VnmrJ / VNMR installation is configured.

Examples: `nuctable(200.057)`
`nuctable:`

Related: `restorenuctable` Calculate and (Re-)store accurate nuctable (M)

numrcvrs **Number of receivers in the system (P)**

Applicability: Systems with multiple receivers.

Description: An integer giving the number of receivers installed in the system. `numrcvrs` is set from the config panel by the `vnmr1` user.

numreg **Return the number of regions in a spectrum (C)**

Syntax: `numreg:number_regions`

Description: Returns the number of regions in a spectrum previously divided by the `region` command, by manual means using the `z` command, or by the Resets button in `ds`. A *region* is the area between two reset points in integral mode, with every other reset point designating the start of a *baseline* region and not included in the count of regions.

Arguments: `number_regions` returns the number of peak regions in the spectrum.

Examples: `numreg:$num`

See also: *User Programming*

Related:	<code>ds</code>	Display a spectrum (C)
	<code>getreg</code>	Get frequency limits of a specified region (C)
	<code>region</code>	Divide spectrum into regions (C)
	<code>z</code>	Add integral reset point at cursor position (C)

numrfch **Number of rf channels (P)**

Description: Holds the number of rf channels available. The value is set with the Number of RF Channels label in the Spectrometer Configuration window. `numrfch` represents the hardware in the system. For example, if the last experiment used the second decoupler, `numrfch` is set to 2. The software then leaves the second decoupler on if it was on and leaves it off if it was off.

CAUTION: Do not reset `numrfch` to eliminate the use of a channel. See the description of `dn2` and `dn3` for the method to disable channels.

Values: The fifth channel can only be used with the deuterium decoupler channel.

See also: *VnmrJ Installation and Administration*

Related:	<code>config</code>	Display current configuration and possibly change it (M)
	<code>dn2</code>	Nucleus for the second decoupler (P)
	<code>dn3</code>	Nucleus for the third decoupler (P)
	<code>dn4</code>	Nucleus for the fourth decoupler (P)

O

off	Make a parameter inactive (C)
on	Make a parameter active or test its state (C)
operator	Operator name (P)
operatorlogin	Sets workspace and parameters for the operator (M)
opx	Open shape definition file for Pbox (M)
oscoef	Digital filter coefficients for over sampling (P)
osfb	Digital filter bandwidth for over sampling (P)
osfilt	Over sampling filter for real-time DSP (P)
oslsfrq	Bandpass filter offset for over sampling (P)
overrange	Frequency synthesizer overrange (P)
oversamp	Over sampling factor for acquisition (P)
owner	Operating system account owner (P)

off **Make a parameter inactive (C)**

Syntax: `off (parameter<, tree>)`

Description: Turns off an active parameter in any tree.

Arguments: `parameter` is the name of the parameter.

`tree` is type of parameter tree: 'current', 'global', 'processed', or 'systemglobal'. The default is 'current'. Refer to the [create](#) command for more information on the types of trees.

Examples: `off ('gf')`
`off ('n', 'global')`

See also: *User Programming*

Related: [create](#) Create new parameter in a parameter tree (C)
[on](#) Make a parameter active or test its state (C)
[typeof](#) Return identifier for argument type (O)

on **Make a parameter active or test its state (C)**

Syntax: `on (parameter<, tree>) <: $active>`

Description: Turns on an inactive parameter in any tree or tests if a parameter is active. Real variables (not strings) can be turned on and off. This can be done in any tree with the commands `on` and `off`, and by entering `name='y'` or `name='n'` to change the active flag for variables in the current tree only. The variable trees are 'current', 'global', 'processed' and 'systemglobal'. The default tree is 'current'.

To test the active flag of a variable, use `on ( . . . ) : $x`. This does not change the active flag of the variable, but sets `$x` to 1, if the variable is active, or to 0, if it is not active. If the variable does not exist, a value of -1 is returned. Care should be taken if using the return value as a test for a conditional statement. For example, in the following fragment,

```
on ('var1') : $e
if $e then
    write('line3', 'if statement is true with value of
```

```
%d', $e)
endif
```

the **write** command will be executed if 'var1' is active, writing the message *if statement is true with value of 1* It will also be executed if 'var1' does not exist, writing the message *if statement is true with value of -1*.

To only execute the **write** command if the variable is active, use something like the following:

```
on('var1'):$e
if ($e > 0.5) then
    write('line3','var1 is active')
endif
```

Arguments: parameter is the name of the parameter to make active or to test.

tree is type of parameter tree: 'current', 'global', 'processed', or 'systemglobal'. The default is 'current'. Refer to the **create** command for more information on the types of trees.

\$active is 1 if the parameter is active, or is 0 if it is not active. Adding a return argument makes on conduct only a test of whether the specified parameter is active and does *not* turn on the parameter if it is inactive.

Examples: on('lb'):\$ison
on('gain','global')

See also: *User Programming*

Related: **create** Create new parameter in a parameter tree (C)
off Make a parameter inactive (C)

operator **Operator name (P)**

Applicability: *VnmrJ Walkup*

Description: Specifies the operator name. It is set when an operator logs into the Walkup interface. Multiple operators may be defined for a single user using the VnmrJ Administrator interface.

Related: **acct** Writes records for operator login and logoff (M)
operatorlogin Sets workspace and parameters for the operator (M)
vnmr_accounting Open Accounting window (U)

operatorlogin **Sets workspace and parameters for the operator (M)**

Syntax: operatorlogin operator email panellevel

Description: Sets the panel display level and other parameters for an operator when the operator logs in. It also clears the new sample area in the study queue, and disables the command line if the operator has insufficient privileges. An operator may be logged in from the Switch operator dialog in the Utilities menu.

Related: **acct** Writes records for operator login and logoff (M)
email Email address (P)
operator Operator name (P)
panellevel Display level for VnmrJ interface pages (P)
vnmr_accounting Open Accounting window (U)

opx **Open shape definition file for Pbox (M)**

Syntax: opx<(name<.ext>)>

Description: Opens the pulse shape/pattern definition input file `shapelib/Pbox.inp` for the Pbox software and writes the file header.

Arguments: `name` is the name of the output shape file.
`ext` is a file name extension that specifies the file type.

Examples: `opx`
`opx('newfile.DEC')`

Related: [Pbox](#) Pulse shaping software (U)

oscoef Digital filter coefficients for over sampling (P)

Description: Specifies number of coefficients used in the digital filter. Enter [addpar](#)('oversamp') to add `oscoef` to the current experiment if `oscoef` does not exist. [addpar](#)('oversamp') creates digital filtering and oversampling parameters [def_osfilt](#), [filtfile](#), `oscoef`, [osfb](#), [osfilt](#), [oslsfrq](#), and [oversamp](#).

Values: The default is $7.5 * \text{oversamp}$ for inline DSP (`dsp='i'`). A larger number of coefficients gives a filter with sharper cutoffs; a smaller number gives a filter with more gradual cutoffs. The value of `oscoef` does not need to be changed when [oversamp](#) is changed because `oscoef` is automatically adjusted by VnmrJ to give filter cutoffs that are the same regardless of the value of [oversamp](#).

The number of coefficients for real-time DSP (`dsp='r'`) is determined by the hardware and is not adjustable.

Related: [addpar](#) Add selected parameters to current experiment (M)
[dsp](#) Type of DSP for data acquisition (P)
[filtfile](#) File of FIR digital filter coefficients (P)
[osfb](#) Digital filter bandwidth for oversampling (P)
[oslsfrq](#) Bandpass filter offset for oversampling (P)
[oversamp](#) Oversampling factor for acquisition (P)
[paros](#) Create additional parameters used by oversampling (M)

osfb Digital filter bandwidth for oversampling (P)

Description: Specifies bandwidth of the digital filter used for oversampling. If `osfb` does not exist in the current experiment, enter [addpar](#)('oversamp') to add it. [addpar](#)('oversamp') creates digital filtering and oversampling parameters [def_osfilt](#), [filtfile](#), `oscoef`, [osfilt](#), [oslsfrq](#), and [oversamp](#).

Values: Number, in Hz. A value less than $sw/2$ rejects frequencies at the edges of the spectrum; a value greater than $sw/2$ aliases noise and signals at frequencies outside of $\pm sw/2$.

'n' sets the bandwidth to $sw/2$.

Related: [addpar](#) Add selected parameters to current experiment (M)
[def_osfilt](#) Default value of `osfilt` (P)
[filtfile](#) File of FIR digital filter coefficients (P)
[oscoef](#) Digital filter coefficients for oversampling (P)
[osfilt](#) Oversampling filter for real-time DSP (P)
[oslsfrq](#) Bandpass filter offset for oversampling (P)
[oversamp](#) Oversampling factor for acquisition (P)

paros Create additional parameters used by oversampling (M)
sw Spectral width in directly detected dimension (P)

osfilt Oversampling filter for real-time DSP (P)

Applicability: Systems with real-time DSP.

Description: Sets the type of real-time digital filter to be used on systems equipped with the real-time DSP hardware option. `osfilt` is normally set automatically by the software based on the user's global parameter `def_osfilt`, so that `osfilt` only needs to be changed if a particular experiment is to be run with a different digital filter than the default.

Values: 'a' or 'A' for the AnalogPlus™ digital filter.
 'b' or 'B' for the brickwall digital filter.
 '' (null string) causes `osfilt` to be set to the value contained in the `def_osfilt` when an acquisition is initiated (with `go`, for example).

Related: `def_osfilt` Default value of `osfilt` (P)
`dsp` Type of DSP for data acquisition (P)

oslsfrq Bandpass filter offset for oversampling (P)

Description: Selects a bandpass filter that is not centered about the transmitter frequency. In this way `oslsfrq` works much like `lsfrq`. If `oslsfrq` does not exist in the current experiment, add it with `addpar('oversamp')`, which creates digital filtering and oversampling parameters, the same as the `paros` macro.

Values: Number, in Hz. A positive value selects a region upfield from the transmitter frequency. A negative value selects a downfield region.

Related: `addpar` Add selected parameters to current experiment (M)
`def_osfilt` Default value of `osfilt` (P)
`filtfile` File of FIR digital filter coefficients (P)
`fsq` Frequency-shifted quadrature detection (P)
`lsfrq` Frequency shift of the `fn` spectrum in Hz (P)
`oscoef` Digital filter coefficients for oversampling (P)
`osfb` Digital filter bandwidth for oversampling (P)
`osfilt` Oversampling filter for real-time DSP (P)
`oversamp` Oversampling factor for acquisition (P)
`paros` Create additional parameters used for oversampling (M)

overrange Frequency synthesizer overrange (P)

Applicability: Systems with optional version X46 of the PTS frequency synthesizer.

Description: Configures whether an rf channel has version X46 of the PTS frequency synthesizer. The value for each channel is set using the label Frequency Overrange in the Spectrometer Configuration window.

Values: Not Present, 10000 Hz, or 100000 Hz
 Not Present indicates that this rf channel does not have the frequency overrange option.
 10000 or 100000 indicate that this rf channel has the frequency overrange option. The **10000 Hz** or **100000 Hz** choices are determined by the letters *H*, *J*, or *K* found in the PTS Synthesizers model number. The normal value for overrange is 10000 Hz. If **Frequency Overrange** is set to 10000 Hz or 100000 Hz, the **Latching** value for that RF channel must also be set to **Present**.

When set to either 10000 Hz or 100000 Hz, `overrange` guarantees a range of phase-continuous frequency jumps of at least 10 kHz or 100 kHz in each jump direction.

See also: *VnmrJ Installation and Administration*

Related: `config` Display current configuration and possibly change it (M)
`latch` Frequency synthesizer latching (P)

oversamp Oversampling factor for acquisition (P)

Description: Specifies the oversampling factor for the acquisition. With inline digital filtering (`dsp= 'i'`), `np*oversamp` data points are acquired at a rate of `sw*oversamp`. The data is then transferred to the host computer, digitally filtered, and downsampled to give `np` points and a spectral width of `sw`.

With real-time digital filtering (`dsp= 'r'`), the oversampling, digital filtering, and down sampling all occur as each data point is collected, so that only `np` data points are ever stored in the acquisition computer memory and subsequently transferred to the host computer.

If `oversamp` does not exist in the current experiment, enter the command `addpar('oversamp')` to add it. `addpar('oversamp')` creates digital filtering and oversampling parameters `def_osfilt`, `filtfile`, `oscoef`, `osfb`, `osfilt`, `oslsfrq`, and `oversamp`.

If `oversamp` is set to a number, then that number represents the amount of oversampling to apply when collecting the data. The `oversamp` value is automatically calculated whenever `sw` is changed, provided `oversamp` is not set to 'n'. That is the distinction between `oversamp= 'n'` and `oversamp=1`. In both cases, no oversampling will be used. This occurs, for example, if the `sw` parameter is greater than half the maximum spectral width. However, if `sw` is reduced so that oversampling is possible, then if `oversamp` is set to 'n', `oversamp` will remain set to 'n' and oversampling will not occur. On the other hand, if `oversamp` is set to 1, then `oversamp` is recalculated and oversampling will occur. Therefore, the `oversamp` parameter accurately represents whether oversampling is performed for a data set. When `oversamp` is automatically determined based on a change to `sw`, it is set to the maximum possible oversampling factor. The value of `oversamp` can be manually reset.

Note that setting `oversamp` greater than 1 means oversampling is selected for the experiment. However, if the oversampling facility is not present in the system (i.e., `dsp= 'n'`), then the `oversamp` parameter is automatically reset to 1, indicating that no oversampling will be performed.

Two other experiment local parameters reflect whether DSP is used during the acquisition of a data set:

- `fb` is set to Not Active if DSP is used.
- `oscoef` reflects whether real-time (`dsp= 'r'`) or inline (`dsp= 'i'`) DSP was used. If real-time, `oscoef` is set to Not Active. If inline, `oscoef` is set to the value used by the inline algorithm.

Values: Number less than or equal to 68. For inline DSP, `sw*oversamp` and `np*oversamp` are limited by the values in the following table:

Maximum <code>sw*oversamp</code>	Maximum <code>np*oversamp</code>
500 kHz	2M
100 kHz	128K

The maximum `np*oversamp` is given for double precision data (`dp= 'y'`). For `dp= 'n'`, multiply this value by 2.

'n' causes normal acquisition to be done without digital filtering.

Related:	<code>addpar</code>	Add selected parameters to current experiment (M)
	<code>def_osfilt</code>	Default value of <code>osfilt</code> parameter (P)
	<code>dp</code>	Double precision (P)
	<code>dsp</code>	Type of DSP for data acquisition (P)
	<code>fb</code>	Filter bandwidth (P)
	<code>filtfile</code>	File of FIR digital filter coefficients (P)
	<code>fsq</code>	Frequency-shifted quadrature detection (P)
	<code>np</code>	Number of data points (P)
	<code>oscoef</code>	Digital filter coefficients for oversampling (P)
	<code>osfb</code>	Digital filter bandwidth for oversampling (P)
	<code>osfilt</code>	Oversampling filter for real-time DSP (P)
	<code>oslsfrq</code>	Bandpass filter offset for oversampling (P)
	<code>paros</code>	Create additional parameters used by oversampling (M)
	<code>sw</code>	Spectral width in directly detected dimension (P)

owner Operating system account owner (P)

Description: Set to the Unix or Linux account owner. It is set when VnmrJ is started.

P

<code>p1</code>	Enter pulse width for p1 in degrees (C)
<code>p1</code>	First pulse width (P)
<code>p2pul</code>	Set up sequence for PFG testing (M)
<code>p31</code>	Automated phosphorus acquisition (M)
<code>p31p</code>	Process 1D phosphorus spectra (M)
<code>pa</code>	Set phase angle mode in directly detected dimension (C)
<code>pal</code>	Set phase angle mode in 1st indirectly detected dimension (C)
<code>pacosy</code>	Plot automatic COSY analysis (C)
<code>pad</code>	Preacquisition delay (P)
<code>padept</code>	Perform adept analysis and plot resulting spectra (C)
<code>page</code>	Submit plot and change plotter page (C)
<code>page</code>	Name of page (P)
<code>panellevel</code>	Display level for VnmrJ interface pages (P)
<code>pap</code>	Plot out “all” parameters (C)
<code>par2d</code>	Create 2D acquisition, processing, and display parameters (M)
<code>par3d</code>	Create 3D acquisition, processing, and display parameters (M)
<code>par3rf</code>	Get display templates for 3rd rf channel parameters (M)
<code>par4d</code>	Create 4D acquisition parameters (M)
<code>paramedit</code>	Edit a parameter and its attributes with user-selected editor (C)
<code>paramvi</code>	Edit a parameter and its attributes with vi editor (M)
<code>pards</code>	Create additional parameters used by down sampling (M)
<code>parfidss</code>	Create parameters for time-domain solvent subtraction (M)
<code>parfix</code>	Update parameter sets (M)
<code>parlc</code>	Create parameters for LC-NMR experiments (M)
<code>par112d</code>	Create parameters for 2D peak picking (M)
<code>parlp</code>	Create parameters for linear prediction (M)
<code>parmax</code>	Parameter maximum values (P)
<code>parmin</code>	Parameter minimum values (P)
<code>paros</code>	Create additional parameters used by over sampling (M)
<code>parstep</code>	Parameter step size values (P)
<code>parversion</code>	Version of parameter set (P)
<code>path3d</code>	Path to currently displayed 2D planes from a 3D data set (P)
<code>paxis</code>	Plot horizontal LC axis (M)
<code>Pbox</code>	Pulse shaping software (U)
<code>pbox_bw</code>	Define excitation band (M)
<code>pbox_bws</code>	Define excitation band for solvent suppression (notch) pulses (M)
<code>pbox_dmf</code>	Extract dmf value from pbox.cal or Pbox shape file (M)
<code>pbox_dres</code>	Extract dres value from pbox.cal or Pbox shape file (M)
<code>pbox_name</code>	Extract name of last shape generated by Pbox from pbox.cal (M)
<code>pbox_pw</code>	Extract pulse length from pbox.cal or Pbox shape file (M)
<code>pbox_pwr</code>	Extract power level from Pbox.cal or Pbox shape file (M)
<code>pbox_pwrf</code>	Extract fine power level from pbox.cal or Pbox shape file (M)
<code>pboxget</code>	Extract Pbox calibration data (M)

P

<code>pboxpar</code>	Add parameter definition to the Pbox.inp file (M)
<code>pboxrst</code>	Reset temporary Pbox variables (M)
<code>pboxunits</code>	Converts to Pbox default units (M)
<code>pcon</code>	Plot contours on a plotter (C)
<code>pcss</code>	Calculate and show proton chemical shifts spectrum (M)
<code>peak</code>	Find tallest peak in specified region (C)
<code>peak2d</code>	Return information about maximum in 2D data (C)
<code>pen</code>	Select a pen or color for drawing (C)
<code>pexpl</code>	Plot exponential or polynomial curves (C)
<code>pexpladd</code>	Add another diffusion analysis to current plot (M)
<code>pfgon</code>	Pulsed field gradient amplifiers on/off control (P)
<code>pfww</code>	Plot FIDs in whitewash mode (C)
<code>pge</code>	Convert parameter set to PGE pulse sequence (M)
<code>pge_calib</code>	Calibrate gradient strengths for PGE pulse sequence (M)
<code>pge_data</code>	Extract data from single element of PGE pulse sequence (M)
<code>pge_output</code>	Output results from PGE pulse sequence (M)
<code>pge_process</code>	Automated processing of data from PGE pulse sequence (M)
<code>pge_results</code>	Calculate diffusion constant for integral region (M)
<code>pge_setup</code>	Set up gradient control parameters for PGE pulse sequence (M)
<code>ph</code>	Set phased mode in directly detected dimension (C)
<code>ph1</code>	Set phased mode in 1st indirectly detected dimension (C)
<code>ph2</code>	Set phased mode in 2nd indirectly detected dimension (C)
<code>phase</code>	Change frequency-independent phase ϕ (M)
<code>phase</code>	Phase selection (P)
<code>phase1</code>	Phase of first pulse (P)
<code>phase2</code>	Phase selection for 3D acquisition (P)
<code>phase3</code>	Phase selection for 4D acquisition (P)
<code>phasing</code>	Control update region during interactive phasing (P)
<code>phfid</code>	Zero-order phasing constant for the np FID (P)
<code>phfid1</code>	Zero-order phasing constant for ni interferogram (P)
<code>phfid2</code>	Zero-order phasing constant for ni2 interferogram (P)
<code>Phosphorus</code>	Set up parameters for ^{31}P experiment (M)
<code>pi3ssbsq</code>	Set up $\pi/3$ shifted sinebell-squared window function (M)
<code>pi4ssbsq</code>	Set up $\pi/4$ shifted sinebell-squared window function (M)
<code>pin</code>	Pneumatics Router Interlock ((P)
<code>pintvast</code>	Plots of integral regions (M)
<code>pir</code>	Plot integral amplitudes below spectrum (C)
<code>pirn</code>	Plot normalized integral amplitudes below spectrum (M)
<code>piv</code>	Plot integral amplitudes below spectrum (M)
<code>pivn</code>	Plot normalized integral amplitudes below spectrum (M)
<code>pl</code>	Plot spectra (C)
<code>pl2d</code>	Plot 2D spectra in whitewash mode (C)
<code>plt2Darg</code>	Plot 2D arguments (P)
<code>plane</code>	Currently displayed 3D plane type (P)
<code>plapt</code>	Plot APT-type spectra automatically (M)
<code>plarray</code>	Plotting macro for arrayed 1D spectra (M)
<code>plate_glue</code>	Define a glue order for plotting and display (U)

<code>plc</code>	Plot a carbon spectrum (M)
<code>plcosy</code>	Plot COSY- and NOESY-type spectra automatically (M)
<code>pldept</code>	Plot DEPT data, edited or unedited (M)
<code>plfid</code>	Plot FIDs (C)
<code>plfit</code>	Plot deconvolution analysis (M)
<code>plgrid</code>	Plot a grid on a 2D plot (M)
<code>plh</code>	Plot proton spectrum (M)
<code>plhet2dj</code>	Plot heteronuclear J-resolved 2D spectra automatically (M)
<code>plhom2dj</code>	Plot homonuclear J-resolved 2D spectra automatically (M)
<code>plhxcor</code>	Plot X,H-correlation 2D spectrum (M)
<code>pll</code>	Plot a line list (M)
<code>pll2d</code>	Plot results of 2D peak picking (C)
<code>pllockport</code>	Port number to use to lock out multiple ProTune processes (P)
<code>plot</code>	Automatically plot spectra (M)
<code>plot1d</code>	Plotting macro for simple (non-arrayed) 1D spectra (M)
<code>plot2D</code>	Plot 2D spectra (M)
<code>plotfile</code>	Plot to a file (M)
<code>plothiresprep</code>	High resolution plot output preparation (M)
<code>plotmanual</code>	Plot manually (M)
<code>plotlogo</code>	Plots a logo (M)
<code>plotside</code>	Plot spectrum on side (M)
<code>plotter</code>	Plotter device (P)
<code>plottop</code>	Plot spectrum on top (M)
<code>plottopside</code>	Plot spectrum on top and side (M)
<code>plp</code>	Plot phosphorus spectrum (M)
<code>plplanes</code>	Plot a series of 3D planes (M)
<code>plt2Darg</code>	Plot 2D arguments (P)
<code>plttext</code>	Plot text file (M)
<code>pltmod</code>	Plotter display mode (P)
<code>plvast</code>	Plot VAST data in a stacked 1D-NMR matrix format (M)
<code>plvast2d</code>	Plot VAST data in a stacked pseudo-2D format (M)
<code>plww</code>	Plot spectra in whitewash mode (C)
<code>pmode</code>	Processing mode for 2D data (P)
<code>poly0</code>	Display mean of the data in regression.inp file (M)
<code>pp</code>	Decoupler pulse length (P)
<code>ppa</code>	Plot a parameter list in plain English (M)
<code>ppcal</code>	Proton decoupler pulse calibration (M)
<code>ppf</code>	Plot peak frequencies over spectrum (C)
<code>pph</code>	Print pulse header (M)
<code>ppmm</code>	Resolution on printers and plotters (P)
<code>pprofile</code>	Plot pulse excitation profile (M)
<code>pps</code>	Plot pulse sequence (C)
<code>prealfa</code>	Specify a delay for longer ring down (P)
<code>prep</code>	Run prepare acquisition macro (M)
<code>Presat</code>	Set up parameters for presat ¹ H experiment (M)
<code>prescan</code>	Study queue prescan (P)
<code>prevpl</code>	Display the previous 3D plane (M)

P

<code>prescan_CoilTable</code>	Read or update the CoilTable File (M)
<code>prescan_tn</code>	Return tn string for a given atomic number (M)
<code>printer</code>	Printer device (P)
<code>printfile</code>	Path to the print-to-file image (P)
<code>printformat</code>	Format of saved-to-file image (P)
<code>printlayout</code>	Layout of printed image (P)
<code>printoff</code>	Stop sending text to printer and start print operation (C)
<code>printon</code>	Direct text output to printer (C)
<code>printregion</code>	Screen region to be printed (P)
<code>printsize</code>	Size of printed image (P)
<code>printsend</code>	Defines where image will print (P)
<code>probe</code>	Probe type (P)
<code>probeConnect</code>	Specify which nucleus can be acquired on each RF channel (P)
<code>Probe_edit</code>	Edit probe for specific nucleus (U)
<code>probe_edit</code>	Edit probe for specific nucleus (M)
<code>probe_protection</code>	Probe protection control (P)
<code>proc</code>	Type of processing on np FID (P)
<code>proc1</code>	Type of processing on ni interferogram (P)
<code>proc1d</code>	Processing macro for simple (non-arrayed) 1D spectra (M)
<code>proc2</code>	Type of processing on ni2 interferogram (P)
<code>proc2d</code>	Process 2D spectra (M)
<code>procarrray</code>	Process arrayed 1D spectra (M)
<code>process</code>	Generic automatic processing (M)
<code>procplot</code>	Automatically process FIDs (M)
<code>profile</code>	Set up pulse sequence for gradient calibration (M)
<code>proj</code>	Project 2D data (C)
<code>Proton</code>	Set up parameters for ^1H experiment (M)
<code>protune</code>	Macro to start ProTune (M)
<code>protune</code>	Shell script to start ProTune operation (U)
<code>protunegui</code>	Macro to start ProTune in graphical user interface (M)
<code>prune</code>	Prune extra parameters from current tree (C)
<code>pscale</code>	Plot scale below spectrum or FID (C)
<code>pseudo</code>	Set default parameters for pseudo-echo weighting (M)
<code>psg</code>	Display pulse sequence generation errors (M)
<code>psggen</code>	Compile a user PSG object library (M,U)
<code>psgset</code>	Set up parameters for various pulse sequences (M)
<code>psgupdateon</code>	Enable update of acquisition parameters (C)
<code>psgupdateoff</code>	Prevent update of acquisition parameters (C)
<code>pshape</code>	Plot pulse shape or modulation pattern (M)
<code>pshapef</code>	Plot the last created pulse shape (M)
<code>pshr</code>	PostScript High Resolution plotting control (P)
<code>pslabel</code>	Pulse sequence label (P)
<code>pslw</code>	PostScript Line Width control (P)
<code>pssl</code>	Plot Arrayed Numbers (C)
<code>ptext</code>	Print out a text file (M)
<code>ptspec3d</code>	Region-selective 3D processing (P)
<code>ptsval</code>	PTS frequency synthesizer value (P)

<code>pulseinfo</code>	Shaped pulse information for calibration (M)
<code>pulsetool</code>	RF pulse shape analysis (U)
<code>purge</code>	Remove macro from memory (C)
<code>puttxt</code>	Put text file into a data file (C)
<code>putwave</code>	Write a wave into Pbox.inp file (M)
<code>pw</code>	Enter pulse width pw in degrees (C)
<code>pw</code>	Pulse width (P)
<code>pw90</code>	90° pulse width (P)
<code>pwd</code>	Display current working directory (C)
<code>pwr</code>	Set power mode in directly detected dimension (C)
<code>pwr1</code>	Set power mode in 1st indirectly detected dimension (C)
<code>pwr2</code>	Set power mode in 2nd indirectly detected dimension (C)
<code>pwsadj</code>	Adjust pulse interval time (M)
<code>pxcal</code>	Decoupler pulse calibration (M)
<code>pxbss</code>	Bloch-Siegert shift correction during Pbox pulse generation (P)
<code>pxrep</code>	Flag to set the level of Pbox reports (P)
<code>pxset</code>	Assign Pbox calibration data to experimental parameters (M)
<code>pxshape</code>	Generates a single-band shape file (M)
<code>Pxsim</code>	Simulate Bloch profile for a shaped pulse (U)
<code>Pxspy</code>	Create shape definition using Fourier coefficients (U)

p1 Enter pulse width for p1 in degrees (C)

Syntax: `p1 (flip_angle<, 90_pulse_width>)`

Description: Calculates the flip time, in μs , given a desired flip angle and the 90° pulse. The value is entered into the pulse width parameter `p1`.

Arguments: `flip_angle` is the desired flip angle, in degrees.

`90_pulse_width` is the 90° pulse, in μs . The default is the value of parameter `pw90` if it exists.

Examples: `p1 (30)`
`p1 (90, 12.8)`

See also: *NMR Spectroscopy User Guide*

Related: `ernst` Calculate the Ernst angle pulse (C)
`p1` First pulse width (P)
`pw90` 90° pulse width (P)

p1 First pulse width (P)

Description: Length of first pulse in the standard two-pulse sequence.

Values: 0, 0.2 μs to 150,000 μs , in 0.1 μs steps
0.1 μs to 8190 sec, smallest value possible is 0.1 μs , finest increment possible is 12.5 ns.

See also: *NMR Spectroscopy User Guide*

Related: `p1` Enter pulse width `p1` in degrees (C)

p1pat Shape of excitation pulse (P)

Applicability: Systems with imaging capabilities.

P

Description: Specifies the shape of pulse `p1` when used in imaging experiments.

Values: 'hard', 'sinc', 'gauss', 'sech', 'sine', or any shape resident in the system pulse shape library or libraries.

See also: *VnmrJ Imaging NMR*

Related: `p1` First pulse width (P)
`pwpat` Shape of refocusing pulse (P)

p2pu1 Set up sequence for PFG testing (M)

Applicability: Systems with the pulsed field gradient (PFG) module. *This sequence is not for NMR applications.*

Description: Sets up the PFG two-pulse sequence, a system checkout sequence for PFG installation. Several modes are controlled by the `cmd` parameter.

- `cmd='twinkle'` sequentially addresses DACs 0 through 4. On the gradient channel interface, lights become a slow binary counter.
- `cmd='pulse'` makes a pulse of value `gzlv11` for a time `gt1`.
- `cmd='bipulse'` makes a pulse of value `gzlv11` for a time `gt1` followed by a pulse of value `-gzlv11` for a time `gzlv11`.

For other modes, see the PFG installation manual.

See also: *Pulsed Field Gradient Modules Installation*

p31 Automated phosphorus acquisition (M)

Syntax: `p31<(solvent)>`

Description: Prepares parameters for automatically acquiring a standard ^{31}P spectrum. The parameter `wexp` is set to 'procplot' for standard processing. If `p31` is used as the command for automation via the `enter` command, then the macro `au` is supplied automatically and should not be entered on the MACRO line of the `enter` program. However, it is possible to customize the standard `p31` macro on the MACRO line by following it with additional commands and parameters. For example, `p31 nt=1` will use the standard `p31` setup but with only one transient.

Arguments: `solvent` is the name of the solvent. The default is `CDC13`. In automation mode, the solvent is supplied by the `enter` program.

Examples: `p31`
`p31('DMSO')`

See also: *NMR Spectroscopy User Guide*

Related: `au` Submit experiment to acquisition and process data (M)
`enter` Enter sample information for automation run (C)
`p31p` Process 1D phosphorus spectra (M)
`proc1d` Processing macro for simple, non-arrayed 1D spectra (M)
`procplot` Automatically process FIDs (M)
`wexp` When experiment completes (P)

p31p Process 1D phosphorus spectra (M)

Syntax: `p31p`

Description: Processes non-arrayed 1D ^{31}P spectra using a set of standard macros. `p31p` is called by the `proc1d` macro but can also be used directly. Fully automatic processing (up to a point where a spectrum could be plotted) is provided:

Fourier transformation (using preset weighting functions), automatic phasing (**aphx** macro), automatic integration (**integrate** macro, if required only), vertical scale adjustment (**vsadjc** macro), avoiding excessive noise (**noislm** macro), threshold adjustment (**thadj** macro), and referencing to the TMS signal, if present (**tmsref** macro).

See also: *NMR Spectroscopy User Guide*

Related:	aphx	Perform and check automatic phasing (M)
	integrate	Automatically integrate 1D spectrum (M)
	noislm	Avoids excessive noise (M)
	p31	Automated phosphorus acquisition (M)
	proc1d	Automatically process non-arrayed 1D fids (M)
	thadj	Adjust threshold (M)
	tmsref	Reference spectrum to TMS line (M)
	vsadjc	Adjust vertical scale for carbon spectra (M)

pa Set phase angle mode in directly detected dimension (C)

Description: Selects the phase angle mode by setting the parameter **dmg**= 'pa '. In the *phase angle display mode*, each real point in the displayed spectrum is calculated from the phase angle of the real and imaginary points comprising each respective complex data point. The phase angle also takes into account the phase parameters **rp** and **lp**.

For 2D data, if **pmode**= 'partial ' or **pmode**= ' ' (two single quotes with no space in between), **pa** has an effect on the data prior to the second Fourier transform. If **pmode**= 'full ', **pa** acts in concert with the commands **pa1**, **av1**, **pwr1**, or **ph1** to yield the resultant contour display for the 2D data.

See also: *NMR Spectroscopy User Guide*

Related:	av	Set abs. value mode in directly detected dimension (C)
	dmg	Data display mode in directly detected dimension (P)
	ft	Fourier transform 1D data (C)
	ft1d	Fourier transform along f_2 dimension (C)
	ft2d	Fourier transform 2D data (C)
	lp	First-order phase in directly detected dimension (P)
	pa1	Set phase angle mode in 1st indirectly detected dimension (C)
	ph	Set phased mode in directly detected dimension (C)
	pmode	Processing mode for 2D data (P)
	pwr	Set power mode in directly detected dimension (C)
	pwr1	Set power mode in 1st indirectly detected dimension (C)
	rp	Zero-order phase in directly detected dimension (P)
	wft	Weight and Fourier transform 1D data (C)
	wft1d	Weight and Fourier transform f_2 of 2D data (M)
	wft2d	Weight and Fourier transform 2D data (M)

pa1 Set phase angle mode in 1st indirectly detected dimension (C)

Description: Selects the phase angle spectra display mode along the first indirectly detected dimension by setting the parameter **dmg1** to the string value 'pa1 '. If the parameter **dmg1** does not exist, **pa1** will create it and set it to 'pa1 '.

In the phase angle mode, each real point in the displayed trace is calculated from the phase angle of the real and imaginary points comprising each respective complex data point. For hypercomplex data, the phase angle uses the real-real and imaginary-real points from each respective hypercomplex data point. The phase angle also takes into account the phase parameters **rp1** and **lp1**.

The `pa1` command is only needed if mixed-mode display is desired. If the parameter `dmg1` does not exist or is set to the null string, the display mode along the first indirectly detected dimension defaults to the display mode of the directly detected dimension (characterized by the parameter `dmg`). For the contour display of multidimensional data, the result of `pa1` is the same as for traces provided that `pmode='partial'` or `pmode=''`.

See also: *NMR Spectroscopy User Guides*

Related:	<code>av1</code>	Set abs. value mode in 1st indirectly detected dimension (C)
	<code>dmg1</code>	Data display mode in 1st indirectly detected dimension (P)
	<code>lp1</code>	First-order phase in 1st indirectly detected dimension (P)
	<code>pa</code>	Set phase angle mode in directly detected dimension (C)
	<code>ph1</code>	Set phased mode in 1st indirectly detected dimension (C)
	<code>pmode</code>	Processing mode for 2D data (P)
	<code>pwr1</code>	Set power mode in 1st indirectly detected dimension (C)
	<code>rp1</code>	Zero-order phase in 1st indirectly detected dimension (P)

pacosy **Plot automatic COSY analysis (C)**

Description: Automatically analyzes and plots a COSY data set with `fn=fn1` and `sw=sw1`. Symmetrization of the data with the command `foldt` is recommended, but not required. First, select a proper threshold and perform a 2D line listing with the command `l12d`. Next, plot the 2D data with the contour plot command `pcon`; leaving enough room at the left side of the plot for the connectivity table. Then, `pacosy` will analyze the data and plot the connectivities on the plotter. `pacosy` gets its input from the file `l12d.out` in the current experiment directory. The command `acosy` performs the same analysis and displays the connectivities on the screen.

See also: *NMR Spectroscopy User Guide*

Related:	<code>acosy</code>	Automatic analysis of COSY data (C)
	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>fn1</code>	Fourier number in 1st indirectly detected dimension (P)
	<code>foldt</code>	Fold COSY-like spectrum along diagonal axis (C)
	<code>hcosy</code>	Automated proton and COSY acquisition (M)
	<code>l12d</code>	Automatic and interactive 2D peak picking (C)
	<code>pcon</code>	Plot contours on plotter (C)
	<code>relayh</code>	Set up parameters for COSY pulse sequence (M)
	<code>sw</code>	Spectral width in directly detected dimension (P)
	<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)

pad **Preacquisition delay (P)**

Description: Each NMR experiment starts with a single delay time equal to `pad` over and above the delay `d1` that occurs before each transient. Normally, `pad` is set to a small, nominal time (0.5 seconds) to allow any hardware changes that may be required at the start of the acquisition to “settle in.” During experiments in which the temperature is changed, the acquisition starts `pad` seconds after the temperature regulation system comes to regulation. Since the sample temperature does not actually come to equilibrium for some time after that, it is generally desirable to increase `pad` to perhaps 300 seconds. This is especially true when running experiments involving arrays of temperatures. The `pad` parameter is most useful for running kinetics experiments. For example, `pad=0, 3600, 3600, 3600, 3600` will run an experiment immediately when `go` is typed (`pad=0`), then wait an hour (3600 seconds), run the second experiment, etc.

Values: 0,0.1 μ s to 8190 sec in 12.5 ns steps
 0,0.2 μ s to 150,000 sec in 0.1 μ s steps.

See also: *NMR Spectroscopy User Guide; VnmrJ Walkup*

Related: [d1](#) First delay (P)
[go](#) Submit experiment to acquisition (C)

padept Perform adept analysis and plot resulting spectra (C)

Syntax: `padept(<('noll'><,'coef'><,'theory'>)>`

Description: Performs the [adept](#) analysis and plots the resulting spectra with a scale and the assigned line listing. Leave enough space at the left end of the display for the line list.

Arguments: The following arguments can be supplied in any order:

'noll' is a keyword that specifies no line listing.

'coef' is a keyword that causes the combination coefficients to be printed.

'theory' is a keyword that causes the theoretical coefficients rather than optimized coefficients to be used.

Examples: `padept('noll','coef')`

See also: *NMR Spectroscopy User Guide*

Related: [adept](#) Automatic DEPT analysis and spectrum editing (C)
[autodept](#) Automated complete analysis of DEPT data (M)
[cdept](#) Automated carbon and DEPT acquisition (C)
[Dept](#) Set up parameters for DEPT experiment
[deptproc](#) Process DEPT data (M)
[hcdept](#) Automated proton, carbon, and DEPT acquisition (C)
[pldept](#) Plot DEPT data, edited or unedited (M)

page Submit plot and change plotter page (C)

Syntax: `page<(number_pages<,'clear'|file>)>`

Description: Submits the current plotter file, which has been created by all previous plotter commands, and changes the paper after the plot has been completed. Actual plotting is controlled by the `vnmrplot` script in the `bin` subdirectory of the system directory. The `page` command can also clear the current plotter file or save the data to a specified file name.

Arguments: `number_pages` is the number of pages to move the plotter forward. The default is 1. If `number_pages` is 0, `page` submits the plot but does not change the paper.

'clear' is a keyword to clear the plot made thus far; that is, clear the data in the current plotter file.

`file` is the name of a file to save the plot for import into a document. If the file already exists, it is overwritten.

Examples: `page`
`page(0)`
`page('clear')`
`page('myplotfile')`

See also: *NMR Spectroscopy User Guide*

Related: [vnmrplot](#) Plot files (U)

P

page Name of page (P)

Description: Specifies the page of a sample. It is saved with a study.

Related: `cgsavestudy` Macro to save study queue parameters (M)
`notebook` Notebook name (P)
`samplename` Sample name (P)
`studypar` Study parameters (P)

panellevel Display level for VnmrJ interface pages (P)

Description: Determines which VnmrJ interface pages are available under the tabs in the parameter page area. The higher the number, the more pages are available. The only time panellevel is changed is during the login process of an operator in the Walkup interface. For the Walkup interface, the value is set by the VnmrJ Administrator (default is 10).

Values: **0-9** — shows the minimum number of pages.

No shim, lock, or processing, and minimal parameter control is available. This may be used for routine automation users.

10-29 — typical for a basic Walkup user.

Shim and lock are available only if there is a sample changer. Basic processing is available. Pages are not fully populated, allowing control of a few basic parameters.

30-100 — typical for the system owner.

All pages are available and fully populated.

See also: VnmrJ Installation and Administration

Related: `operator` Operator name (P)
`operatorlogin` Sets workspace and parameters for the operator (M)

pap Plot out “all” parameters (C)

Syntax: `pap(<template><,x><,y><,character_size>)>`

Description: Plots a parameter list containing “all” parameter names and values.

Arguments: `template` is the name of a template that controls the display. The default is the string parameter `ap`, which can be modified using `paramvi('ap')`. See the manual *User Programming* for rules on building a template.

`x` is the starting position in the x direction of the plot on the paper, in mm. The default is a preset value.

`y` is the starting position in the y direction of the plot on the paper, in mm. If `y` is specified, the `x` position must be also. The default is a preset value.

`character_size` is the character size of the list and is specified as a multiplier. The default is 0.70 (not available on all plotters or printers acting as plotters).

Examples: `pap`
`pap(wcmax-40)`
`pap(10,wc2max*.9)`
`pap('newpap',wcmax-50,100,1.4)`

See also: *NMR Spectroscopy User Guide, User Programming*

Related: `ap` Print out “all” parameters (C)
`ap` “All” parameters display control (P)
`hpa` Plot parameters on special preprinted chart paper (C)

`paramvi` Edit a variable and its attributes using `vi` text editor (M)
`ppa` Plot a parameter list in “English” (M)

par2d Create 2D acquisition, processing, and display parameters (M)

Description: Creates the acquisition parameters `ni`, `sw1`, and `phase`, which can be used to acquire a 2D data set. `par2d` also creates any missing processing and display parameters for the `ni` (or second) dimension, including `flcoef`, `reffrq1`, `refpos1`, and `refsource1`. The `par2d` macro is functionally the same as `addpar('2d')`.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to the current experiment (M)
`flcoef` Coefficient to construct F1 interferogram (P)
`ni` Number of increments in 1st indirectly detected dimension (P)
`phase` Phase selection (P)
`reffrq1` Reference frequency of reference line in 1st indirect dimension (P)
`refpos1` Position of reference line in 1st indirect dimension (P)
`refsource1` Center frequency in 1st indirect dimension (P)
`set2d` General setup for 2D experiments (M)
`sw1` Spectral width in 1st indirectly detected dimension (P)

par3d Create 3D acquisition, processing, and display parameters (M)

Description: Creates the acquisition parameters `ni2`, `sw2`, `d3`, and `phase2` that can be used to acquire a 3D data set. `par3d` also creates any missing processing or display parameters for the `ni2` (or third) dimension, including `f2coef`, `fiddc3d`, `specdc3d`, and `ptspec3d`. The `par3d` macro is functionally the same as `addpar('3d')`.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to the current experiment (M)
`d3` Incremented delay in 2nd indirectly detected dimension (P)
`f2coef` Coefficient to construct F2 interferogram (P)
`fiddc3d` 3D time-domain dc correction (P)
`ni2` Number of increments in 2nd indirectly detected dimension (P)
`phase2` Phase selection for 3D acquisition (P)
`ptspec3d` Region-selective 3D processing (P)
`specdc3d` 3D spectral drift correction (P)
`sw2` Spectral width in 2nd indirectly detected dimension (P)

par3rf Get display templates for 3rd rf channel parameters (M)

Applicability: Systems with a second decoupler.

Description: Retrieves the `dg2` and modified `ap` display templates from the parameter set `s2pul3rf` in the system `parlib` directory. These two templates support the display of second decoupler acquisition parameters and 3D acquisition and processing parameters.

See also: *User Programming*

Related: `ap` “All” parameters display control (P)
`dg2` Control `dg2` parameter group display (P)

par4d Create 4D acquisition parameters (M)

Applicability: Systems with a third decoupler.

Description: Creates the acquisition parameters `ni3`, `sw3`, `d4`, and `phase3` that can be used to acquire a 4D data set. The `par4d` macro is functionally the same as `addpar('4d')`.

See also: *NMR Spectroscopy User Guide*

Related:

<code>addpar</code>	Add selected parameters to the current experiment (M)
<code>d4</code>	Incremented delay for 3rd indirectly detected dimension (P)
<code>ni3</code>	Number of increments in 3rd indirectly detected dimension (P)
<code>phase3</code>	Phase selection for 4D acquisition (P)
<code>sw3</code>	Spectral width in 3rd indirectly detected dimension (P)

paramedit **Edit a parameter and its attributes with user-selected editor (C)**

Syntax: `paramedit(parameter<,tree>)`

Description: Opens a parameter file for editing with a user-selected text editor. The default editor is `vi`. If `vi` is used as the editor, `paramedit` is functionally the same as the `paramvi` command. To select another editor, set the UNIX environmental variable `vnmreditor` to the editor name (change `.login` line `setenv vnmreditor old_editor` to become `setenv vnmreditor new_editor` (e.g., `setenv vnmreditor emacs`) and make sure a script with the prefix `vnmr_` followed by the name of the editor is placed in the `bin` subdirectory of the system directory (e.g., `vnmr_emacs`). The script file makes adjustments for the type of graphic interface in use.

Scripts in the software release include `vnmr_vi` and `vnmr_textedit`. To create other scripts, refer to the `vnmr_vi` script for non-window editor interfaces and to `vnmr_textedit` for window-based editor interfaces. The `vnmreditor` variable must be set before starting `VnmrJ`.

Arguments: `parameter` is the name of the parameter file to be edited.
`tree` is a keyword for one of the parameter trees 'current', 'global', or 'processed'. The default is 'current'.

Examples: `paramedit('ap')`
`paramedit('b','global')`

See also: *NMR Spectroscopy User Guide; User Programming*

Related:

<code>paramvi</code>	Edit a parameter and its attributes with <code>vi</code> editor (M)
<code>vi</code>	Edit text file with the <code>vi</code> text editor (C)

paramvi **Edit a parameter and its attributes with vi editor (M)**

Syntax: `paramvi(parameter<,tree>)`

Description: Opens a parameter file for editing using the UNIX `vi` text editor. The parameter file contains various attributes of the parameter in a format documented in the manual *User Programming*. Be sure you understand the format before modifying the parameter because if an error in the format is made, the parameter will not load. When the editor is exited, the modified parameter is reloaded into the system.

Arguments: `parameter` is the name of the parameter file to be edited.
`tree` is a keyword for one of the parameter trees 'current', 'global', or 'processed'. The default is 'current'.

Examples: `paramvi('ap')`
`paramvi('b','global')`

See also: *NMR Spectroscopy User Guide, User Programming*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>destroy</code>	Destroy a parameter (C)
	<code>destroygroup</code>	Destroy parameters of a group in a tree (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>fread</code>	Read parameters from file and load them into a tree (C)
	<code>fsave</code>	Save parameters from a tree to a file (C)
	<code>groupcopy</code>	Copy parameters of group from one tree to another (C)
	<code>paramedit</code>	Edit a parameter and its attributes with user-selected editor (C)
	<code>prune</code>	Prune extra parameters from current tree (C)
	<code>setgroup</code>	Set group of a parameter in a tree (C)
	<code>setlimit</code>	Set limits of a parameter in a tree (C)
	<code>setprotect</code>	Set protection mode of a parameter (C)
	<code>vi</code>	Edit text file with the <code>vi</code> text editor (C)

pards Create additional parameters used by downsampling (M)

Description: Creates the parameters `downsamp`, `dscoef`, `dsfb`, `dsfsfrq`, and `filtfile` necessary for digital filtering and downsampling. The `pards` macro is functionally the same as `addpar ( 'dowsamp' )`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to current experiment (M)
	<code>downsamp</code>	Downsampling factor applied after digital filtering (P)
	<code>dscoef</code>	Digital filter coefficients for downsampling (P)
	<code>dsfb</code>	Digital filter bandwidth for downsampling (P)
	<code>dsfsfrq</code>	Bandpass filter offset for downsampling (P)
	<code>filtfile</code>	File of FIR digital filter coefficients (P)
	<code>movedssw</code>	Set downsampling parameters for selected spectral region (M)

parfidss Create parameters for time-domain solvent subtraction (M)

Description: Creates solvent subtraction parameters `ssfilter`, `ssfsfrq`, `ssntaps`, and `ssorder`. Entering `addpar ( 'ss' )` is functionally equivalent to `parfidss`.

In a 1D transform, subtraction of the zero-frequency component from the time-domain data, usually in the context of solvent subtraction, is selected by setting `ssorder` and `ssfilter` to desired values and entering `wft`:

- The zfs (zero-frequency suppression) option is selected if both `ssfilter` and `ssorder` are set to a value other than “Not Used.”
- The lfs (low-frequency suppression) option is selected if `ssfilter` is set to a value other than “Not Used” and `ssorder` is set to “Not Used.”
- The zfs and lfs options are both turned off if `ssfilter` is set to “Not Used.”

The zfs option leads to the following series of processing events: (1) the raw FID is frequency-shifted by `ssfsfrq` Hz, (2) the raw FID is subjected to a low-pass digital filter, (3) the filtered FID is fit to a polynomial of order `ssorder`, (4) the polynomial function is subtracted from the raw FID, and (5) the resulting FID is frequency-shifted by `-ssfsfrq` Hz.

The lfs option does not include a polynomial fit (step 3 of the zfs option), which leads to the following series of processing events: (1) the raw FID is frequency-shifted by `ssfsfrq` Hz, (2) the raw FID is subjected to a low-pass digital filter, (3) the filtered FID is directly subtracted from the raw FID, (4) the resulting FID is frequency-shifted by `-ssfsfrq` Hz.

The quality of filtering with `zfs` diminishes rapidly as the solvent peak moves off the exact center of the digital filter. It may be necessary to adjust `lsfrq` or `sslsfrq` to move the solvent peak to within ± 0.2 Hz of the center of the filter to obtain optimal solvent suppression. The `lfs` option is less sensitive to small offsets, but typically removes or distorts peaks near to the solvent peak.

In a 2D transform, solvent correction to the t_2 FIDs is invoked in the same manner with the `ft1d`, `ft2d`, `wft1d`, and `wft2d` commands and with the `ft2da`, `ft1da`, `wft2da`, and `wft1da` macros.

In a 3D transform, solvent suppression works on t_3 FIDs of 3D spectra just like in the 1D and 2D cases.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>ft</code>	Fourier transform 1D data (C)
	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>ft2d</code>	Fourier transform 2D data (C)
	<code>ft3d</code>	Perform a 3D Fourier transform on a 3D FID data set (M,U)
	<code>lsfrq</code>	Frequency shift of the f_n spectrum in Hz (P)
	<code>ntype3d</code>	N-type peak selection in f_1 or f_2 (P)
	<code>ssfilter</code>	Full bandwidth of digital filter to yield a filtered FID (P)
	<code>sslsfrq</code>	Center of solvent-suppressed region of spectrum (P)
	<code>ssorder</code>	Order of polynomial to fit digitally filtered FID (P)
	<code>ssntaps</code>	Number of coefficients to be used in the digital filter (P)
	<code>wft</code>	Weight and Fourier transform 1D data (C)

parfix **Update parameter sets (M)**

Description: Corrects upper limits, lower limits, and step sizes of a number of parameters in the current experiment. In addition, the template parameter `dgs` is updated. This is automatically done via the macro `fixpar` if the parameter `parversion` is less than 4.3. `parfix` is used by the macro `updatepars` to correct saved data. This macro has been applied to all parameters as of VNMR version 4.3 and should be run on older parameter sets (e.g., `rtp('pars')` `svp('pars')` update a parameter set named `pars`).

See also: *NMR Spectroscopy User Guide*

Related:	<code>ap</code>	“All” parameters display control (P)
	<code>dgs</code>	Control <code>dgs</code> parameter group display (P)
	<code>fixpar</code>	Correct parameter characteristics in experiment (M)
	<code>parversion</code>	Version of parameter set (P)
	<code>updatepars</code>	Update all parameter sets saved in a directory (M)

parlc **Create parameters for LC-NMR experiments (M)**

Applicability: Systems with LC-NMR accessory.

Description: Creates the following parameters used for a variety of LC-NMR experiments: `curscan`, `dtrig`, `inject`, `ntrig`, and `savefile`. The `parlc` macro also creates `ni` and `sw1` (if they don't exist) for use in isocratic runs. Finally, it creates a display parameter `dglc`, so that the `dg('dglc')` command (or the equivalent macro `dglc`) can be used to display all the LC-related parameters.

Note that `parlc` can be used without worrying about losing existing values or attributes; if the parameters already exist, they are left untouched.

See also: *NMR Spectroscopy User Guide*

Related:	<code>curscan</code>	Scan currently in progress (P)
	<code>dglc</code>	Control LC-NMR parameter display (P)

<code>dtrig</code>	Delay to wait for another trigger or acquire a spectrum (P)
<code>inject</code>	Trigger the injection of a sample (P)
<code>ntrig</code>	Number of trigger signals to wait before acquisition (P)
<code>savefile</code>	Base file name for saving FIDs or data sets (P)

par112d Create parameters for 2D peak picking (M)

Description: Creates additional parameters `th2d` and `xdiag` for use with `112d` 2D peak picking program. `par112d` is functionally the same as `addpar('112d')`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>112d</code>	Automatic and interactive 2D peak picking (C)
	<code>th2d</code>	Threshold for integrating peaks in 2D spectra (P)
	<code>xdiag</code>	Threshold for excluding diagonal peaks when peak picking (P)

parlp Create parameters for linear prediction (M)

Syntax: `parlp<(dimension)>`

Description: Creates parametrized options for linear prediction (LP) in the current experiment. The display template for the `dglp` macro is also created if necessary. `parlp` is functionally the same as `addpar('lp')`.

Arguments: `dimension` is the dimension of a multidimensional data set. The default is to create the LP parameters `lpalg`, `lpopt`, `lpfilt`, `lpnupts`, `strtlp`, `lpext`, `strtext`, `lptrace`, and `lpprint`.

`parlp(1)` creates LP parameters `lpalg1`, `lpopt1`, `lpfilt1`, `lpnupts1`, `strtlp1`, `lpext1`, `strtext1`, `lptrace1`, and `lpprint1`. `addpar('lp',1)` is functionally equivalent to `parlp(1)`.

`parlp(2)` creates LP parameters `lpalg2`, `lpopt2`, `lpfilt2`, `lpnupts2`, `strtlp2`, `lpext2`, `strtext2`, `lptrace2`, and `lpprint2`. `addpar('lp',2)` is functionally equivalent to `parlp(2)`.

Examples: `parlp`
`parlp(1)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>lpalg</code>	LP algorithm for np dimension (P)
	<code>lpext</code>	LP data extension for np dimension (P)
	<code>lpfilt</code>	LP coefficients to calculate for np dimension (P)
	<code>lpnupts</code>	LP number of data points for np dimension (P)
	<code>lpopt</code>	LP algorithm data extension for np dimension (P)
	<code>lpprint</code>	LP print output for np dimension (P)
	<code>lptrace</code>	LP output spectrum for np dimension (P)
	<code>proc</code>	Type of processing on np FID (P)
	<code>proc1</code>	Type of processing on n1 interferogram (P)
	<code>proc2</code>	Type of processing on n12 interferogram (P)
	<code>strtext</code>	Starting point for LP data extension for np dimension (P)
	<code>strtlp</code>	Starting point for LP calculation for np dimension (P)

parmax Parameter maximum values (P)

Description: An array that holds the maximum values of other parameters. The maximum value of a parameter is an index into the array, and more than one parameter can have the same index into `parmax`. Several global parameters set in the Spectrometer Configuration window are part of `parmax`. To display all `parmax` values, enter `display('parmax','systemglobal')`.

See also: *User Programming*

Related:	<code>config</code>	Display current configuration and possibly change it (M)
	<code>display</code>	Display parameters and their attributes (C)
	<code>paramedit</code>	Edit a parameter and its attributes with user-selected editor (C)
	<code>paramvi</code>	Edit a parameter and its attributes using vi text editor (M)
	<code>parmin</code>	Parameter minimum values (P)
	<code>parstep</code>	Parameter step size values (P)

parmin **Parameter minimum values (P)**

Description: An array that holds the minimum values for other parameters. The minimum value of a parameter is the index into the `parmin` array. More than one parameter may have the same index into the array. To display all the values in `parmin`, enter `display('parmin','systemglobal')`.

See also: *User Programming*

Related:	<code>paramvi</code>	Edit a parameter and its attributes using vi text editor (M)
	<code>display</code>	Display parameters and their attributes (C)
	<code>paramedit</code>	Edit a parameter and its attributes with user-selected editor (C)
	<code>parmax</code>	Parameter maximum values (P)
	<code>parstep</code>	Parameter step size values (P)

paros **Create additional parameters used by oversampling (M)**

Description: Creates the parameters `def_osfilt`, `filtfile`, `oscoef`, `osfb`, `osfilt`, `oslsfrq`, and `oversamp` for oversampling and digital filtering. `paros` is functionally the same as `addpar('oversamp')`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to current experiment (M)
	<code>def_osfilt</code>	Default value of <code>osfilt</code> parameter (P)
	<code>filtfile</code>	File of FIR digital filter coefficients (P)
	<code>oscoef</code>	Digital filter coefficients for oversampling (P)
	<code>osfb</code>	Digital filter bandwidth for oversampling (P)
	<code>osfilt</code>	Oversampling filter for real-time DSP (P)
	<code>oslsfrq</code>	Bandpass filter offset for oversampling (P)
	<code>oversamp</code>	Oversampling factor for acquisition (P)

parstep **Parameter step size values (P)**

Description: An array that holds the step size values for other parameters. The step size value of a parameter is the index into the array. More than one parameter can have the same index into `parstep`. Several configuration parameters set in the Spectrometer Configuration window are part of `parstep`. To display all `parstep` values, enter `display('parstep','systemglobal')`.

See also: *User Programming*

Related:	<code>config</code>	Display current configuration and possibly change it (M)
	<code>display</code>	Display parameters and their attributes (C)
	<code>paramedit</code>	Edit a parameter and its attributes with user-selected editor (C)
	<code>paramvi</code>	Edit a parameter and its attributes using vi text editor (M)
	<code>parmax</code>	Parameter maximum values (P)
	<code>parmin</code>	Parameter minimum values (P)

parversion Version of parameter set (P)

Description: Stores the version of a parameter set. When a parameter set is updated with `updatepars` or `parfix`, `parversion` is set to 4.3 to indicate that fact. When a parameter set is retrieved into an experiment, `fixpar` checks `parversion` to determine if other parameters need to be updated using `parfix`.

See also: *NMR Spectroscopy User Guide*

Related: `fixpar` Correct parameter characteristics in experiment (M)
`parfix` Update parameter sets (M)
`updatepars` Update all parameter sets saved in a directory (M)

path3d Path to currently displayed 2D planes from a 3D data set (P)

Description: Stores the absolute path to the current 3D data directory tree. If `path3d` does not exist, it is created by the macro `par3d`. The command `select`, as well as the many macros that make use of `select`, require `path3d` in order to know where the 2D planes extracted from a 3D data set can be found.

`path3d` is set automatically by the macros `ft3d` and `getplane`:

- `ft3d` sets `path3d` to `curexp/datadir3d` if `ft3d` is not supplied with a directory path for the transformed 3D data. If `ft3d` is supplied with such a directory path (e.g., `/home/data/test3D`), `path3d` is set equal to that directory path. In this case, the 3D spectral data would reside in the directory `/home/data/test3D/data`.
- `getplane` sets `path3d` to `curexp/datadir3d` if `getplane` is not supplied with a directory path to the transformed 3D data. If `getplane` is supplied with such a directory path (e.g., `/home/data/test3D`), `path3d` is set equal to that directory path. In this case, the extracted 3D planes would reside in the directory `/home/data/test3D/extr`.

See also: *NMR Spectroscopy User Guide*

Related: `dplane` Display a 3D plane (M)
`dproj` Display a 3D plane projection (M)
`dsplanes` Display a series of 3D planes (M)
`ft3d` Perform a 3D Fourier transform on a 3D FID data set (M)
`getplane` Extract planes from a 3D spectral set (M)
`nextpl` Display the next 3D plane (M)
`par3d` Create 3D acquisition, processing, display parameters (C)
`plane` Currently displayed 3D plane type (P)
`plplanes` Plot a series of 3D planes (M)
`prevpl` Display the previous 3D plane (M)
`select` Select a spectrum or 2D plane without displaying it (C)

paxis Plot horizontal LC axis (M)

Applicability: Systems with the LC-NMR accessory.

Syntax: `paxis(time,major_tic,mino_tic)`

Description: Plots a horizontal LC axis. Horizontal axes are assumed to be used with “LC plots” of an entire LC run are labeled accordingly. It is assumed that relevant parameters (e.g., `sc`, `wc`, `vo`, `vp`) have not been changed after plotting the data.

Arguments: `time` is the time scale, in minutes (decimal values are fine), of the axis.
`major_tic` is spacing, in minutes (decimal values are fine), of major tics.
`minor_tic` is spacing, in minutes (decimal values are fine), of minor tics.

See also: *NMR Spectroscopy User Guide*

Pbox **Pulse shaping software (U)**

Syntax: `Pbox file options`

Description: Main Pbox (Pandora's Box) program for the generation of shape files for RF and gradients. (See *NMR Spectroscopy User Guide* manual for description of interactive Pbox usage).

Arguments: `file` is the name of a shape file.

`options` is any of the Pbox parameters initialized by the '-' sign and followed by the parameter value. The following options can be in any order and combinations:

<code>-b time</code>	Activates Bloch simulator, sets <code>simtime</code> , in sec.
<code>-c</code>	Calibrate only, do not create a shape file.
<code>-f file</code>	Set name of the output file.
<code>-h wave</code>	Print wave file header.
<code>-i wave</code>	Print wave file parameters.
<code>-l ref_pw90</code>	Length, in μ s, of reference pw90 pulse.
<code>-o</code>	List options.
<code>-p ref_pwr</code>	Reference power level, in dB.
<code>-r file</code>	Reshape Pbox pulse.
<code>-s stepsize</code>	Define length, in μ s, of a single step in waveform.
<code>-t wave</code>	Print wave title.
<code>-w wavestr</code>	Set wave data string.
<code>-v</code>	Run in verbose mode. Also print Pbox version.
<code>-value</code>	Sets reps to value.

Examples: `Pbox -i eburp2`
`Pbox newshape -wc 'eburp1 450 -1280.0' -1`
`Pbox sel.RF -w 'eburp1 420 -800' 'eburp1 420 1200'`
`Pbox -w 'eburp1 200 -1200' -attn e -p1 45 54.2 -b`
`Pbox tst -w 'esnob 20p 170p' -sfrq 150.02 -refofs 55p`
`-ref_pwr 45 -ref_pw90 54.2`

See also: *NMR Spectroscopy User Guide*

Related:	<code>cpx</code>	Create Pbox shape file (M)
	<code>dprofile</code>	Display pulse excitation profile from Pbox software (M)
	<code>dshape</code>	Display pulse shape (M)
	<code>dshapef</code>	Display last generated pulse shape (M)
	<code>dshapei</code>	Display pulse shape interactively (M)
	<code>opx</code>	Open shape definition file for Pbox (M)
	<code>pbox_bw</code>	Define excitation band (M)
	<code>pbox_bws</code>	Define excitation band for solvent suppression (notch) pulses (M)
	<code>pbox_dmf</code>	Extract dmf value from Pbox shape file (M)
	<code>pbox_dres</code>	Extract dres value from Pbox shape file (M)
	<code>pbox_name</code>	Extract name of last shape file generated by Pbox (M)
	<code>pbox_pw</code>	Extract pulse length from Pbox shape file (M)
	<code>pbox_pwr</code>	Extract pulse power from Pbox shape file (M)
	<code>pbox_pwrf</code>	Extract pulse fine power from Pbox (M)
	<code>pboxget</code>	Extract all calibration data from a Pbox shape file (M)

<code>pboxpar</code>	Add parameter definition to the pbox.inp file (M)
<code>pboxrst</code>	Reset temporary Pbox/VnmrJ variables (M)
<code>pboxunits</code>	Converts to Pbox default units (M)
<code>pph</code>	Print pulse header (M)
<code>pprofile</code>	Plot pulse excitation profile from Pbox software (M)
<code>pshape</code>	Plot pulse shape (M)
<code>pshapef</code>	Display pulse shape or modulation pattern interactively (M)
<code>putwave</code>	Write a wave into Pbox.inp file (M)
<code>pxset</code>	Assign Pbox calibration data to experimental parameters (M)
<code>pxshape</code>	Generates a single-band shape file (M)
<code>Pxsim</code>	Simulate Bloch profile for a shaped pulse (M)
<code>Pxspy</code>	Create shape definition using Fourier coefficients (U)
<code>selex</code>	Defines excitation band (M)
<code>setwave</code>	Sets a single excitation band in Pbox.inp file (M)
<code>shdec</code>	Shaped observe excitation sequence (M)

pbox_bw Define excitation band (M)

Syntax: `pbox_bw< (shapename) >`

Description: Defines the excitation band from the position of cursors in the graphics window and reports them to user. It also sets `r1` to excitation bandwidth and `r2` to offset. This macro is used mainly in Pbox menus and macros.

Arguments: `shapename` is the name of a shape as in `wavelib`; mainly for use with menus.

See also: *NMR Spectroscopy User Guide*

Related: `Pbox` Pulse shaping software (U)

pbox_bws Define excitation band for solvent suppression (notch) pulses (M)

Syntax: `pbox_bws< (shapename) >`

Description: Defines the excitation band from the position of cursors in the graphics window and reports them to user. It also sets `r1` to excitation bandwidth and `r2` to offset. Note, the left cursor should be placed on the left side of the excitation band and the right cursor on resonance of the solvent signal. This macro is mainly used in Pbox menus and macros.

Arguments: `shapename` is the name of a shape file as in `wavelib`, mainly for use with menus.

See also: *NMR Spectroscopy User Guide*

Related: `Pbox` Pulse shaping software (U)

pbox_dmf Extract dmf value from pbox.cal or Pbox shape file (M)

Syntax: `pbox_dmf< (shapefile.DEC) >:exp_param`

Description: Extracts the `dmf` value from the file `shapefile.DEC` created by `Pbox` or, if file name is not provided, from the `pbox.cal` file containing parameters of the last created Pbox shape file.

Arguments: `shapefile.DEC` is the name of a shape file.

`exp_param` is a `dmf` type experiment parameter.

Examples: `pbox_dmf('myfile.DEC'):mydmf`
`pbox_dmf:dmf2`

See also: *NMR Spectroscopy User Guide*

Related: **dmf** Decoupler modulation frequency for first decoupler (P)
Pbox Pulse shaping software (U)

pbox_dres Extract dres value from pbox.cal or Pbox shape file (M)

Syntax: `pbox_dres<(shapefile.DEC)>:exp_param`

Description: Extracts the **dres** value from the file `shapefile.DEC` created by **Pbox** or, if file name is not provided, from the `Pbox.cal` file containing parameters of the last created Pbox shape file.

Arguments: `shapefile.DEC` is the name of a shape file.
`exp_param` is a `dres` type experiment parameter.

Examples: `pbox_dres('myfile.DEC'):mydres`
`pbox_dres:dres2`

See also: *NMR Spectroscopy User Guide*

Related: **dres** Tip-angle resolution for first decoupler (P)
Pbox Pulse shaping software (U)

pbox_name Extract name of last shape generated by Pbox from pbox.cal (M)

Syntax: `pbox_name:exp_name`

Description: Extracts name of the last shape file generated by **Pbox** and stored in the `Pbox.cal` file. Note, that the file name extension is not stored explicitly and is not provided by this macro.

Arguments: `exp_name` returns the name of last shape file.

Examples: `pbox_pw:shname`
`pbox_pw:pwpat`

See also: *NMR Spectroscopy User Guide*

Related: **Pbox** Pulse shaping software (U)

pbox_pw Extract pulse length from pbox.cal or Pbox shape file (M)

Syntax: `pbox_pw<(shapefile.RF)>:exp_param`

Description: Extracts pulse length from the file `shapefile.RF` generated by **Pbox** or, if file name is not provided, from `pbox.cal` file containing parameters of the last created Pbox shape file. Returns the pulse length, in μ s.

Arguments: `shapefile.RF` is the shape file name, including the extension.
`exp_param` is a `pw` type experiment parameter.

Examples: `pbox_pw('myfile.RF'):softpw`
`pbox_pw:selpw`

See also: *NMR Spectroscopy User Guide*

Related: **Pbox** Pulse shaping software (U)

pbox_pwr Extract power level from Pbox.cal or Pbox shape file (M)

Syntax: `pbox_pwr<(shapefile.ext)>:exp_param`

Description: Extracts the power lever from the file `shapefile.ext` generated by **Pbox** or, if file name is not provided, from the `pbox.cal` file containing parameters of the last created Pbox shape file. Returns the power level, in dB. The

`exp_param` parameter will not be changed by this macro if the parameter is previously set to 'n' (not used).

Arguments: `shapefile.ext` is the name of the shape file.
`exp_param` is a power type experiment parameter.

Examples: `pbox_pwr('myfile.DEC'):mypwr`
`pbox_pwr:dpwr2`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

pbox_pwrf Extract fine power level from pbox.cal or Pbox shape file (M)

Syntax: `pbox_pwrf<(shapefile.ext)>:exp_param`

Description: Extracts the fine power level from the file `shapefile.ext` generated by [Pbox](#) or, if file name is not provided, from the `pbox.cal` file containing parameters of the last created Pbox shape file. Returns the value of fine power, in dB. Note that the parameter will not be changed by this macro if it was previously set to 'n' (not used).

Arguments: `shapefile.ext` is the name of the shape file.
`exp_param` is a fine power type experiment parameter.

Examples: `pbox_pwrf('myfile.DEC'):mypwrf`
`pbox_pwrf:dpwrf`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

pboxget Extract Pbox calibration data (M)

Syntax: `pboxget<(shfile.ext)>:$name,$pw,$pwr,$pwrf,$dres,$dmf`

Description: Extracts calibration data from the file `shfile.ext` generated by [Pbox](#) or, if a file name is not provided, from the `pbox.cal` file containing parameters of the last created Pbox shape file. Returns shape name and the values of total pulse length (in μ s), power (dB), fine power, `dres`, and `dmf`. The parameter will not be changed by this macro if the parameter was previously set to 'n' (not used).

Arguments: `shfile.ext` is the name of the shape file, including the extension.
`name` is the experiment parameter receiving the shape name (without the extension).
`pw` is the experiment parameter receiving the total pulse length, in μ s.
`pwr` is the experiment parameter receiving the power level, in dB.
`pwrf` is the experiment parameter receiving the fine power level.
`dres` is the experiment parameter receiving the decoupler resolution.
`dmf` is the experiment parameter receiving the decoupler modulation frequency.

Examples: `pboxget('myfile.DEC'):dseq,r1,dpwr,dpwrf,dres,dmf`
`pboxget('selshape.RF'):pwpat,selpw,selpwr`
`pboxget:dseq2,r1,dpwr2,dpwrf2,dres2,dmf2`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

P

pboxpar Add parameter definition to the Pbox.inp file (M)

Syntax: `pboxpar (param, value)`

Description: Adds a parameter definition to the `Pbox.inp` file.

Arguments: `param` is the parameter name
`value` is the value of the parameter.

Examples: `pboxpar('name', 'myfile.DEC')`
`pboxpar('bsim', 'y')`
`pboxpar('T1', 0.24)`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

pboxrst Reset temporary Pbox variables (M)

Description: Resets `r1=0`, `r2=0`, `r3=0`, `r4=0`, `n2='n'`, `n3=''`, and adds some standard comment lines to the `Pbox.inp` file. This macro is used in menus and other Pbox macros.

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

pboxunits Converts to Pbox default units (M)

Syntax: `pboxunits`

Description: Used by Pbox menus to scale parameters related to time or frequency down to Pbox default units (Hz or seconds) before the parameter is stored in the `Pbox.inp` file.

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

pcon Plot contours on a plotter (C)

Syntax: `pcon(<'pos' | 'neg'><, 'noaxis'><, levels><, spacing>)>`

Description: Plots positive and negative peaks of a contour plot display using different colors. Specifically, if [maxpen](#) is set for `n` pens, positive peaks are plotted using colors 1 through $(n+1)/2$, and negative peaks are plotted using colors $((n+1)/2)+1$ through `n` (i.e., half the colors for each, plus one extra for positive if an odd number of pens is specified). Pen 1 is always used for the axes, and the lowest contour of the positive peaks is also plotted with `pen1`. In all cases, the pen colors are cycled if more contours are to be plotted than there are pens available.

To plot both negative and positive contours of a phase-sensitive spectrum on a monochrome device such as a LaserJet or a plotter with a single pen, different numbers of contours may be plotted for the different sign. For example, `pcon('pos', 10, 1.4)` `pcon('neg', 1)` will plot ten closely spaced positive contours and one negative contour.

Arguments: `'pos'` is a keyword specifying that phase-sensitive spectra plot positive peaks only. The default is to plot both positive and negative peaks.

`'neg'` is a keyword specifying that phase-sensitive spectra plot negative peaks only. The default is to plot both positive and negative peaks.

`'noaxis'` is a keyword to omit outlining the plot and omit plotting the horizontal and vertical axes.

`levels` is maximum number of contour levels to plot. The default is 4.

spacing is relative intensity of successive contour levels. The default is 2.

Examples: `pcon`
`pcon(4,1.4)`
`pcon('pos','noaxis')`
`pcon('neg',3)`

See also: *NMR Spectroscopy User Guide*

Related: `dpcon` Display plotted contours (C)
`maxpen` Maximum number of pens to use (P)

pcss Calculate and show proton chemical shifts spectrum (M)

Syntax: `pcss(<threshold><,max_cc><,max_width>)`

Description: Calculates and shows the proton chemical shifts spectrum. The `dsp` command is used to display the results. The list of chemical shifts is saved in the file `pcss.outpar`. The original spectrum can be calculated by the `wft` command.

Arguments: `threshold` sets the level whether a point belongs to a peak or is noise. The default is that `pcss` automatically calculates the threshold.

`max_cc` is the maximum allowable coupling constant in the spectrum. The default is 20 Hz.

`max_width` is the maximum width of a spin multiplet in the spectrum. The default is 60 Hz.

Examples: `pcss`
`pcss(10)`
`pcss(9,20,80)`

See also: *NMR Spectroscopy User Guide*

Related: `do_pcss` Calculate proton chemical shifts spectrum (C)
`dsp` Display pulse sequence (C)
`wft` Weight and Fourier transform 1D data (C)

peak Find tallest peak in specified region (C)

Syntax: `peak(<min_freq,max_freq><:height,freq>`

Description: Returns the height and frequency of the tallest peak in the selected region, including any referencing (i.e., the same frequency that you would measure by placing a cursor on the peak). A spectrum need not actually be displayed for `peak` to work.

Arguments: With no return arguments, `peak` displays on the screen information about peak height and frequency. If two cursors are displayed, `peak` without arguments finds the tallest peak between the cursors.

`min_freq` is minimum frequency limit of the region to be searched. The default value is `sp`.

`max_freq` is maximum frequency limit, in Hz, of the region to be searched. The default value is `sp + wp`.

`height` returns the height, in mm, of the tallest peak in the selected region.

`freq` returns the frequency, in Hz, of the tallest peak in the selected region.

Examples: `peak:$ht,$freq`
`peak(0,2000):r3`
`peak:$ht,cr`

P

See also: *User Programming*

Related: **sp** Start of plot (P)
wp Width of plot (P)

peak2d Return information about maximum in 2D data (C)

Syntax: `peak2d:$maximum_intensity<,$trace,$point>`

Description: Searches the area defined by **sp**, **wp**, **sp1**, and **wp1** in a 2D data set for a maximum intensity.

Arguments: `$maximum_intensity` returns the maximum intensity value found.
`$trace` returns the trace number of the maximum. The parameter **trace** defines whether f_1 or f_2 traces are counted.
`$point` returns the data point number of the maximum on that trace.

See also: *NMR Spectroscopy User Guide*

Related: **sp** Start of plot (P)
sp1 Start of plot in 1st indirectly detected dimension (P)
trace Mode for n -dimensional data display (P)
wp Width of plot (P)
wp1 Width of plot in 1st indirectly detected dimension (P)

pen Select a pen or color for drawing (C)

Syntax: `pen(<'graphics' | 'plotter', ><'xor' | 'normal', >
pen|color)`

Description: Selects the pen number for a plotter or the color for the graphics screen. This command is part of a line drawing capability that includes the **move** and **draw** commands. **move** sets the coordinates from which the line starts. **draw** draws a line from that point to the new coordinates specified by **draw**. Refer to the description of **draw** for examples of using the line drawing capability.

Arguments: **'graphics'** and **'plotter'** are keywords selecting the output device. The default is **'plotter'**. The output selected is passed to subsequent **pen**, **move**, or **draw** commands and remains active until a different output is specified.

'xor' and **'normal'** are keywords selecting the drawing mode for the **'graphics'** output device. In the **'xor'** mode, if a line is drawn such that one or more points of the line are in common with a previously drawn line, the common points are erased. In the **'normal'** mode, the common points remain. The mode selected is passed to subsequent **pen**, **draw**, or **move** commands and remains active until a different mode is specified. The default mode is **'normal'**.

pen is the plotter pen number: **'pen1'**, **'pen2'**, **'pen3'**, etc.

color is the active color for the graphics screen: **'red'**, **'green'**, **'blue'**, **'cyan'**, **'magenta'**, **'yellow'**, **'black'**, or **'white'**.

Examples: `pen('pen2')`
`pen('graphics', 'red')`

See also: *NMR Spectroscopy User Guide*

Related: **draw** Draw line from current location to another location (C)
move Move to an absolute location (C)

pexpl **Plot exponential or polynomial curves (C)**

Syntax: `pexpl(<options,><line1,line2, ...>`

Description: Plots exponential curves resulting from T_1 , T_2 , or kinetics analysis. Also plots polynomial curves from diffusion or other types of analysis. The `analyze.out` file is the data input file used to make the plot. Refer to the [expl](#) entry for the format of this file. The parameters `sc`, `wc`, `sc2`, and `wc2` control the size of the plot.

Arguments: `options` are any of the following keywords:

- `'linear'`, `'square'`, and `'log'` provide for plotting of the data points against the square or log of the data. `'linear'` controls x-axis scale, `'square'` controls the y-axis. The default is `'linear'`.
- `'link'` causes the data points to be connected rather than a plot of the theoretical curve.
- `'nocurve'` produces a plot of data points only.
- `'oldbox'` plots an additional curve on an existing plot. Only the first data set in `analyze.out` is plotted. It causes the program to get box and scale description from `expfit.out` in the current experiment.
- `'file'` followed by a file name replaces `analyze.out` as the input.

`line1`, `line2`, ... specify curves to be plotted. The default is to plot the first six curves (if that many exist) along with the data points.

Examples: `pexpl`
`pexpl(1,3,6)`

See also: *NMR Spectroscopy User Guide, User Programming*

Related:	expl	Display exponential or polynomial curves (C)
	sc	Start of chart (P)
	sc2	Start of chart in second direction (P)
	wc	Width of chart (P)
	wc2	Width of chart in second direction (P)

pexpladd **Add another diffusion analysis to current plot (M)**

Applicability: Systems with the diffusion option.

Syntax: `pexpladd(integral_region)`

Description: Adds results of another diffusion analysis to the currently plotted results.

Arguments: `integral_region` specifies the number of the region whose results are to be added to the existing plot.

Examples: `pexpladd(1)`

See also: *NMR Spectroscopy User Guide*

Related:	expl	Display exponential or polynomial curves (C)
	pexpl	Plot exponential or polynomial curves (C)
	expladd	Add another diffusion analysis to current display (M)

pfgon **Pulsed field gradient amplifiers on/off control (P)**

Applicability: Systems with pulsed field gradient (PFG) modules.

Description: A global string parameter controlling the X, Y, and Z gradients for the PFG current amplifiers. Entering `su` or `go` sets the amplifiers at the current value of `pfgon`. For `pfgon` to take effect, `gradtype` must equal `p`, `q`, `l`, `t`, or `u` for the corresponding X, Y, or Z gradient, and a `su` or a `go` must be issued.

P

Values: A three-character string, with the first character controlling the X gradient, the second the Y gradient, and the third the Z gradient. For each gradient, setting the value to y turns on an amplifier and setting the value to n turns it off. For example, `pfgon= 'nny'` turns on only the PFG amplifier on the Z channel, and `pfgon= 'nnn'` turns off the PFG amplifiers on all channels.

See also: *NMR Spectroscopy User Guide*

Related:

<code>go</code>	Submit experiment to acquisition (M)
<code>gradtype</code>	Gradients for X, Y, and Z axes (P)
<code>setup</code>	Set up parameters for basic experiments (M)
<code>su</code>	Submit a setup experiment to acquisition (M)

p f w w Plot FIDs in whitewash mode (C)

Syntax: `p f w w <(<start><, finish><, step><, 'all' | 'imag'>)>`

Description: Plots FIDs in whitewash mode (after the first FID, each FID is blanked out in regions in which it is behind an earlier FID). The position of the first FID is governed by parameters `wc`, `sc`, and `vpf`.

Arguments: `start` is the index of a particular FID for arrayed 1D or 2D data sets. For multiple FIDs, `start` is the index of the first FID.

`finish` is the index of the last FID for multiple FIDs.

`step` specifies the increment for the FID index. The default is 1.

`'all'` is a keyword to plot all of the FIDs. This is the default.

`'imag'` is a keyword to plot only the imaginary FID channel. The default is `'all'`.

Examples: `p f w w`
`p f w w (4,10,2, 'imag')`

See also: *NMR Spectroscopy User Guide*

Related:

<code>dfs</code>	Display stacked FIDs (C)
<code>dfww</code>	Display FIDs in whitewash mode (C)
<code>plfid</code>	Plot FIDs (C)
<code>sc</code>	Start of chart (P)
<code>vpf</code>	Current vertical position of FID (P)
<code>wc</code>	Width of chart (P)

p g e Convert parameter set to PGE pulse sequence (M)

Applicability: Systems with the diffusion option.

Description: Adds all necessary parameters to perform the PGE (Pulse Gradient Experiment) pulse sequence, taking those parameters from the file `/vnmr/parlib/pge`.

See also: *NMR Spectroscopy User Guide*

Related:

<code>pge_calib</code>	Calibrate gradient strengths for PGE pulse sequence (M)
<code>pge_data</code>	Extract data from single element of PGE pulse sequence (M)
<code>pge_output</code>	Output results from PGE pulse sequence (M)
<code>pge_process</code>	Automated processing of data from PGE pulse sequence (M)
<code>pge_results</code>	Calculate diffusion constant for integral region (M)
<code>pge_setup</code>	Set up gradient control parameters for PGE pulse sequence (M)

p g e _ c a l i b Calibrate gradient strengths for PGE pulse sequence (M)

Applicability: Systems with the diffusion option.

Description: Calibrates the parameters `grad_cw_coef` and `grad_p_coef`, which relate the DAC values (in DAC units) to the gradient strengths (in gauss/cm). Given a diffusion constant measurement (made with `pge_results`) for a known diffusion constant, `pge_calib` then adjusts the calibration parameters to produce the correct diffusion constant.

See also: *NMR Spectroscopy User Guide*

Related: `pge` Calibrate gradient strengths for PGE pulse sequence (M)
`pge_results` Calculate diffusion constant for integral region (M)

pge_data Extract data from single element of PGE pulse sequence (M)

Applicability: Systems with the diffusion option.

Syntax: `pge_data (array_index)`

Description: Extracts integral information from a currently displayed element of a PGE (Pulse Gradient Experiment) and writes the results in the current experiment directory as the file `info_#`, where # is the value of the `array_index` argument (e.g., if `array_index` is 5, the file is `info_5`)

Arguments: `array_index` is the number of the array element from which the data is extracted.

Examples: `pge_data (5)`

See also: *NMR Spectroscopy User Guide*

Related: `pge` Calibrate gradient strengths for PGE pulse sequence (M)

pge_output Output results from PGE pulse sequence (M)

Applicability: Systems with the diffusion option.

Description: Prints the calculated results from the PGE (Pulse Gradient Experiment) pulse sequence on a printer and plots the graphs of calculated decay curves.

See also: *NMR Spectroscopy User Guide*

Related: `pge` Calibrate gradient strengths for PGE pulse sequence (M)

pge_process Automated processing of data from PGE pulse sequence (M)

Applicability: Systems with the diffusion option.

Syntax: `pge_process`

Description: Performs full automated processing of data from a PGE (Pulse Gradient Experiment) pulse sequence.

See also: *NMR Spectroscopy User Guide*

Related: `pge` Calibrate gradient strengths for PGE pulse sequence (M)

pge_results Calculate diffusion constant for integral region (M)

Applicability: Systems with the diffusion option.

Syntax: `pge_results (integral_region<, reference_region>)`

Description: Calculates a diffusion coefficient based on a single integral region in the spectrum (if one input argument) or calculates diffusion coefficient of an integral region consisting of two components (if two input arguments).

Arguments: `integral_region` is the number of the integral region on which to perform the analysis

reference_region is the number of the integral region used to get the value of the diffusion coefficient.

Examples: `pge_results(2)`
`pge_results(1,3)`

See also: *NMR Spectroscopy User Guide*

Related: [pge](#) Calibrate gradient strengths for PGE pulse sequence (M)

pge_setup Set up gradient control parameters for PGE pulse sequence (M)

Applicability: Systems with the diffusion option.

Syntax: `pge_setup<('no')>`

Description: Prompts the user for the values of the `g_max`, `g_min`, `g_steps`, `g_array`, `nt_first`, `nt_array`, and other parameters for the PGE (Pulse Gradient Experiment) pulse sequence. These parameters are then used to calculate the `grad_p1` and `nt` arrays.

Arguments: 'no' is a keyword to turn off prompting the user and instead use the current values of the parameters to calculate the `grad_p1` and `nt` arrays.

Examples: `pge_setup`
`pge_setup('no')`

See also: *NMR Spectroscopy User Guide*

Related: [pge](#) Calibrate gradient strengths for PGE pulse sequence (M)

ph Set phased mode in directly detected dimension (C)

Description: Selects the phased mode by setting the parameter `dmg='ph'`. In the *phased spectra display mode*, each real point in the displayed spectrum is calculated from a linear combination of the real and imaginary points comprising each respective complex data point. The coefficients for this linear combination are derived from the phase parameters `rp` and `lp`.

For 2D data, if `pmode='partial'` or `pmode=''` (two single quotes with no space in between), `ph` has an effect on the data prior to the second Fourier transform. If `pmode='full'`, `ph` acts in concert with the commands `ph1`, `av1`, or `pwr1` to yield the resultant contour display for the 2D data.

See also: *NMR Spectroscopy User Guide*

Related:

<code>av</code>	Set abs. value mode in directly detected dimension (C)
<code>av1</code>	Set abs. value mode in 1st indirectly detected dimension (C)
<code>dmg</code>	Data display mode in directly detected dimension (P)
<code>ft</code>	Fourier transform 1D data (C)
<code>ft1d</code>	Fourier transform along f_2 dimension (C)
<code>ft2d</code>	Fourier transform 2D data (C)
<code>lp</code>	First-order phase in directly detected dimension (P)
<code>pa</code>	Set phase angle mode in directly detected dimension (C)
<code>pa1</code>	Set phase angle mode in 1st indirectly detected dimension (C)
<code>ph1</code>	Set phased mode in 1st indirectly detected dimension (C)
<code>ph2</code>	Set phased mode in 2nd indirectly detected dimension (C)
<code>pmode</code>	Processing mode for 2D data (P)
<code>pwr</code>	Set power mode in directly detected dimension (C)
<code>pwr1</code>	Set power mode in 1st indirectly detected dimension (C)
<code>rp</code>	Zero-order phase in directly detected dimension (P)
<code>wft</code>	Weight and Fourier transform 1D data (C)
<code>wft1d</code>	Weight and Fourier transform f_2 of 2D data (M)
<code>wft2d</code>	Weight and Fourier transform 2D data (M)

ph1 Set phased mode in 1st indirectly detected dimension (C)

Description: Selects the phased spectra display mode along the first indirectly detected dimension by setting the parameter **dmg1** to the string value 'ph1'. If the parameter **dmg1** does not exist, ph1 will create it and set it to 'ph1'.

In the phased mode, each real point in the displayed trace is calculated from a linear combination of the real and imaginary points comprising each respective complex data point. For hypercomplex data, the linear combination uses the real-real and imaginary-real points from each respective hypercomplex data point. The coefficients for this linear combination are derived from the phase parameters **rp1** and **lp1**.

The ph1 command is only needed if mixed-mode display is desired. If the parameter **dmg1** does not exist or is set to the null string, the display mode along the first indirectly detected dimension defaults to the display mode of the directly detected dimension (characterized by the parameter **dmg**). For the contour display of multidimensional data, the result of ph1 is the same as for traces provided that **pmode**='partial' or **pmode**=' '.

See also: *NMR Spectroscopy User Guide*

Related:	av1	Set abs. value mode in 1st indirectly detected dimension (C)
	dmg1	Data display mode in 1st indirectly detected dimension (P)
	lp1	First-order phase in 1st indirectly detected dimension (P)
	pa	Set phase angle mode in directly detected dimension (C)
	pa1	Set phase angle mode in 1st indirectly detected dimension (C)
	ph	Set phased mode in directly detected dimension (C)
	pmode	Processing mode for 2D data (P)
	pwr1	Set power mode in 1st indirectly detected dimension (C)
	rp1	Zero-order phase in 1st indirectly detected dimension (P)

ph2 Set phased mode in 2nd indirectly detected dimension (C)

Description: Selects phased spectrum display mode processing along the second indirectly detected dimension by setting the parameter **dmg2**='ph2'. If **dmg2** does not exist or is set to the null string, ph2 creates **dmg2** and sets it to 'ph2'.

In the phased mode, each real point in the displayed trace is calculated from a linear combination of the real and imaginary points comprising each respective complex data point. For hypercomplex data, the linear combination uses the real-real and imaginary-real points from each respective hypercomplex data point. The coefficients for this linear combination are derived from the phase parameters **rp2** and **lp2**.

The ph2 command is only needed if mixed-mode display is desired. If the parameter **dmg2** does not exist or is set to the null string, the display mode along the second indirectly detected dimension defaults to the display mode of the directly detected dimension (characterized by the parameter **dmg**). For the contour display of multidimensional data, the result of ph2 is the same as for traces provided that **pmode**='partial' or **pmode**=' '.

See also: *NMR Spectroscopy User Guide*

Related:	av2	Set abs. value mode in 2nd indirectly detected dimension (C)
	dmg2	Data display mode in 2nd indirectly detected dimension (P)
	ft1d	Fourier transform along f_2 dimension (C)
	ft2d	Fourier transform 2D data (C)
	lp2	First-order phase in 2nd indirectly detected dimension (P)
	ph	Set phased mode in directly detected dimension (C)
	pmode	Processing mode for 2D data (P)
	pwr2	Set power mode in 2nd indirectly detected dimension (C)
	rp2	Zero-order phase in 2nd indirectly detected dimension (P)

P

phase **Change frequency-independent phase *rp* (M)**

Syntax: `phase (phase_change)`

Description: Changes the phase of all peaks in the spectrum by adding a value to the current *rp* value. Any excess over 360° is removed.

Arguments: *phase_change* is the value to be added to the current *rp* value (i.e., $new\ rp = old\ rp + phase\_change$).

Examples: `phase(45)`

See also: *NMR Spectroscopy User Guide*

Related: *rp* Zero-order phase in directly detected dimension (P)

phase **Phase selection (P)**

Description: Selects the phase cycling that determines the experiment type. To create the parameters *phase*, *ni*, and *sw1* for acquisition of a 2D data set in the current experiment, enter `addpar ( ' 2d ' )`.

Values: The following values are generally used in experiments with phase cycling. For more details, see the specific pulse sequence.

phase=0 selects an absolute-value 2D experiment.

phase=1 , 2 selects the required two components of a hypercomplex (States-Haberkorn) experiment.

phase=3 selects TPPI (Time Proportional Phase Incrementation).

See also: *NMR Spectroscopy User Guide*

Related: *addpar* Add selected parameters to the current experiment (M)

cosyps Set up parameters for phase-sensitive COSY (M)

Dqcosy Set up parameters for double quantum filtered COSY (M)

Hmqc Set up parameters for HMQC pulse sequence (M)

hmqcr Set up parameters for HMQCR pulse sequence (M)

inadqt Set up parameters for INADEQUATE pulse sequence (M)

mqcosy Set up parameters for MQCOSY pulse sequence (M)

Noesy Set up parameters for NOESY pulse sequence (M)

Roesy Set up parameters for ROESY pulse sequence (M)

Tocsy Set up parameters for TOCSY pulse sequence (M)

phase1 **Phase of first pulse (P)**

Applicability: Systems with a solids NMR module.

Description: Controls the first pulse phase in the cycle, in multipulse experiments.

See also: *NMR Spectroscopy User Guide*

Related: *br24* Set up BR24 multiple pulse experiment (M)

flipflop Set up sequences for multipulse (M)

phase2 **Phase selection for 3D acquisition (P)**

Description: Selects phase cycling type for 3D data acquisitions. Also selects the phase of the second pulse in the sequence set up by *flipflop*. To create the parameters *phase2*, *d3*, *ni2*, and *sw2* for acquisition of a 3D data set in the current experiment, enter `addpar ( ' 3d ' )`.

See also: *NMR Spectroscopy User Guide; User Guide: Solid-State NMR*

Related: *addpar* Add selected parameters to the current experiment (M)

d3 Incremented delay for 2nd indirectly detected dimension (P)

<code>flipflop</code>	Set up sequences for multipulse (M)
<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)
<code>par3d</code>	Create 3D acquisition, processing, display parameters (C)
<code>sw2</code>	Spectral width in 2nd indirectly detected dimension (P)

phase3 **Phase selection for 4D acquisition (P)**

Description: Selects phase cycling type for 4D data acquisitions. To create the parameters `phase3`, `d4`, `ni3`, and `sw3` for acquisition of a 4D data set in the current experiment, enter `addpar('4d')`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>d4</code>	Incremented delay for 3rd indirectly detected dimension (P)
	<code>ni3</code>	Number of increments in 3rd indirectly detected dimension (P)
	<code>par4d</code>	Create 4D acquisition parameters (C)
	<code>sw3</code>	Spectral width in 3rd indirectly detected dimension (P)

phasing **Control update region during interactive phasing (P)**

Description: Controls the percentage of the spectrum updated during interactive phasing using the `ds` command.

Values: 10 to 100, in percent, where 100 causes the entire spectrum to be updated, and 20 causes the area between the two vertical cursors to be updated.

See also: *NMR Spectroscopy User Guide*

Related:	<code>ds</code>	Display a spectrum (C)

phfid **Zero-order phasing constant for the np FID (P)**

Description: Specifies the angle of zero-order rotation. This zero-order rotation is executed as a part of retrieving the time-domain data into the active region of the memory and can be used instead of the parameter `rp` applied to the frequency-domain data. `phfid` is used only in a complex phase rotation.

`phfid` (and related parameters `lsfid` and `lsfrq`) operate on complex `np` FID data, referred to as the t_2 dimension in a 2D experiment or as the t_3 dimension in a 3D experiment. `phfid` is in the processing group and is properly handled through the `wti` display.

Values: -360.0 to +360.0, in degrees; 'n'

See also: *NMR Spectroscopy User Guide*

Related:	<code>dfid</code>	Display a single FID (C)
	<code>ds</code>	Display a spectrum FID (C)
	<code>ft</code>	Fourier transform 1D data (C)
	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>ft2d</code>	Fourier transform 2D data (C)
	<code>lsfid</code>	Number of complex points to left-shift the <code>np</code> FID (P)
	<code>lsfrq</code>	Frequency shift of the <code>fn</code> spectrum in Hz (P)
	<code>np</code>	Number of data points (P)
	<code>phfid1</code>	Zero-order phasing constant for <code>ni</code> interferogram (P)
	<code>phfid2</code>	Zero-order phasing constant for <code>ni2</code> interferogram (P)
	<code>rp</code>	Zero-order phase in directly detected dimension (P)
	<code>wft</code>	Weight and Fourier transform 1D data (C)
	<code>wft1d</code>	Weight and Fourier transform f_2 of 2D data (M)
	<code>wft2d</code>	Weight and Fourier transform 2D data (M)
	<code>wti</code>	Interactive weighting (C)

P

phfid1 Zero-order phasing constant for ni interferogram (P)

Description: Specifies the angle of zero-order rotation. This zero-order rotation is executed as a part of retrieving the time-domain data into the active region of the memory and can be used instead of the parameter **rp1** applied to the frequency-domain data. **phfid1** is used in a complex phase rotation for complex t_1/t_2 interferograms and in a hypercomplex phase rotation for hypercomplex t_1/t_2 interferograms.

phfid1 (and related parameters **lsfid1** and **lsfrq1**) operate on **ni** interferogram data, both hypercomplex and complex. **ni** interferogram data are referred to as the t_1 dimension in both a 2D and a 3D experiment. **phfid1** is in the processing group and is properly handled through the **wti** display; that is, a **wti** operation on an **ni** interferogram applies the parameters **phfid1**, **lsfid1**, and **lsfrq1**, if selected, to the time-domain data prior to the Fourier transformation.

Values: -360.0 to +360.0, in degrees; 'n'.

See also: *NMR Spectroscopy User Guide*

Related:	lsfid1	Number of complex points to left-shift the ni interferogram (P)
	lsfrq1	Frequency shift of the fn1 spectrum in Hz (P)
	ni	Number of increments in 1st indirectly detected dimension (P)
	phfid	Zero-order phasing constant for np FID (P)
	phfid2	Zero-order phasing constant for ni2 interferogram (P)
	rp1	Zero-order phase in 1st indirectly detected dimension (P)
	wti	Interactive weighting (C)

phfid2 Zero-order phasing constant for ni2 interferogram (P)

Description: Specifies the angle of zero-order rotation. This zero-order rotation is executed as a part of retrieving the time-domain data into the active region of the memory and can be used instead of the parameter **rp2** applied to the frequency-domain data. **phfid2** is used in a complex phase rotation for complex t_1/t_2 interferograms and in a hypercomplex phase rotation for hypercomplex t_1/t_2 interferograms.

phfid2 (and related parameters **lsfid2** and **lsfrq2**) operate on **ni2** interferogram data, both hypercomplex and complex. **ni2** interferogram data are referred to as the t_2 dimension in a 3D experiment. **phfid2** is in the processing group and is properly handled through the **wti** display.

Values: -360.0 to +360.0, in degrees; 'n'.

See also: *NMR Spectroscopy User Guide*

Related:	lsfid2	Number of complex points to left-shift ni2 interferogram (P)
	lsfrq2	Frequency shift of the fn2 spectrum in Hz (P)
	ni2	Number of increments in 2nd indirectly detected dimension (P)
	phfid	Zero-order phasing constant for np FID (P)
	phfid1	Zero-order phasing constant for ni interferogram (P)
	rp2	Zero-order phase in 2nd indirectly detected dimension (P)
	wti	Interactive weighting (C)

Phosphorus Set up parameters for ³¹P experiment (M)

Description: Set up parameters for ³¹P experiment.

pi3ssbsq Set up pi/3 shifted sinebell-squared window function (M)

Syntax: pi3ssbsq(<t1_inc>,<t2_inc>)>

Description: Sets up a $\pi/3$ unshifted sinebell-squared window function in 1, 2, or 3 dimensions. The macro checks whether the data is 1D, 2D, and 3D.

Arguments: `t1_inc` is the number of t1 increments. The default is `ni`.
`t2_inc` is the number of t2 increments. The default is `ni2`.

See also: *NMR Spectroscopy User Guide*

Related: `gaussian` Set up unshifted Gaussian window function (M)
`ni` Number of increments in 1st indirectly detected dimension (P)
`ni2` Number of increments in 2nd indirectly detected dimension (P)
`pi4ssbsq` Set up $\pi/4$ shifted sinebell-squared window function (M)
`sqcosine` Set up unshifted cosine-squared window function (M)
`sq sinebell` Set up unshifted sinebell-squared window function (M)

pi4ssbsq Set up $\pi/4$ shifted sinebell-squared window function (M)

Syntax: `pi4ssbsq(<t1_inc>,<t2_inc>)>`

Description: Sets up a $\pi/4$ unshifted sinebell-squared window function in 1, 2, or 3 dimensions. The macro checks whether the data is 1D, 2D, and 3D.

Arguments: `t1_inc` is the number of t1 increments. The default is `ni`.
`t2_inc` is the number of t2 increments. The default is `ni2`.

See also: *NMR Spectroscopy User Guide*

Related: `gaussian` Set up unshifted Gaussian window function (M)
`ni` Number of increments in 1st indirectly detected dimension (P)
`ni2` Number of increments in 2nd indirectly detected dimension (P)
`pi3ssbsq` Set up $\pi/3$ shifted sinebell-squared window function (M)
`sqcosine` Set up unshifted cosine-squared window function (M)
`sq sinebell` Set up unshifted sinebell-squared window function (M)

pin Pneumatics Router Interlock ((P))

Description: This parameter controls the effect of a Pneumatics Router Fault. The Pneumatic Router can fault in four ways:

- Intake pressure < 20 psi
- Solids narrow bore stack temperature fault
- VT air flow exceeded.
- Power supply fault

When either of these fault occur, and interrupt alerts the console of the problem and this parameter determines how the fault is handled. Once a fault is registered, all subsequent acquisitions will see the error according to 'pin'. The error must be cleared and re-armed with `sethw('pneufault','clear')`

Values: `'n'` -- the fault is ignored
`'w'` -- a warning msg is printed, acquisition continues
`'y'` -- an error msg is printed, acquisition is aborted

Related: `tin` Temperature interlock (P)
`vtairflow` VT air flow (P)
`vtairlimits` VT air flow limits (P)

pintvast Plots of integral regions (M)

Applicability: Systems with VAST accessory.

P

Syntax: `pintvast (last)`

Description: `pintvast` plots the integrals of the partial regions of each spectra from wells 0 to `last`.

Arguments: `last` is the number last sample well. The default is 96.

See also: *NMR Spectroscopy User Guide*

Related: `intvast` Builds text file the integral regions (M)

pir Plot integral amplitudes below spectrum (C)

Description: Plots integral amplitudes below the appropriate spectral regions.

See also: *NMR Spectroscopy User Guide*

Related: `dpf` Display peak frequencies over spectrum (C)
`dpir` Display integral amplitudes below spectrum (C)
`dpirn` Display normalized integral amplitudes below spectrum (M)
`pirn` Plot normalized integral amplitudes below spectrum (M)
`ppf` Plot peak frequencies over spectrum (M)

pirn Plot normalized integral amplitudes below spectrum (M)

Description: Equivalent to the command `pir` except that the sum of the integrals is normalized to the value of the parameter `ins`.

See also: *NMR Spectroscopy User Guide*

Related: `dpirn` Display normalized integral amplitudes below spectrum (M)
`ins` Integral normalization scale (P)
`pir` Plot integral amplitudes below spectrum (C)

piv Plot integral values below spectrum (M)

Syntax: `piv<(vertical_position)>`

Description: Labels integrals with a bracket below the spectrum and a vertical number indicating the integral value. See `dpiv` for description and use.

Related: `dpir` Display integral amplitudes below spectrum (C)
`dpiv` Display integral amplitudes below spectrum (M)
`dpirn` Display normalized integral amplitudes below spectrum (C)
`dpivn` Display normalized integral amplitudes below spectrum (M)
`pirn` Plot normalized integral amplitudes below spectrum (C)
`pir` Plot integral amplitudes below spectrum (C)
`pivn` Plot normalized integral amplitudes below spectrum (M)

pivn Plot normalized integral values below spectrum (M)

Syntax: `pivn<(vertical_position)>`

Description: Labels integrals with a bracket below the spectrum and a vertical number indicating the integral value. See `dpiv` for description and use.

Related: `dpir` Display integral amplitudes below spectrum (C)
`dpiv` Display integral amplitudes below spectrum (M)
`dpirn` Display normalized integral amplitudes below spectrum (C)
`dpivn` Display normalized integral amplitudes below spectrum (M)

<code>pirn</code>	Plot normalized integral amplitudes below spectrum (C)
<code>pir</code>	Plot integral amplitudes below spectrum (C)
<code>piv</code>	Plot integral amplitudes below spectrum (M)

p1 **Plot spectra (C)**

Syntax: `p1(<start,finish,<step>><,<'int'><,<'all'><,<options>>>`

Description: Plots one or more spectra. When a single spectrum is plotted, integral plotting is controlled by the parameter `intmod` as follows: `intmod='off'` turns off the integral plot, `intmod='full'` plots the entire integral, and `intmod='partial'` plots every other integral region.

For arrayed 1D spectra or for 2D spectra, a particular trace can be plotted by supplying the index number as an argument. For 2D data sets, spectra can be plotted from either the f_1 or f_2 domain by setting the parameter `trace` to `'f1'` or `'f2'`, respectively. After the command `ft1d`, interferogram can be plotted by setting `trace='f1'` and then typing `p1`. Multiple spectra can be plotted by supplying the indexes of the first and last spectra.

The position of the first spectrum is governed by the parameters `wc`, `sc`, and `vp`. For 1D data, subsequent spectra are positioned relative to the preceding spectrum by the vertical and horizontal offset parameters `vo` and `ho`. For 2D data, `ho` defines the total horizontal offset between the first and last spectrum. Also for 2D data, `vo` is inactive while the parameter `wc2` defines the total vertical offset between the first and last spectrum.

The parameter `cutoff`, if it exists and is active, defines the distance above and below the current vertical position `vp` at which peaks are truncated. By arraying `cutoff` to have two different values, truncation limits above and below the current vertical position can be controlled. For example, `cutoff=50` truncates peaks at `vp+50` mm and `vp-50` mm. `cutoff=50,10` truncates peaks at `vp+50` mm and `vp-10` mm.

Arguments: `start` is the index of a particular trace for arrayed 1D or 2D spectra. For multiple spectra, `start` is the index of the first spectrum.

`finish` is the index of the last spectrum for multiple spectra.

`step` specifies the increment for the spectral index. The default is 1.

`'int'` is a keyword that specifies displaying only the integral, independently of the value of `intmod`.

`'all'` is a keyword to plot all of the spectra. This value is the default.

`options` can be any of the following keywords:

- `'top'` or `'side'` cause the spectrum to be plotted either above or at the left edge of a contour plot. This assumes that the parameters `sc`, `wc`, `sc2`, and `wc2` are those used to position the contour plot.
- `'dodc'` causes all spectra to be drift corrected independently.
- `'pen1'`, `'pen2'`, `'pen3'`, etc. specify a pen number on a plotter.

Examples: `p1`
`p1(1,6,2)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>cutoff</code>	Data truncation limit (P)
	<code>dssa</code>	Display stacked spectra automatically (C)
	<code>dsww</code>	Display spectra in whitewash mode (C)
	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>ho</code>	Horizontal offset (P)
	<code>intmod</code>	Integral display mode (P)

<code>plww</code>	Plot spectra in whitewash mode (C)
<code>pshr</code>	PostScript High Resolution plotting control (P)
<code>pslw</code>	PostScript Line Width control (P)
<code>sc</code>	Start of chart (P)
<code>sc2</code>	Start of chart in second direction (P)
<code>shownumx</code>	x position counting from bottom left of every spectrum (P)
<code>shownumy</code>	y position counting from bottom left of every spectrum (P)
<code>trace</code>	Mode for 2D data display (P)
<code>vo</code>	Vertical offset (P)
<code>vp</code>	Vertical position of spectrum (P)
<code>wc</code>	Width of chart (P)
<code>wc2</code>	Width of chart in second direction (P)

p12d **Plot 2D spectra in whitewash mode (C)**

Syntax: `p12d<('nobase' | 'fill' | 'fillnb')>`

Description: Plots a stacked plot of 2D spectra in whitewash mode (after the first spectra, each spectra is blanked out in regions in which it is behind an earlier spectra). Color does not represent intensity (unlike `dcon`), since intensity can be seen visually, but instead successive traces are displayed in different colors so that color represents frequency. The horizontal offset parameter `ho` is not active for this command.

Arguments: `'nobase'` is a keyword to activate `th` to suppress intensity below `th`.
`'fill'` is a keyword to fill in the peaks. Note that if `'fill'` (or `'fillnb'`) is used, `th` operates linearly and not logarithmically (with factors of 2) as it does in contour or color intensity displays.
`'fillnb'` is a keyword to combine base suppression and peak filling.

Examples: `p12d`
`p12d('nobase')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dcon</code>	Display noninteractive color intensity map (C)
	<code>ds2d</code>	Display 2D spectra in whitewash mode (C)
	<code>dsww</code>	Display spectra in whitewash mode (C)
	<code>ho</code>	Horizontal offset (P)
	<code>plww</code>	Plot spectra in whitewash mode (C)
	<code>th</code>	Threshold (P)

plane **Currently displayed 3D plane type (P)**

Description: Stores the type of 3D plane currently displayed within VnmrJ. If `plane` does not exist, it is created by the macro `par3d`. The command `select`, as well as the many macros that make use of `select`, requires the parameter `plane` to exist for 3D data sets and to contain an appropriate value.

`plane` is set automatically by the macro `getplane`; it can also be set by the macro `ft3d` if automatic plane extraction is requested at the end of the 3D FT. The order of priority for the plane types is `'f1f3'`, `'f2f3'`, and then `'f1f2'`. In other words, if `getplane` is requested to extract the f_1f_3 and the f_2f_3 planes, `plane` will be set to `'f1f3'`. `plane` can also be set manually.

Values: `'f1f3'`, `'f3f1'`, `'f2f3'`, `'f3f2'`, `'f1f2'`, or `'f2f1'`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dplane</code>	Display a 3D plane (M)
	<code>dproj</code>	Display a 3D plane projection (M)

<code>dsplanes</code>	Display a series of 3D planes (M)
<code>ft3d</code>	Perform a 3D Fourier transform on a 3D FID data set (M,U)
<code>getplane</code>	Extract planes from a 3D spectral set (M)
<code>nextpl</code>	Display the next 3D plane (M)
<code>par3d</code>	Create 3D acquisition, processing, display parameters (C)
<code>path3d</code>	Number of complex points to left-shift np FID (P)
<code>plplanes</code>	Plot a series of 3D planes (M)
<code>prevpl</code>	Display the previous 3D plane (M)
<code>select</code>	Select a spectrum or 2D plane without displaying it (C)

plapt **Plot APT-type spectra automatically (M)**

Syntax: `plapt <(13Cexp_number)>`

Description: Automatically plots APT spectra. The APT spectrum is plotted on top of a standard carbon spectrum if either an experiment with such data is specified or if a file C13 is found in `curexp+ '/subexp'`. If neither such a subfile is found nor an experiment with standard carbon data is specified, the APT spectrum is plotted alone.

Arguments: `13Cexp_number` specifies the number, from 1 to 9, of an experiment with a standard ^{13}C spectrum.

Examples: `plapt`
`plapt (2)`

See also: *NMR Spectroscopy User Guide*

Related: `curexp` Current experiment directory (P)

plarray **Plotting macro for arrayed 1D spectra (M)**

Description: A generic macro for plotting arrayed 1D spectra. `plarray` is called by the `plot` macro, but can also be used directly. For the plot layout, `proccarray` distinguishes between arrays with few elements (6 or less), which will be stacked vertically (no horizontal offset), and spectra with many (greater than 6) elements. Those are stacked horizontally by default, unless there are too many lines, in which case a diagonally stacked display is chosen. Horizontal stacking is mostly adequate for pulse and power calibrations, where there are usually few lines only; diagonally stacked displays/plots are frequently chosen for T_1 and T_2 experiments on entire spectra, often with many lines.

The automatic stacking mode can be overridden by creating and setting a string parameter `stackmode` in the startup macro or before calling `procplot` or `proccarray`. Possible values for `stackmode` are 'horizontal', 'vertical', or 'diagonal'. DEPT-type spectra can, in principle, also be processed with `proccarray`, but no DEPT editing occurs, of course.

See also: *NMR Spectroscopy User Guide*

Related: `aexppl` Automatic expansion plot (M)
`plc` Plot carbon spectrum (M)
`plh` Plot proton spectrum (M)
`plot` Automatically plot spectra (M)
`proccarray` Process arrayed 1D spectra (M)
`stackmode` Stack control for processing arrayed 1D spectra (P)

plate_glue **Define a glue order for plotting and display (U)**

Applicability: Systems with VAST accessory

P

Description: In a Unix terminal or shell window type `plate_glue`. The glue order is determined by clicking on the wells to be displayed. Save the glue order file in the user's `vnmr/sys/templates/glue` directory.

See also: *NMR Spectroscopy User Guide*

Related:

<code>dsvast2d</code>	Display VAST data in a pseudo-2D format (M)
<code>plvast</code>	Plot VAST data in a stacked 1D-NMR matrix (M)
<code>plvast2d</code>	Plot VAST data in a pseudo-2D format (M)

plc **Plot a carbon spectrum (M)**

Syntax: `plc<(pltmod)>`

Description: Plots a carbon spectrum based on the parameters `pltmod` (the options 'off', 'full', and 'fixed' are implemented) and `intmod` ('off', 'full', and 'partial' are implemented). Peak frequency labels, in ppm, are usually plotted.

Arguments: `pltmod` is an alternate value of `pltmod` for this macro only. The value of the `pltmod` parameter is not changed.

Examples:

```
plc
plc('full')
```

See also: *NMR Spectroscopy User Guide*

Related:

<code>intmod</code>	Integral display mode (P)
<code>pltmod</code>	Plotter display mode (P)

plcosy **Plot COSY- and NOESY-type spectra automatically (M)**

Syntax: `plcosy(<'pos' | 'neg'><, ><levels<, spacing<, exp1D>>>)`

Description: Automatically plots 2D COSY- and NOESY-type spectra (homonuclear correlated spectra). Features include the following:

- Keeps the orientation (f_1 , f_2) of the spectrum on the screen.
- Plot area is optimized.
- Number of contour levels and their spacing can be selected.
- Negative or positive contours can be suppressed.
- 1D traces can be plotted along both axes; such 1D traces are taken from a full (or reduced) 1D spectrum in an other experiment, or from a subfile from within the current experiment.
- Works correctly for expansions.
- 1D traces can be suppressed, allowing a larger area for the 2D spectrum.
- 1D spectrum can be in any experiment.
- With phase-sensitive spectra using a plotter with one pen or a printer such as a LaserJet, if 'pos' or 'neg' are not selected, seven positive levels (or the specified number of positive contours) and one negative level are plotted, to distinguish positive and negative signals.

In multiexperiment mode, for the first plot, the experiment with the 1D spectrum should be specified (at least if it is not in `exp1`). From then on, the 1D spectrum will be stored *within* the experiment with the 2D spectrum, which allows much faster switching between spectra and also frees the other (1D) experiment for other tasks. Because of this internal storage, the `exp1D` argument is not required for subsequent plots.

Arguments: 'pos' is a keyword to plot only positive contours.

'neg' is a keyword to plot only negative contours.

levels is the number of contour levels. The default is 7.

spacing is the spacing between the contours. The default is 2.

exp1D is the experiment in which the proton 1D spectrum resides. This can be a full 1D spectrum, but the referencing must be the same as for the 2D. A negative number suppresses the proton trace. The default is from a subfile.

Examples: `plcosy`
`plcosy(12,1.5)`
`plcosy('pos',7,2,3)`
`plcosy(7,2,-1)`
`plcosy('neg')`

See also: *NMR Spectroscopy User Guide*

pldept **Plot DEPT data, edited or unedited (M)**

Description: Plots out DEPT data, either edited or not edited.

See also: *NMR Spectroscopy User Guide*

Related: `adept` Automatic DEPT analysis and spectrum editing (C)
`autodept` Automated complete analysis of DEPT data (M)
`deptproc` Process DEPT data (M)
`padept` Perform adept analysis and plot resulting spectra (C)

plfid **Plot FIDs (C)**

Syntax: `plfid(<start><,finish><,step><,'all' | 'imag'>
<,pen>>`

Description: Plots one or more FIDs. The position of the first FID is governed by the parameters `wc`, `sc`, and `vpf`. A subsequent FID is positioned relative to the preceding FID by the vertical and horizontal offset parameters `vo` and `ho`.

Arguments: `start` is the index of a particular FID for arrayed 1D or 2D data sets. For multiple FIDs, `start` is the index of the first FID.
`finish` is the index of the last FID for multiple FIDs. To include all FIDs, set `start` to 1 and `finish` to the parameter `arraydim` (see example).
`step` specifies the increment for the FID index. The default is 1.
'all' is a keyword to plot all of the FIDs. This is the default.
'imag' is a keyword to plot the imaginary FID channel only. The default is 'all'.
`pen` is a keyword with the plotter pen number: 'pen1', 'pen2', 'pen3', etc. The default is 'pen1'.

Examples: `plfid(1,arraydim,3)`

See also: *NMR Spectroscopy User Guide*

Related: `arraydim` Dimension of experiment (P)
`dfs` Display stacked FIDs (C)
`dfww` Display FIDs in whitewash mode (C)
`ho` Horizontal offset (P)
`sc` Start of chart (P)
`vo` Vertical offset (P)
`vpf` Current vertical position of FID (P)
`wc` Width of chart (P)

P

plfit **Plot deconvolution analysis (M)**

Description: Produces a complete output plot of a deconvolution analysis, plotting the observed spectrum, the full calculated spectrum, each individual component, as well as the numerical results of the analysis.

See also: *NMR Spectroscopy User Guide*

Related: **fitspec** Perform spectrum deconvolution (C)
showfit Display numerical results of deconvolution (M)
usemark Use “mark” output as deconvolution starting point (M)

plgrid **Plot a grid on a 2D plot (M)**

Syntax: (1) `plgrid(<spacing><, ><pen>)>`
 (2) `plgrid(start_f2, incr_f2, start_f1, incr_f1<, pen>)>`

Description: Plots grid lines over a 2D plot.

Arguments: `spacing` specifies the approximate spacing of the grid lines, in cm. The default is intervals of approximately 1 cm, rounded so that the intervals fall at a multiple of 1, 2, or 5 (in Hz) or 1p, 2p, or 5p (in ppm).

`pen` is a keyword with the plotter pen number: 'pen1', 'pen2', 'pen3', etc. The default is 'pen1'.

`start_f2`, `incr_f2`, `start_f1`, `incr_f1` define the starting and increment frequencies in both f_2 and f_1 for a grid. Add the p suffix to a value to enter it in ppm (see last example below).

Examples: `plgrid`
`plgrid(2)`
`plgrid('pen5')`
`plgrid(1.5, 'pen2')`
`plgrid(1p, 0.5p, 3p, 0.5p)`

See also: *NMR Spectroscopy User Guide*

Related: **grid** Draw a grid on a 2D display (C)

plh **Plot proton spectrum (M)**

Syntax: `plh<(pltmod)>`

Description: Plots a proton spectrum based on the parameters **pltmod** (the options 'off', 'fixed', 'full', and 'variable' are implemented) and **intmod** ('off', 'full', and 'partial' are implemented).

Arguments: `pltmod` is an alternate value of the parameter **pltmod** for this macro only. The value of the **pltmod** parameter is not changed.

Examples: `plh`
`plh('full')`

See also: *NMR Spectroscopy User Guide*

Related: **intmod** Integral display mode (P)
pltmod Plotter display mode (P)
sp Start of plot (P)
wp Width of plot (P)

plhet2dj **Plot heteronuclear J-resolved 2D spectra automatically (M)**

Syntax: `plhet2dj('pos' | 'neg'<, levels<, spacing<, exp1D>>>)>`

Description: Automatically plots 2D spectra of type HET2DJ (heteronuclear J-resolved 2D spectra) with the following features:

- Displayed portion of the spectrum is plotted in f2-mode
- Plot area is optimized
- Number of contour levels and their spacing can be selected
- Negative or positive contours can be suppressed
- A 1D trace can be plotted along the f_2 axis; such a 1D trace is taken from a full (or reduced) 1D spectrum in an other experiment, or from a file from within the current experiment.
- Expansions are handled correctly
- The 1D trace can be suppressed, which allows using a larger area for the 2D spectrum
- The 1D spectrum can be in any experiment
- With phase-sensitive spectra, if 'pos' or 'neg' are not selected and the plotter has only one pen (also for printers like the LaserJet), the specified number of positive contours are plotted (default is 7), but only one negative level, to distinguish positive and negative signals.

In multiexperiment mode, for the first plot the experiment with the 1D spectrum should be specified (at least if it is not in exp1). From then on, the 1D spectrum is stored *within* the experiment with the 2D spectrum, which allows much faster switching between the spectra and also frees the other 1D experiment for other tasks. Because of this internal storage, the exp1D argument is not required for subsequent plots.

Arguments: 'pos' is a keyword to only plot positive contours

'neg' is a keyword to only plot negative contours

levels is the number of contour levels. The default is 7.

spacing is the spacing between the contours. The default is 2.

exp1D is the number from 1 to 9 of the experiment in which the 1D spectrum resides. This can be a full 1D spectrum, but the referencing must be the same as for the 2D. A negative number will suppress the 1D trace. The default is 1 (for exp1).

Examples: `plhet2dj`
`plhet2dj(12,1.5)`
`plhet2dj('pos',7,2,3)`
`plhet2dj(7,2,-1)`

See also: *NMR Spectroscopy User Guide*

plhom2dj Plot homonuclear J-resolved 2D spectra automatically (M)

Syntax: (1) `plhom2dj<(levels<, spacing<, exp1D>>) >`
 (2) `plhom2dj('pos' | 'neg'<, levels<, spacing<, exp1D>>>)`

Description: Automatically plots 2D spectra of type HOM2DJ (homonuclear J-resolved 2D spectra). Features include the following:

- The displayed portion of the spectrum is plotted in f2-mode
- The plot area is optimized
- Number of contour levels and their spacing can be selected
- Negative or positive contours can be suppressed

- A 1D trace can be plotted along the f_2 axis; such a 1D trace is taken from a full (or reduced) 1D spectrum in an other experiment, or from a file from within the current experiment.
- It also works correctly for expansions
- The 1D trace can be suppressed, which allows using a larger area for the 2D spectrum
- The 1D spectrum can be in any experiment
- With phase-sensitive spectra, if 'pos' or 'neg' are not selected and the plotter has only 1 pen (also for printers like the LaserJet) 7 or the specified number of positive contours are plotted, but only one negative level, to distinguish positive and negative signals.

In multiexperiment mode, for the first plot the experiment with the 1D spectrum should be specified (at least if it is not in `exp1`). From then on, the 1D spectrum will be stored *within* the experiment with the 2D spectrum, which allows much faster switching between the spectra and also frees the other (1D) experiment for other tasks. Because of this internal storage, the `exp1D` argument is not required for subsequent plots.

Arguments: `levels` is the number of contour levels. The default is 7.
`spacing` is the spacing between the contours. The default is 2.
`exp1D` is a number from 1 to 9 for the experiment in which the 1D spectrum resides. The spectrum can be a full 1D spectrum but the referencing must be the same as for the 2D. A negative number will suppress the 1D trace. The default is 1 (for `exp1`).
 'pos' specifies only plot positive contours.
 'neg' specifies only plot negative contours.

Examples: `plhom2dj`
`plhom2dj (25, 1.2)`
`plhom2dj ('pos', 7, 2, 3)`
`plhom2dj (7, 2, -1)`

See also: *NMR Spectroscopy User Guide*

plhxcor **Plot X,H-correlation 2D spectrum (M)**

Syntax: `plhxcor (<'pos' | 'neg'> <, > <levels>, spacing
 <, exp1D_H<, exp1D_X>>>)`

Description: Automatically plots 2D spectra of type HETCOR, COLOC, HMQC, HMBC (direct and indirect detection). Features include the following:

- Keeps the orientation (f_1 , f_2) of the spectrum on the screen.
- Plot area is optimized.
- Number of contour levels and their spacing can be selected.
- Negative or positive contours can be suppressed.
- 1D proton and X traces can be plotted along both axes; such 1D traces are taken from full (or reduced) 1D spectra in other experiments or subfile within the current experiment.
- Works correctly for expansions.
- 1D traces can be suppressed, allowing a larger area for the 2D spectrum.
- 1D spectra can be in any experiment.

Arguments: 'pos' is a keyword to plot only positive contours.
 'neg' is a keyword to plot only negative contours.

`levels` is the number of contour levels. The default is 7.

`spacing` is the spacing between the contours. The default is 2.

`exp1D_H` is a number from 1 to 9 of the experiment in which the proton 1D spectrum resides; this can be a full 1D spectrum, but the referencing must be the same as for the 2D. A negative number will suppress the proton trace. The default is a subfile in the current experiment.

`exp1D_X` is a number from 1 to 9 of the experiment in which the X 1D spectrum resides. A negative number suppresses the X trace. the default is a subfile in the current experiment.

Examples: `plhxcor(12,1.5)`
`plhxcor(7,2,3)`
`plhxcor(7,2,1,3)`
`plhxcor('pos',7,2,-1,3)`
`plhxcor(7,2,-1,-1)`
`plhxcor('neg')`

See also: *NMR Spectroscopy User Guide*

Related: [hetcor](#) Set up parameters for HETCOR pulse sequence (M)

p11 Plot a line list (M)

Syntax: `p11<(x,y,minimum_y)>`

Description: Produces a columnar line list on a plotter, similar to what would appear on a printer. `p11` is quite different from the alternative method of plotting peak frequencies using [ppf](#). The output of `p11` is automatically formatted into multiple columns, depending on the number of lines.

Arguments: `x` is the `x` position of the upper left of the line list.

`y` is the `y` position of the upper left of the line list.

`minimum_y` is the minimum `y` at which to reset back to top.

Examples: `p11`
`p11(20,150)`
`p11(5,wc2max*.8,wc2max*.5)`

See also: *NMR Spectroscopy User Guide*

Related: [ppf](#) Plot peak frequencies over spectrum (M)

p112d Plot results of 2D peak picking (C)

Syntax: `p112d<(options)>`

Description: Plots the results of applying the [112d](#) command to pick 2D peaks in a 2D spectrum or a 2D plane of a 3D spectrum. Refer to the description of [112d](#) for a description of the process and the options available.

See also: *NMR Spectroscopy User Guide*

Related: [112d](#) Automatic and interactive 2D peak picking (C)

plockport Port number to use to lock out multiple ProTune processes (P)

Syntax: `plockport=<value>`

Description: The parameter must be created as a real local parameter before it can be used. The parameter is used to override a default port number that is used internally in ProTune to prevent two Java ProTune process from running simultaneously.

Related:	protune	Macro to start ProTune (M)
	create	Create new parameter in a parameter tree (C)

plot Automatically plot spectra (M)

Description: A universal plotting macro normally called through the [procplot](#) macro (which by itself serves as processing and plotting facility for automatic experiments). `plot` can also be used directly by the user who then doesn't have to remember specific plotting macros. Of course, the specialized macros can still be called directly if the user know their names.

The main purpose of `plot` is to automatically call the correct specialized plotting macro, depending on the user definition or otherwise on the type of data in the experiment. A plotting macro is selected automatically as follows:

APT spectra:	plapt
other, non-arrayed 1D data:	plot1d
DEPT type arrayed spectra:	pldept
other arrayed 1D spectra:	plarray
J-resolved 2D spectra:	pl2dj
homonuclear correlation 2D spectra:	plcosy
heteronuclear correlation 2D spectra:	plhxcor

Other types of 2D spectra (mostly multiple-quantum 2D spectra such as 2D-INADEQUATE) are not plotted automatically at this time. For phase-sensitive 2D spectra, automatic plotting is only provided if they were acquired using the method described by States, Haberkorn, and others; TPPI spectra are not covered.

Note that `plot` macros in general should not adjust the phase, the vertical scale, or change the integral size and reset points; these are assumed to be adjusted either by hand or by a suitable processing macro like [procplot](#) and the macros called therein. The plotting macros only make adjustments in order to make spectrum and parameters fit onto the page the desired way.

See also: *NMR Spectroscopy User Guide*

Related:	apptype	Application type (P)
	execpars	Set up the exec parameters (M)
	execplot	Execute plotting macro (P)
	plapt	Plot APT spectra (M)
	plarray	Plot arrays (M)
	plcosy	Plot homonuclear 2D correlation spectra (M)
	pldept	Plot DEPT type spectra (M)
	plhxcor	Plot heteronuclear correlation spectra (M)
	plot1d	Plot 1D spectra (M)
	plt2Darg	Plot 2D arguments (P)
	procplot	Automatically process FIDs (M)

plot1d Plotting macro for simple (non-arrayed) 1D spectra (M)

Description: A generic macro for plotting non-arrayed 1D spectra using a set of standard macros. `plot1d` is called by the [plot](#) macro, but can also be used directly. `plot1d` first tries to find a specific macro (e.g., [plh](#), [plc](#), [plp](#)) for the current observe nucleus. If such a macro exists, it is called. If a nucleus-specific macro is not found in the command path, a “minimal” 1D plot is produced.

See also: *NMR Spectroscopy User Guide*

Related: `plc` Plot carbon spectrum (M)
`plh` Plot proton spectrum (M)
`plp` Plot phosphorus spectrum (M)
`plot` Automatically plot spectra (M)

plot2D Plot 2D spectra (M)

Syntax: `plot2D('pos'|'neg'|'both', levels, spacing, \`
`'top'|'notop'|'proj', 'side'|'noside'|'proj')`

Description: Checks for the presence of appropriate proton or carbon high-resolution spectra in the directory `userdir+' /data/' +sample` and decides to plot high resolution spectra or a projection depending on whether or not the proton or carbon spectrum exists.

Arguments: The `plot2D` macro accepts the following arguments:

<code>'pos'</code>	keyword to plot positive contours
<code>'neg'</code>	keyword to plot negative contours.
<code>'both'</code>	keyword to plot both positive and negative contours.
<code>levels</code>	number of levels to be plotted.
<code>spacing</code>	spacing between contour levels.
<code>'top'</code>	keyword to plot a high-resolution spectrum on the top.
<code>'notop'</code>	keyword to plot a non-high-resolution spectrum or projection.
<code>'proj'</code>	keyword to plot a projection on top.
<code>'side'</code>	keyword to plot a high-resolution spectrum on the side.
<code>'noside'</code>	keyword to plot a non-high-resolution spectrum or projection.
<code>'proj'</code>	keyword that plots a projection on the side.

Examples: `plot2D('pos', 2, 5, 'top', 'side')`

See also: *NMR Spectroscopy User Guide*

Related: `plot` Automatically plot spectra (M)
`plotside` Plot spectrum on side (M)
`plottop` Plot spectrum on top (M)
`plottopside` Plot spectrum on top and side (M)

plotfile Plot to a file (M)

Syntax: `plotfile('argument')`

Description: plots automatically to a file. Supported output formats are: `ps`, `pdf`, `jpg`, `pcl`, `hpgl`, and `png`.

Arguments: `auto` — plots automatically.

`manual` — plots contents of printer queue to a file.

`Path and file name` — plots to specified file in the directory specified. Plots to the data directory using the supplied name if no path is specified.

Examples: `plotfile('xxx.fid/myplotfile.PDF')` plots will go into saved data directory.

`plotfile('myplotfile.PDF')` - plots will go to `vnmr/sys/plots` if FID has not been saved.

P

plothiresp High resolution plot output preparation (M)

Description: Required for the operation of the "Plot HiRes..." popup window to interactively use `plottop`/`plotside` of spectra in work spaces EXPn - creates necessary variables.

plotmanual Plot manually (M)

Description: Makes correct choice of printer (for preview) and correct alignment with respect to parameter output, resets back screen to original size & position based on selections made on the Plot page.

plotlogo Plots a logo (M)

Description: Plots a logo Varian logo using image file located in `/vnmr/iconlib/varianlogo.gif` or a custom logo from location specified in the parameter `plotlogo`.

Reads value for `doplotlogo` (n/y), `plotlogox` (x dimension image), and `plotlogy` (y dimensions image), and image file in `iconlib`.

plotpreview Creates temporary plots of the current plot output (M)

Syntax: `plotpreview<('argument')>`

Description: Creates preview of the output from auto-plotting the current spectrum and starts an Acrobat PDF reader. The preview output can be saved in PS, PDF, PCL, HPGL, JPG or PNG formats.

Arguments: `no argument` — creates preview of whatever is ready to send to the plotter.
`auto` — creates preview of auto-plot based upon plot macro
`manual` — creates preview of the contents of the print queue.

plotside Plot spectrum on side (M)

Description: Plots projection or high-resolution spectrum on the side of a 2D spectrum. `plotside` is used with `plot2D` and is not useful by itself.

See also: *NMR Spectroscopy User Guide*

Related: `plot2D` Plot 2D spectra (M)

plotter Plotter device (P)

Description: Sets the plotter in use on the system.

Values: A string with entries such as 'DraftPro', 'ThinkJet_96', 'LaserJet_300', 'jim', 'varian1', and 'Laser1'.

See also: *NMR Spectroscopy User Guide*

Related: `setplotdev` Return characteristics of a named plotter (C)
`showplotter` Show list of currently defined plotters and printers (M)

plottop Plot spectrum on top (M)

Description: Plots projection or high resolution spectra on the top of a 2D spectrum. `plottop` is used with `plot2D` and is not useful by itself.

See also: *NMR Spectroscopy User Guide*

Related: `plot2D` Plot 2D spectra (M)

plottopside **Plot spectrum on top and side (M)**

Description: Plots projection or high-resolution spectrum on the top and side of a 2D spectrum. `plottopside` is used with `plot2D` and is not useful by itself.

See also: *NMR Spectroscopy User Guide*

Related: `plot2D` Plot 2D spectra (M)

plp **Plot phosphorus spectrum (M)**

Syntax: `plp<(pltmod)>`

Description: Plots a phosphorus spectrum based on the parameters `pltmod` (the options 'off', 'full', and 'fixed' are implemented) and `intmod` ('off', 'full', and 'partial' are implemented). Peak frequency labels, in ppm, are usually plotted.

Arguments: `pltmod` is an alternate value of `pltmod` for this macro only. The value of the `pltmod` parameter is not changed.

Examples: `plp`
`plp('full')`

See also: *NMR Spectroscopy User Guide*

Related: `intmod` Integral display mode (P)
`plh` Plot proton spectrum (M)
`pltmod` Plotter display mode (P)

plplanes **Plot a series of 3D planes (M)**

Syntax: `plplanes(start_plot,stop_plot<,'pos' | 'neg'>
<,number_levels><,spacing>)`

Description: Creates the 2D contour plots for a subset of the 3D planes specified by the parameter `plane`.

Arguments: `start_plot` specifies the number, greater than 0, of the 3D plane with which plotting is to begin.

`stop_plot` specifies the number of the 3D plane with which plotting is to end. If `start_plot` is greater than `stop_plot`, only the first plane, whose number is `start_plot`, is plotted. The range of `stop_plot` depends on the value of the parameter `plane`:

- if `plane`='f1f3', `stop_plot` is between 0 and `fn2`/2
- if `plane`='f2f3', `stop_plot` is between 0 and `fn1`/2
- if `plane`='f1f2', `stop_plot` is between 0 and `fn`/2

'pos' is a keyword specifying that phase-sensitive spectra plot positive peaks only. The default is to plot both positive and negative peaks.

'neg' is a keyword specifying that phase-sensitive spectra plot negative peaks only. The default is to plot both positive and negative peaks.

`levels` is maximum number of contour levels to plot. The default is 4.

`spacing` is relative intensity of successive contour levels. The default is 2.

Note that the optional arguments 'pos' | 'neg', `number_levels`, and `spacing` are for the VnmrJ plotting command `pcon`.

Examples: `plplanes(1,3)`
`plplanes(2,3,'pos',4)`

P

See also: *NMR Spectroscopy User Guide*

Related:	<code>dplane</code>	Display a 3D plane (M)
	<code>dproj</code>	Display a 3D plane projection (M)
	<code>dsplanes</code>	Display a series of 3D planes (M)
	<code>getplane</code>	Extract planes from 3D spectral data set (M)
	<code>nextpl</code>	Display the next 3D plane (M)
	<code>path3d</code>	Path to currently displayed 2D planes from a 3D data set (P)
	<code>pcon</code>	Plot contours on a plotter (C)
	<code>plane</code>	Currently displayed 3D plane type (P)
	<code>prevpl</code>	Display the previous 3D plane (M)

plt2Darg **Plot 2D arguments (P)**

Applicability: Liquids

Description: Specifies options for contours and 1D projections on 2D plots, used by the `plot2D` macro. The plot options are selected on the Defaults page in the Acquire folder for most 2D sequences.

Related: `plot2D` Plot 2D spectra (M)

plttext **Plot text file (M)**

Syntax: `plttext(<file><,x<,y<,width>>>)>`
`<:$x_next,$y_next,$y_increment>`

Description: Plots a text file.

Arguments: `file` is the name of a text file. The default is the current experiment text file.
`x` and `y` are coordinates, in mm, of the first line of text. This positions the location of the output. The default is the upper left-hand corner of the page.
`width` is the maximum column text width, in characters. `plttext` uses a word wrap to make the text fit into the width specified.
`$x_next` and `$y_next` are the coordinates where the start of the next line would have been plotting. This is useful for subsequent character plotting.
`$y_increment` is the vertical increment between lines.

Examples: `plttext`
`plttext(wcmax-70)`
`plttext(userdir+'/exp3/text')`
`plttext(100,100)`
`plttext(userdir+'/exp4/text',200,200,24)`
`plttext:$x,$y,$dy`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dtext</code>	Display a text file in the graphics window (C)
	<code>ptext</code>	Print out a text file (M)
	<code>text</code>	Display text or set new text for current experiment (C)
	<code>userdir</code>	User directory (P)

pltmod **Plotter display mode (P)**

Description: Controls plotting of a proton, carbon, or phosphorus spectrum.

Values: `'off'` sets no plotting.
`'fixed'` takes `sp` and `wp` as is.
`'full'` adjusts `sp` and `wp` to plot the full spectrum.

'variable' adjusts `sp` and `wp` to plot only the region of interest.

See also: *NMR Spectroscopy User Guide*

Related:	<code>plc</code>	Plot carbon spectrum (M)
	<code>plh</code>	Plot proton spectrum (M)
	<code>plp</code>	Plot phosphorus spectrum (M)
	<code>sp</code>	Start plot (P)
	<code>wp</code>	Width of plot (P)

plvast Plot VAST data in a stacked 1D-NMR matrix format (M)

Applicability: Systems with the VAST accessory.

Syntax: `plvast<(display order, number of columns plotted)>`

Description: `plvast` arranges and plots the traces from a reconstructed 2D data set (see `vastglue`) as an array of 1D spectra in a convenient format (as a matrix of 1D spectra). If no arguments are provided, the number of rows and columns are determined by the periodicity of the display order. For example, if a block of 96 spectra, as is typical for a microtiter-plate, have been acquired using VAST automation, the spectra is plotted in a matrix 8 rows and 12 columns.

The default is to plot the spectra from 1 through `arraydim` (the number of spectra in the 2D data set). An optional argument (`plvast (##)`) allows one to specify that only spectra from 1 through `##` should be plotted.

Arguments: `display order` is optional and its default value is the glue order as listed in `glueorderarray`.

`number of columns plotted`. The default value of is deduced by examining the periodicity of the requested display order. The `number of columns plotted` can entered as the second argument or as the first argument if the default `display order` is used.

Examples: `plvast`
`plvast(12)`
`plvast('glue_file', 4)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dsast2d</code>	Display VAST data in a pseudo-2D format (M)
	<code>dsvast</code>	Display VAST data in a stacked 1D-NMR matrix (M)
	<code>plvast2d</code>	Plot VAST data in a pseudo-2D format (M)
	<code>plate_glue</code>	define a display order (U)

plvast2d Plot VAST data in a stacked pseudo-2D format (M)

Applicability: Systems with the VAST accessory.

Syntax: `plvast2d<(number)>`

Description: If an array of 1D spectra have been acquired (in particular if a block of 96 spectra has been acquired using VAST automation, especially in a microtiter-plate format) and if these spectra have been glued into a reconstructed 2D dataset (see `vastglue`), `plvast2d` will arrange and plot them (on the plotter) in a convenient pseudo-2D format (almost like an LC-NMR chromatogram). Well labels are not attached to the spectra and spectra are plotted with 12 spectra per row.

Arguments: `number` specifies that only spectra from 1 through `number` should be plotted. The default is to plot all the spectra (from 1 through `arraydim`).

See also: *NMR Spectroscopy User Guide*

Related:	dsast2d	Display VAST data in a pseudo-2D format (M)
	dsvast	Display VAST data in a stacked 1D-NMR matrix (M)
	plvast	Plot VAST data in a stacked 1D-NMR matrix (M)

plww **Plot spectra in whitewash mode (C)**

Syntax: `plww<(start,finish,step><,'all'>>`

Description: Plots one or more spectra in whitewash mode (after the first spectra, each spectra is blanked out in regions in which it is behind an earlier spectra).

Arguments: **start** — index of the first spectra when plotting multiple spectra. It is also the index number of a particular trace to be plotted when plotting arrayed 1D spectra or 2D spectra. The default is to plot all spectra.

finish — index of the last spectra when plotting multiple spectra.

step — increment for the spectral index when plotting multiple spectra, default is 1.

'all' — (default) keyword to plot all spectra in the array.

See also: *NMR Spectroscopy User Guide*

Related:	dss	Display stacked spectra (C)
	dsww	Display spectra in whitewash mode (C)
	pl	Plot spectra (C)

pmode **Processing mode for 2D data (P)**

Description: Specifies the type of 2D spectral data that the 2D Fourier transform (FT) will yield. **pmode** is in the processing group.

Values: **' '** (null string, shown by two single quotes with no space in between) specifies a processing mode in which it is not possible to change either the f_2 or f_1 display mode after the 2D FT. If the f_2 display mode has been set to phased (**dmg**= 'ph'), each f_2 spectrum is phase rotated using the phase constants **rp** and **lp** prior to the FT along the second dimension. If the f_2 display mode has been set to power (**dmg**= 'pwr') or absolute-value (**dmg**= 'av'), however, the f_2 spectrum is not processed any further after the first FT. The complex t_1 interferograms are handled in a similar manner. If the f_1 display mode has been set to phased (**dmg1**= 'ph1'), each f_1 spectrum is phased using the phase constants **rp1** and **lp1**. If the display mode has been set to power (**dmg1**= 'pwr1') or to absolute value (**dmg1**= 'av1'), the appropriate magnitude calculation is performed, with the result being placed in the real part of the appropriate complex datum and a 0 being placed in the imaginary part. At the end of the 2D transform, the spectral data file `datdir/data` is reduced from complex data to real data ("VnmrJ REDUCE" display message).

'partial' specifies a processing mode in which it is not possible to change the f_2 display mode after the 2D FT. It is possible, however, to select between the three f_1 display modes without having to reprocess the 2D data. If the f_2 display mode has been set to phased (**dmg**= 'ph'), each f_2 spectrum is phase rotated using the phase constants **rp** and **lp** prior to FT along the second dimension. If the f_2 display mode is set to power (**dmg**= 'pwr') or absolute value (**dmg**= 'av'), the f_2 spectrum is not processed any further after the first FT. Regardless of the requested f_1 display mode, no further processing is performed by **ft2d** on the f_1 spectra after the second FT. The calculations on 2D spectral data necessary to achieve the requested f_1 display mode are performed by **dcon** or **dconi**. If **pmode** does not exist, it is assigned a value of **'partial'** internal to VnmrJ.

'full' specifies a processing mode in which it is possible to select between the three display modes for each dimension without having to reprocess the 2D data. Regardless of any requested display mode, no display mode processing is performed by **ft2d** on the f_2 spectra after the first or second FT.

The hypercomplex data structure for the 2D time domain data is:

$$\{ \text{Re}(t_1) \text{Re}(t_2), \text{Re}(t_1) \text{Im}(t_2), \text{Im}(t_1) \text{Re}(t_2), \\ \text{Im}(t_1) \text{Im}(t_2) \}$$

and is experimentally composed by the pulse sequence generation arraying mechanism. The hypercomplex data structure for the t_1 interferograms is:

$$\{ \text{Re}(t_1) \text{Re}(F_2), \text{Re}(t_1) \text{Im}(F_2), \text{Im}(t_1) \text{Re}(F_2), \\ \text{Im}(t_1) \text{Im}(F_2) \}$$

where Re represents the real part and Im represents the imaginary part. A hypercomplex FT along t_1 yields a hypercomplex 2D spectrum with the following data structure per hypercomplex point:

$$\{ \text{Re}(F_1) \text{Re}(F_2), \text{Re}(F_1) \text{Im}(F_2), \text{Im}(F_1) \text{Re}(F_2), \\ \text{Im}(F_1) \text{Im}(F_2) \}$$

Note that if `pmode='full'`, the **ft2d** program will require an array index or coefficients for the construction of the t_1 interferograms.

See also: *NMR Spectroscopy User Guide*

Related:	av	Set abs. value mode in directly detected dimension (C)
	av1	Set abs. value mode in 1st indirectly detected dimension (C)
	dcon	Display noninteractive color intensity map (C)
	dconi	Interactive 2D data display (C)
	dmg	Data display mode in directly detected dimension (P)
	dmg1	Data display mode in 1st indirectly detected dimension (P)
	ft1d	Fourier transform along f_2 dimension (C)
	ft2d	Fourier transform 2D data (C)
	ph	Set phased mode in directly detected dimension (C)
	ph1	Set phased mode in indirectly detected dimension (C)
	pwr	Set power mode in directly detected dimension (C)
	pwr1	Set power mode in 1st indirectly detected dimension (C)
	wft1d	Weight and Fourier transform 2D data (C)
	wft2d	Weight and Fourier transform 2D data (C)

poly0 **Display mean of the data in regression.inp file (M)**

Description: Calculates and displays the mean of data in the file `regression.inp`.

See also: *User Programming*

Related:	averag	Calculate average and standard deviation of input (C)
	expl	Display exponential or polynomial curves (C)

pp **Decoupler pulse length (P)**

Description: Sets the decoupler pulse length for use by pulse sequences such as DEPT, HET2DJ, and HETCOR.

See also: *NMR Spectroscopy User Guide*

Related:	AC1-AC9	Automatic calibration (M)
	Dept	Set up parameters for DEPT experiment
	dhp	Decoupler high-power control with class C amplifier (P)
	dpwr	Power level for first decoupler with linear amplifier (P)
	hetcor	Set up parameters for HETCOR pulse sequence (M)

`p1` First pulse width (P)
`pw` Pulse width (P)

ppa Plot a parameter list in plain English (M)

Syntax: `ppa<(x<,y>)>`

Description: Plots parameters in plain English (instead of in a table with parameter names and their values as plotted by the parameter `pap`).

Arguments: `x` controls the `x` offset, in mm, from the lower left of the plot to the starting position (upper left) of the parameter list. The default is a preset position on the page (upper left corner).

`y` controls the `y` offset, in mm, from the lower left of the plot to the starting position (upper left) of the parameter list. Default is a preset position on the page (upper left corner).

Examples: `ppa`
`ppa(10)`
`ppa(wcmax-80,wc2max*.9)`

See also: *NMR Spectroscopy User Guide*

Related: `bpa` Plot boxed parameters (M)
`hpa` Plot parameters on special preprinted chart paper (C)
`pap` Plot out “all” parameters (C)
`plttext` Plot a text file (M)

ppcal Proton decoupler pulse calibration (M)

Description: Proton decoupler pulse calibration for DEPT, HETCOR, INEPT, etc.

See also: *NMR Spectroscopy User Guide*

Related: `AC1S-AC11S` Automatic calibration (M)
`d2pul` Set up parameters for D2PUL pulse sequence (M)
`Dept` Set up parameters for DEPT experiment
`hetcor` Set up parameters for HETCOR pulse sequence (M)
`inept` Set up parameters for INEPT pulse sequence (M)

ppf Plot peak frequencies over spectrum (C)

Syntax: (1) `ppf<(<'noll'><,'pos'><,noise_mult><,'top'>)>`
(2) `ppf<(<'noll'><,'pos'><,noise_mult><,'leader'><,length>)>`

Description: Plots peak frequencies, in units specified by the `axis` parameter, in the plotter device. Only those peaks greater than `th` high are selected. Two basic modes of label positioning are available: labels placed at the top, with long “leaders” extending down to the tops of the lines (syntax 1 using the `'top'` keyword), or labels positioned just above each peak, with short leaders (syntax 2 using the `'leader'` keyword). The default is short leaders.

Arguments: `'noll'` is a keyword to plot frequencies using the last previous line listing.

`'pos'` is a keyword to plot positive peaks only (`'noneg'` is the same as `'pos'`).

`noise_mult` is a numerical value that determines the number of noise peaks plotted for broad, noisy peaks. The default is 3. A smaller value results in more peaks, a larger value results in fewer peaks, and a value of 0.0 results in a line listing containing all peaks above the threshold `th`. Negative values of

`noise_mult` default to 3. The `noise_mult` argument is inactive when the `'noll'` keyword is specified.

`'top'` is a keyword to plot labels at the top with long leaders. In this mode, the height of labels is varied by changing the parameter `wc2`.

`'leader'` is a keyword to plot labels positioned just above each peak with short leaders.

`length` specifies the leader length, in mm, if labels are positioned just above each peak. The default length is 20 mm.

Examples: `ppf('pos')`
`ppf('leader',30)`
`ppf('top','noll')`
`ppf('pos',0.0,'leader',30)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>axis</code>	Axis label for displays and plots (P)
	<code>dpf</code>	Display peak frequencies over spectrum (C)
	<code>dpir</code>	Display integral amplitudes below spectrum (C)
	<code>dpirn</code>	Display normalized integral amplitudes below spectrum (M)
	<code>pir</code>	Plot integral amplitudes below spectrum (C)
	<code>pirn</code>	Plot normalized integral amplitudes below spectrum (M)
	<code>th</code>	Threshold (P)

pph **Print pulse header (M)**

Syntax: `pph(file)`

Description: Prints out the shape file header (i.e., all lines starting with #).

Arguments: `file` is the name of the shape file, including the extension.

Examples: `pph('shgrad.GRD')`

See also: *NMR Spectroscopy User Guide*

Related: `Pbox` Pulse shaping software (U)

ppmm **Resolution on printers and plotters (P)**

Description: An internal software parameter, selected automatically based on the plotter configuration, that contains the resolution in dots/mm on raster graphics printers. On pen plotters, `ppmm` contains the resolution of points drawn. On PostScript printers, `ppmm` adjusts linewidths.

pprofile **Plot pulse excitation profile (M)**

Syntax: `pprofile<(axisflag<,profile<,shapefile>>)>`

Description: Plots the X, Y and Z excitation (inversion) profile for a pulse shape that has been generated with the `Pbox` software. If shape names is not provided, the last simulation data stored in the `shapelib/pbox.sim` file are plotted.

Arguments: The `axisflag` and `profile` arguments can be given in any order.

`axisflag` is 'y' to display the full spectrum and a frequency scale, or 'n' to suppress the scale and spectrum. The default is 'n'.

`profile` is a character string identifying the desired profile. 'xyz' selects X, Y, and Z (inversion) profiles; 'xy' selects only the excitation (transverse) profiles; 'x' selects only the X transverse excitation profile; and 'z' selects only the inversion profile. The default is 'xyz'.

`shapefile` is the name of a *.RF or *.DEC file, including the extension.

P

Examples: `pprofile`
`pprofile('y','x')`
`pprofile('xy','n','softpls.RF')`

See also: *NMR Spectroscopy User Guide*

Related: `dprofile` Display pulse excitation profile (M)
`Pbox` Pulse shaping software (U)

pps Plot pulse sequence (C)

Syntax: `pps<(file<,x,y,width,height)>>`

Description: Plots pulse sequences. The plotted picture consists of three to five parts. At the top is the transmitter pulse sequence. Below that is the decoupler pulse sequence. Next is the second decoupler pulse sequence or gradients, depending on the program. At the bottom is the status.

The parameter of each pulse is plotted if its length is less than 30 letters. The value of each pulse is also plotted. If its value is less than zero, a question mark “?” is plotted. The time units are displayed as letters (s, m, or u). The height of pulses are plotted according to their power level.

Arguments: `file` specifies the pulse sequence to be plotted. The default is `seqfil`.

`x, y` specifies the start of the plotting position with respect to the lower-left corner of the plotter.

`width, height` are in proportion to `wcmax` and `wc2max`.

Examples: `pps`
`pps('s2pul')`
`pps(3,50)`

See also: *NMR Spectroscopy User Guide*

Related: `dps` Display pulse sequence (C)
`seqfil` Pulse sequence name (P)
`wcmax` Maximum width of chart (P)
`wc2max` Maximum width of chart in second direction (P)

prealfa Specify a delay for longer ring down (P)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Specify a delay to be used in situations when there is a longer ring down of rf following the last rf pulse.

This parameter is only active when `qcomp='y'`. `prealfa` should be created as a local parameter of type `pulse` or `delay`. This parameter must be created as a local parameter of the type `pulse` for SpinCad Sequences.

If it is desired to use the software computed value for this delay, destroy the `prealfa` parameter.

Values: User set `prealfa` value that may be slightly adjusted by the software to better optimize the DSP parameters.

prep Run prepare acquisition macro (M)

Applicability: Imaging

Description: Run the prepare acquisition macro specified by the `execprep` parameter. Usually only called from panels.

Related: `execprep` Execute prepare macro (P)

Presat Set up parameters for presat ¹H experiment (M)

Description: Set up parameters for presat ¹H experiment with solvent suppression.

prevpl Display the previous 3D plane (M)

Description: Displays 2D color map of the previous 3D plane in the set of planes defined by the parameters `plane` and `path3d`. For example, if `dplane(40)` has just been executed, `prevpl` results in the display of 3D plane 39 of that set. (If `prevpl` immediately follows the command `dproj`, an error results because there is no 3D plane whose number is -1.) `prevpl` is more efficient than `dplane` or `dproj` because the 3D parameter set (`procp3d`) is not loaded into VnmrJ. It is assumed to have already been loaded by, for example, `dplane` or `dproj`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dplane</code>	Display a 3D plane (M)
	<code>dproj</code>	Display a 3D plane projection (M)
	<code>dsplanes</code>	Display a series of 3D planes (M)
	<code>getplane</code>	Extract planes from a 3D spectral data set (M)
	<code>nextpl</code>	Display the next 3D plane (M)
	<code>path3d</code>	Path to currently displayed 2D planes from a 3D data set (P)
	<code>plane</code>	Currently displayed 3D plane type (P)
	<code>plplanes</code>	Plot a series of 3D planes (M)

prescan Study queue prescan (P)

Description: This parameter keeps track of the type and status of the prescans in the study queue.

Related:	<code>cqexp</code>	Load experiment from protocol (M)
	<code>cqrset</code>	Reset study queue parameters (M)
	<code>sqexp</code>	Load experiment from protocol (M)
	<code>sqreset</code>	Reset study queue parameters for imaging (M)

prescan_CoilTableRead or update the CoilTable File (M)

Syntax: `prescan_CoilTable(action, rfcoil)`

Description: Manages the CoilTable file in `~/vnmrsys`. Reads information about `rfcoil` into the global parameter `coil_param`; updates/adds information for `rfcoil` from `coil_param`; removes the `rfcoil` entry from CoilTable.

Arguments: actions for the specified `rfcoil` are:

```
read
add
update
remove
```

Examples: `prescan_CoilTable('read', 'main')`

prescan_tn Return tn string for a given atomic number (M)

Syntax: `prescan_tn(number):str`

Description: Returns `tn` string for a given atomic number; for H1, C13, F19, P31, Na23, Xe129 only.

Arguments: Number is the atomic number.

P

`str` is a string that can be assigned to `tn`.

Examples: `prescan_tn(23):tn`

printer **Printer device (P)**

Description: Selects the printer in use on the system.

Values: A string with entries such as 'ThinkJet_96', 'LaserJet_300', 'jim', 'varian1', and 'Laser1'.

See also: *NMR Spectroscopy User Guide*

Related: [showplotter](#) Show list of currently defined plotters and printers (M)

printfile **Path to the print-to-file image (P)**

Description: Defines the path where an image is saved if it is printed to a file.

printformat **Format of saved-to-file image (P)**

Description: The format of the image to be printed to a file.

Values: 'jpeg', 'gif', 'tiff', 'bmp'

printlayout **Layout of printed image (P)**

Description: The layout of the printed image.

Values: 'portrait' or 'layout'

printoff **Stop sending text to printer and start print operation (C)**

Syntax: `printoff<('clear'|file)>`

Description: Stops redirection of output to printer caused by the [printon](#) command and starts the print operation. **The command `printoff` must be entered to obtain output on the printer.** Actual printing is controlled by the [vnmrprint](#) script in the `bin` subdirectory of the system directory. `printoff` can also clear the data in the current print file or save data to a specified file name (i.e., print or plot to a file).

Arguments: 'clear' is a keyword to clear the print file made so far.

`file` specifies the name of a file to save the printout. If the file already exists, it is overwritten.

Examples: `printoff`
`printoff('clear')`
`printoff('vnmrsys/papers/peaks.list')`

See also: *NMR Spectroscopy User Guide*

Related: [printon](#) Direct text output to printer (C)
[vnmrprint](#) Print text files (U)

printon **Direct text output to printer (C)**

Description: Sends information to the printer that is normally displayed in the text window. After using `printon`, output from commands that use the text window, such as [dg](#) and [cat](#), is sent to the printer and does not appear on the screen. The value of the parameter [printer](#) is used to select which printer is used.

See also: *NMR Spectroscopy User Guide*

Related: `cat` Output one or more files to output text window (C)
`dg` Display group of acquisition/processing parameters (C)
`printer` Printer device (P)
`printoff` Stop sending text to printer and start print operation (C)

printregion Screen region to be printed (P)

Description: The region of the screen to be printed or saved to a file.

Values: `'vnmrj'` -- entire VnmrJ interface.
`'graphics'` -- the graphics area of the VnmrJ interface.
`'frames'` -- selected frames from the graphics area.

printsize Size of printed image (P)

Description: The size of the printed image.

Values: `'quarterpage'`, `'halfpage'`, `'page'`

printsend Defines where image will print (P)

Description: Defines whether the selected image will sent to a file or a printer.

Values: `'file'` or `'printer'`

probe Probe type (P)

Description: Contains a string with the name of the probe currently in the magnet. This parameter is set automatically when the `addprobe` macro is entered. The `getparam` and `setparams` macros use `probe` to retrieve and write parameters into the current probe file.

See also: *NMR Spectroscopy User Guide*

Related: `addnucleus` Add new nucleus to existing probe file (M)
`addprobe` Create new probe directory and probe file (M)
`getparam` Receive parameter from probe file (M)
`setparams` Write parameter to current probe file (M)

probeConnect Specify which nucleus can be acquired on each RF channel (P)

Applicability: VNMRS and 400 MR

Syntax: `probeConnect = 'nucl nuc2 nuc3...'`

Description: Global string parameter that does not exist by default. If present, PSG uses it to determine which RF channel to connect to a given nucleus. The string consists of a series of space-separated nuclei. A nucleus 'X' may be used only once in the string to match any nucleus. The parameter must match the hardware connections. If the parameter does not match the hardware connections or does not exist, default settings are used. Default settings are to use the first channel for `tn` for high band observe, and the second channel for `tn` for low band observe.

Values: Any nucleus name used for `tn`, or 'X'.

Examples: `create('probeConnect','string','global')`
`probeConnect = 'H1 C13'` maps H1 to channel 1, C13 to channel 2
`probeConnect = 'H1 P31 X'` maps H1 to channel 1, P31 to channel 2, any nucleus to channel 3.

See also: *VnmrJ User Programming*

Related:	<code>tn</code>	Nucleus for observe transmitter (P)
	<code>dm</code>	Nucleus for first decoupler (P)
	<code>dm2</code>	Nucleus for second decoupler (P)
	<code>dm3</code>	Nucleus for third decoupler (P)

Probe_edit Edit probe for specific nucleus (U)

Syntax: (UNIX) `Probe_edit probe nucleus`

Description: Opens a dialog box showing all the parameters related to a specific nucleus from the probe table.

Arguments: `probe` is the name of the probe.
`nucleus` is the specified nucleus from the probe table.

Examples: `Probe_edit 5mmSW H1`

Related: `probe_edit` Edit probe for specific nucleus (M)

probe_edit Edit probe for specific nucleus (M)

Syntax: `probe_edit (probe, nucleus)`

Description: Opens a dialog box showing all the parameters related to a specific nucleus from the probe table.

Arguments: `probe` is the name of the probe.
`nucleus` is the specified nucleus from the probe table.

Examples: `probe_edit ('5mmSW', 'H1')`
`probe_edit (probe, tn)`

Related: `Probe_edit` Edit probe for a specific nucleus (U)

probe_protectionProbe protection control (P)

Description: Controls the power check for probe protection.

See also: *NMR Spectroscopy User Guide*

proc Type of processing on np FID (P)

Description: Specifies the type of data processing to be performed upon the `np` (t_2) FID. Similarly, parameters `proc1` and `proc2` specify the type of data processing on the `ni` (t_1) and `ni2` interferograms, respectively.

All Varian data must be processed along `np` with a complex Fourier transform (FT). Sequentially sampled Bruker data (the usual case) must be processed along this dimension with a real FT, while simultaneously sampled Bruker data must be processed with a complex FT.

Pure absorptive 2D data collected by the States-Haberhorn (hypercomplex) method must be processed along `ni` or `ni2` with a complex FT.

Pure absorptive 2D data collected by the TPPI method on a Varian spectrometer can be processed in one of two ways, depending upon how the data was collected:

`phase=3` Complex FT, i.e., `proc1='ft'` (standard way)
`phase=1,4` Real FT, i.e., `proc1='rft'` (new way)
`phase2=3` Complex FT, i.e., `proc2='ft'`
`phase2=1,4` Real FT, i.e., `proc2='rft'`

Pure absorptive 2D data collected by TPPI method on a Bruker spectrometer must be processed along `ni` with a real FT (i.e., `proc1='rft'`).

Values: `'ft'` specifies complex FT data processing.

`'rft'` specifies real FT data processing.

`'lp'` specifies linear prediction processing on complex data. If `'lp'` is selected, additional parameters must be set to fully define how the time-domain data is to be processed; see the description of the `addpar` command.

See also: *NMR Spectroscopy User Guide*

Related:

<code>addpar</code>	Add selected parameters to the current experiment (M)
<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
<code>np</code>	Number of data points (P)
<code>parlp</code>	Create parameters for linear prediction (C)
<code>phase</code>	Phase selection (P)
<code>phase2</code>	Phase selection for 3D acquisition (P)
<code>proc1</code>	Type of processing on <code>ni</code> interferogram (P)
<code>proc2</code>	Type of processing on <code>ni2</code> interferogram (P)

proc1 Type of processing on ni interferogram (P)

Description: Specifies the type of data processing to be performed upon the `ni` (`t1`) interferogram (2D). Refer to the description of `proc` for further information.

Values: `'ft'` specifies complex Fourier transform (FT) data processing.

`'rft'` specifies real FT data processing.

`'lp'` specifies linear prediction processing on complex data. If `'lp'` is selected, additional parameters must be set to fully define how the time-domain data is to be processed; see the description of the `addpar` command.

`'ht'` specifies Hadamard transform processing. If `'ht'` is selected, additional parameters must be set with the `addpar` command. In addition, the data set must be acquired using a Hadamard pulse sequence.

See also: *NMR Spectroscopy User Guide*

Related:

<code>addpar</code>	Add selected parameters to the current experiment (M)
<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
<code>proc</code>	Type of processing on <code>np</code> FID (P)

proc1d Processing macro for simple (non-arrayed) 1D spectra (M)

Description: A generic macro for processing non-arrayed 1D spectra using a set of standard macros. `proc1d` is called by the `procplot` macro, but can also be used directly. `proc1d` first tries to find a macro of the form `{tn}p` with the name of the observe nucleus in lower case (e.g., `h1p`, `c13p`). If such a macro exists, it is called. If such a nucleus-specific macro is not found in the command path, minimal 1D processing is performed (the intent is to provide a well-processed spectrum in most cases): Fourier transformation (using pre-set weighting functions), automatic phasing (`aphx` macro), automatic integration (`integrate` macro), vertical scale adjustment (`vsadj` macro), avoiding excessive noise (`noislm` macro), and threshold adjustment (`thadj` macro).

`proc1d` does not work with arrayed 1D spectra: use `deptproc` (for DEPT-type spectra) or `procarrray` (for all other arrayed 1D data).

See also: *NMR Spectroscopy User Guide*

Related:	<code>aphx</code>	Perform optimized automatic phasing (M)
	<code>c13p</code>	Process 1D carbon spectra (M)
	<code>deptproc</code>	Process arrayed dept type spectra (M)
	<code>h1p</code>	Process 1D proton spectra (M)
	<code>integrate</code>	Automatically integrate 1D spectrum (M)
	<code>noislm</code>	Avoids excessive noise (M)
	<code>procarrray</code>	Process arrayed 1D spectra (M)
	<code>procplot</code>	Automatically process FIDs (M)
	<code>thadj</code>	Adjust threshold (M)
	<code>vsadj</code>	Adjust vertical scale (M)

proc2 Type of processing on ni2 interferogram (P)

Description: Specifies the type of data processing to be performed upon the `ni2` interferogram (3D). Refer to the description of `proc` for further information.

Values: `'ft'` specifies complex Fourier transform (FT) data processing.
`'rft'` specifies real FT data processing.
`'lp'` specifies linear prediction processing on complex data. If `'lp'` is selected, additional parameters must be set to fully define how the time-domain data is to be processed; see the description of the `addpar` command.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)
	<code>proc</code>	Type of processing on np FID (P)

proc2d Process 2D spectra (M)

Description: A general 2D processing macro that tries to do the appropriate processing for as many types of 2D experiments as possible. It uses `wft2da` for phase-sensitive spectra, `wft2d` for absolute-value 2D spectra, `wft2d('ptype')` for HOM2DJ and COSYPS (absolute value). Symmetric homonuclear correlation spectra (`fn=fn1`, `sw=sw1`) in absolute-value mode is symmetrized using `foldt`. The resulting spectrum is then normalized (adjustment of `vs` and `th`) using `nm2d` and displayed (if not in background mode). `proc2d` is called as part of the `procplot` macro, but can also be used directly by the user.

See also: *NMR Spectroscopy User Guide*

Related:	<code>fn</code>	Fourier number in the directly detected dimension (P)
	<code>fn1</code>	Fourier number in 1st indirectly detected dimension (P)
	<code>foldt</code>	Fold COSY-like spectrum along diagonal axis (C)
	<code>nm2d</code>	Normalize intensity of 2D spectrum (M)
	<code>procplot</code>	Automatically process FIDs (M)
	<code>sw</code>	Spectral width in the directly detected dimension (P)
	<code>sw1</code>	Spectral width in the 1st indirectly detected dimension (P)
	<code>th</code>	Threshold (P)
	<code>vs</code>	Vertical scale (P)
	<code>wft2d</code>	Weight and Fourier transform 2D data (C)
	<code>wft2da</code>	Weight and Fourier transform for pure absorption 2D data (M)

procarrray Process arrayed 1D spectra (M)

Description: A generic macro for processing arrayed 1D data. It is called within the **procplot** macro, but can also be called directly. It transforms all traces, phase the trace with the largest signal, scale the traces appropriately, and set up the display parameters such that the data can be plotted directly. The plotting is done in a separate macro **plarray** that is also called in the **procplot** macro.

For the display setup, **procarrray** distinguishes between arrays with 6 or less elements, which are stacked vertically (no horizontal offset), and spectra with greater than 6 elements, which are stacked horizontally by default, unless there are too many lines, in which case a diagonally stacked display is chosen.

Horizontal stacking is mostly adequate for pulse and power calibrations, where there are usually only a few lines. Diagonally stacked displays and plots are frequently chosen for T_1 and T_2 experiments on entire spectra, often with many lines. The automatic stacking mode can be overridden by creating and setting a string parameter **stackmode** in the startup macro, or before calling **procplot** or **procarrray**. Possible values for **stackmode** are 'horizontal', 'vertical', and 'diagonal'. DEPT-type spectra can, in principle, be also processed with **procarrray** but, of course, no DEPT editing occurs.

See also: *NMR Spectroscopy User Guide*

Related:	deptproc	Process arrayed dept type spectra (M)
	plarray	Plot arrayed 1D spectra (M)
	proc1d	Processing macro for simple (non-arrayed) 1D spectra (M)
	procplot	Automatically process FIDs (M)
	stack	Set stacking control parameter (M)
	stackmode	Stack control for processing arrayed 1D spectra (P)

process Generic automatic processing (M)

Description: Processes a wide range of data types. If the **apptype** parameter is set, it runs the **execprocess** macro if it exists. If the **apptype** parameter is not set it selects a macro depending on the type of data. For simple 1D spectra, **process** looks for a macro of form {**tn**}**p** with the observe nucleus in lower case (e.g., **h1p**, **c13p**, **f19p**). If no such macro is found, **process** calls **proc1d**, a generic processing macro for 1D spectra. For DEPT type data, **deptproc** is called. For other arrays of 1D spectra, **procarrray** is called. For 2D spectra, **proc2d** is called. **process** by itself is called within the **procplot** macro.

See also: *NMR Spectroscopy User Guide*

Related:	apptype	Application type (P)
	c13p	Processing of 1D carbon spectra (M)
	deptproc	Process array of DEPT spectra (M)
	execpars	Set up the exec parameters (M)
	execprocess	Execute processing macro (P)
	f19p	Processing of 1D fluorine spectra (M)
	h1p	Processing of 1D proton spectra (M)
	proc1d	Automatically process non-arrayed 1D fids (M)
	proc2d	Process 2D spectra (M)
	procarrray	Process arrayed 1D spectra (M)
	procplot	Automatically process FIDs (M)
	tn	Nucleus for observe transmitter (P)

procplot Automatically process FIDs (M)

Syntax: **procplot**<(pltmod_value)>

Description: Universal FID processing macro called usually with `wexp='procplot'` by automatic acquisition macros such as `h1`, `c13`, `hcap`, and `hcosy`. The purpose of `procplot` is not the data processing itself, but rather the selection of the appropriate processing macro for a given data set.

First, `procplot` calls a macro `process` that calculates spectra; that macro by itself then selects an appropriate processing macro, like `proc1d` for non-arrayed 1D spectra. Depending whether the parameter `pltmod` is set to 'none' or not, `procplot` then calls `plot`, a universal plotting macro. The setting of the parameter `pltmod` can be temporarily overridden by specifying an alternative value as argument to `procplot`.

One of the concepts behind `procplot` is that the user should never have to modify any processing macro for customizing the processing or the output of automatic experiments or processing; this outcome can happen by selecting a parameter in the calling macro or before calling `procplot`.

Arguments: `pltmod_value` is an alternate value for the parameter `pltmod` that is only used for the current call. The values 'none' and 'off' suppress plotting. The range of possible (active) values for `pltmod_value` depends on the plotting macros. Often, the parameter `pltmod` has no effect other than turning on or off plotting. Note that if only the calculation of a spectrum is desired, it is usually easier to call the `process` macro.

Examples: `procplot`
`procplot('none')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>deptproc</code>	Process arrayed dept type spectra (M)
	<code>plot</code>	Automatically plot spectra (M)
	<code>pltmod</code>	Determine plot mode (P)
	<code>proc1d</code>	Processing macro for simple (non-arrayed) 1D spectra (M)
	<code>proc2d</code>	Process 2D spectra (M)
	<code>procarray</code>	Process arrayed 1D spectra (M)
	<code>process</code>	Automatically calculate spectra (M)

profile **Set up pulse sequence for gradient calibration (M)**

Applicability: Systems with the pulsed field gradients (PFG) module.

Description: Performs an rf and gradient echo sequence that gives a high quality profile of the sample. This sequence is used with the macro `setgcal` to provide gradient strength calibration.

See also: *Perform a Pulsed Field Gradient Module Installation; Pulsed Field Gradient Modules Installation; User Programming*

Related:	<code>gcal</code>	Gradient calibration constant (P)
	<code>setgcal</code>	Calibrate gradient strength from measured data (M)

proj **Project 2D data (C)**

Syntax: `proj (exp_number<, 'sum'><, start<, width>>)`

Description: Projects 2D data onto the axis parallel to the screen x-axis, which can be f_1 or f_2 , depending upon the parameter `trace`. Two projections are available:

- *Summing projection.* The data at each frequency are summed and the result becomes the projection.
- *Skyline projection.* The data are searched and the maximum intensity at any given frequency becomes the intensity in the projection (similar to looking

at the skyline of a city where only the largest building along any given line of sight is visible).

Phase-sensitive data can be projected, but the resulting projection can only be displayed in an absolute-value mode

Arguments: `exp_number` is the number of the experiment, from 1 through 9, in which the resulting spectrum is stored.

'sum' is a keyword to use the summing projection. The default is skyline.

`start` defines the starting trace, in Hz. The default is to project all data.

`width` defines the width of the traces, in Hz, to be projected. The default is to project all data. If `width` is supplied as zero, a single trace corresponding to the start frequency will be stored.

Examples: `proj(3)`
`proj(5, 'sum')`
`proj(4, 3*sfrq, 6*sfrq)`

See also: *NMR Spectroscopy User Guide*

Related: [trace](#) Select mode for 2D data display (P)

Proton **Set up parameters for ^1H experiment (M)**

Description: Set up parameters for ^1H experiment.

protune **Macro to start ProTune (M)**

Applicability: Liquids, Walkup, Automation

Syntax: `protune(freq1 <, match1 <, freq2 <, match2>>>)`
`protune('argument', <$nucleus, <$target>>)`
`protune('exec', command1 <, command2, ...)`

Description: Tunes to frequency `freq1` MHz if the first argument is the frequency in MHz. Executes a sequence of arbitrary tuning commands if the first argument is the keyword `exec`. Any command that can be typed into the command line box in the ProTune GUI display is allowed.

Arguments: First case:

`freq1` MHz — first tuning frequency in MHz

`match1` — % of optimum for the first frequency, 5% is the default

`freq2` MHz — optional second tuning frequency in MHz

`match2` — % of optimum for the second frequency, 5% is the default.

Second case:

'argument' may have the following values:

no argument or 'popup'	opens Tune Probe dialog for probe tuning. Select the nucleus to tune and how coarse to tune using the buttons and menus in the dialog box.
'calibrate'	open ProTune calibration interface.
'nucleus'	tune using specified nucleus – <code>\$nucleus</code> must be specified.

`$nucleus` — Nucleus to tune to, 'H1', 'C13' ...

`$target` — Tune target level, 0.1(finest) to 100 (coarsest), defaults to 5 if no value is specified.

Third case:

`exec` — keyword that precedes a command or string of commands.

Examples: `protune('exec', 'setTuneFrequency 0 599.96e6')`

Tunes the probe to 599.96 MHz.

See also: User Guide Liquids and VnmrJ Walkup

Related:	<code>atune</code>	ProTune present (P)
	<code>protunegui</code>	Macro to start ProTune in graphical user interface (M)
	<code>plockport</code>	Port number to use to lock out multiple ProTune processes (P)
	<code>probeConnect</code>	Specify which nucleus can be tuned on each RF channel (P)
	<code>settune</code>	set up tune parameters for automation
	<code>showprotunegui</code>	show the graphical interface while tuning (P)
	<code>tchan</code>	RF channel number used for tuning (P)
	<code>tugain</code>	Receiver gain used in tuning (P)
	<code>tunehf</code>	Tune both H1 and F19 on an HFX probe (M)
	<code>tunesw</code>	Width of the tuning sweep in Hz (P)
	<code>tunematch</code>	Default match target, in percent of optimum (P)
	<code>tupwr</code>	Transmitter power used in tuning (P)
	<code>tuneResult</code>	Message indicating how well the tuning succeeded (P)
	<code>tunemethod</code>	Method to use for tuning (P)
	<code>wtune</code>	Specify when to tune (P)
	<code>wtunedone</code>	What to do after tuning is done (P)
	<code>xmtune</code>	Check tune parameter during automation (M)

protune **Shell script for start ProTune operation (U)**

Applicability: Automation

Description: Starts and stops ProTune. Usually called from Protune macros.

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `protune` (M) Macro to start ProTune (M)

protunegui **Macro to start ProTune in graphical user interface (M)**

Applicability: Liquids, VnmrJ Walkup, Automation

Syntax: `protune('argument', <$nucleus, <$target>>)`

Description: Starts ProTune in graphical mode.

Arguments: see `protune` (M)

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `protune` Macro to start ProTune (M)

prune **Prune extra parameters from current tree (C)**

Syntax: `prune(file)`

Description: Destroys parameters in the current parameter tree that are not also defined in the supplied parameter file. `prune` is used to remove leftover parameters from previous experimental setups. Recalling a new parameter set into an experiment has a similar effect and, in general, `prune` is not required.

Arguments: `file` is the path of a parameter file.

Examples: `prune(systemdir+'/parlib/cosyps.par/procpar')`
`prune('/vnmr/par400/stdpar/H1.par/procpar')`
`prune(userdir+'/exp3/curpar')`

See also: *User Programming*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>destroy</code>	Destroy a parameter (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>fread</code>	Read parameters from file and load them into a tree (C)
	<code>fsave</code>	Save parameters from a tree to a file (C)

pscale **Plot scale below spectrum or FID (C)**

Syntax: `pscale(<rev><, axis><, label><, vp0><, sp0><, color><, pen>) >`

Description: Plots a scale under a spectrum or FID.

Arguments: `rev` – reverses the direction of the scale. That is, the smaller numbers will be at the left side of the scale. If used, '`rev`' must be the first argument.

`axis` – If the letter `p`, `h`, `k`, etc. is supplied, it will be used instead of the current value of the parameter `axis`. For an FID scale, if the letter `s`, `m`, or `u` is supplied, it will be used instead of the current value of the parameter `axisf`.

`label` – If a string of 2 or more characters is supplied, it will be used as the axis label.

`vp0` – This is supplied as the first real number. It defines the vertical position where the scale is drawn. The default is 5 mm below the current value of the parameter `vp`.

`sp0` – This is supplied as the second real number. It is a modified start of plot. If, for example, the display is from 347 to 447 hz, but the scale is desired to read 0 to 100 hz., `sp0` would be input as 0.

`wp0` – This is supplied as the third real number. It is a modified width of plot. If, for example, the display is from 347 to 447 hz, but the scale is desired to read 0 to 550 Units. `sp0` would be input as 0, `wp0` would be 550, and the label would be 'Units'.

An optional color or pen number can be supplied to `dscale` or `pscale`. The available colors and pens are: '`red`', '`green`', '`blue`', '`cyan`', '`magenta`', '`yellow`', '`black`', '`white`', '`pen1`', '`pen2`', '`pen3`', ..., '`pen8`'

Examples: `pscale`
`pscale(20)`
`pscale('h', 0, 'pen2')`
`pscale('fid', 'm')`
`pscale('h', vp-10, 0)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>axis</code>	Axis label for displays and plots (P)
	<code>axisf</code>	Axis label for FID displays and plots (P)
	<code>dscale</code>	Display scale below spectrum or FID (C)
	<code>vp</code>	Vertical position of spectrum (P)

pseudo **Set default parameters for pseudo-echo weighting (M)**

Syntax: `pseudo(<C1, C2, C3, C4> >`

Description: Generates an initial guess at good weighting parameters for absolute-value 2D experiments. To generate modified guesses, four coefficients are allowed to set the values of the weighting functions.

Arguments: `C1` sets `lb=-0.318/(C1*at)`. The default value of `C1` is 0.0625.

`C2` sets `gf=C2*at`. The default value of `C2` is 0.25.

C3 sets `lb1` = $-0.318 / (C3 * (ni / sw1))$ but is used with 2D experiments only. The default value of C3 is 0.0625.

C4 sets `gf1` = $C4 * (ni / sw1)$ but is used with 2D experiments only. The default value of C4 is 0.25.

Examples: `pseudo`
`pseudo(.1, .4, .2, .5)`

See also: *NMR Spectroscopy User Guide*

Related: `sinebell` Select default parameters for sinebell weighting (M)

psg Display pulse sequence generation errors (M)

Description: Helps identify the problem if, after entering `go` or `su`, etc., the message is returned that pulse sequence generation (PSG) aborted abnormally. Any parameters that are not found are listed. This information is stored in the user's directory (`vnmrsys`) in a text file named `psg.error`. If the message "Maximum communication retries exceeded, Experiment unable to be sent" is displayed, a program communications problem is indicated. Consult the system operator for assistance.

See also: *User Programming*

psggen Compile a user PSG object library (M,U)

Description: A user PSG (pulse sequence generation) kit is supplied that allows editing low-level pulse sequence code. `psggen` compiles these edits so that subsequent pulse sequence generation with the `seqgen` command uses the customized pulse sequence source.

See also: *User Programming*

psgset Set up parameters for various pulse sequences (M)

Syntax: `psgset(file, par1, par2, ..., parN)`

Description: Sets up parameters for various pulse sequences using information in a `parlib` file. Rather than returning the entire parameter file, `psgset` returns the parameters listed. `psgset`, in general, is never entered from the keyboard but is used as part of experiment setup macros.

Arguments: `file` is the file from the user or system `parlib` that provides information on setting up the parameters listed. The parameters `seqfil` and `pslabel` are set to the supplied file name.

`par1, par2, ..., pN` are 1 to 11 parameters to be returned from `parlib`.

Examples: `psgset('cosy', 'dg', 'ap', 'ss', 'd1', 'axis', 'phase')`

See also: *User Programming*

Related: `pslabel` Pulse sequence label (P)
`seqfil` Pulse sequence name (P)

psgupdateon Enable update of acquisition parameters (C)

Description: Permits the interactive updating of acquisition parameters.

See also: *SpinCAD*

Related: `psgupdateoff` Prevent update of acquisition parameters (C)
`updtparam` Update specified acquisition parameters (C)

psgupdateoff Prevent update of acquisition parameters (C)

Description: Prevents the interactive updating of acquisition parameters.

See also: *SpinCAD*

Related: [psgupdateon](#) Enable update of acquisition parameters (C)
[updtparam](#) Update specified acquisition parameters (C)

pshape Plot pulse shape or modulation pattern (M)

Syntax: `pshape<(pattern.ext)>`

Description: Plots the real (X) and imaginary (Y) components of a shaped pulse. Any type of waveform (.RF, .DEC or .GRD) can be plotted.

Arguments: `pattern` is the name of a shape or pattern file specified by an absolute file name, relative file name, or a simple pattern file name. `ext` is a file name extension that specifies the file type. In the case of a simple file name, [dshape](#) searches for the file in the local directory, then in the user's `shapelib`, and finally in the directory `/vnmr/shapelib`. If `pattern.ext` is not given, `pshape` displays the last created waveform stored in the `pbox.fid` file.

Examples: `pshape`
`pshape('my_shape.DEC')`

See also: *NMR Spectroscopy User Guide*

Related: [dshape](#) Display the last created pulse shape (M)
[Pbox](#) Pulse shaping software (U)

pshapef Plot the last created pulse shape (M)

Description: Plots real (X) and imaginary (Y) components of the last created shaped pulse.

See also: *NMR Spectroscopy User Guide*

Related: [dshape](#) Display the last created pulse shape (M)
[Pbox](#) Pulse shaping software (U)

pshr PostScript High Resolution plotting control (P)

Applicability: ALL

Syntax: `pshr=<value>`

Description: Global parameter that controls whether a 1D spectrum is plotted in hi-resolution mode or not. A hi-resolution plot is one in which every data point is represented in the plot. The standard resolution plot determines maximum and minimum values over small regions and plots those. The parameter `pshr` can have the values 1 for hi-res and 0 for standard plot.

Values: 0 for standard resolution
 1 for high resolution.

Related: [pl](#) Plot spectra (C)
[pslw](#) PostScript Line Width control (P)

pslabel Pulse sequence label (P)

Description: Contains the text to be displayed in the `Seq:` field on the top line of the screen. This string may be different from the pulse sequence name selected with [seqfil](#). However, the string in [seqfil](#) is the name of the pulse sequence

searched for when an experiment is started. Generally `seqfil=pslabel`, and when `seqfil` is set, the system sets `pslabel` to the same string.

See also: *NMR Spectroscopy User Guide*

Related: `seqfil` Pulse sequence name (P)

pslw PostScript Line Width control (P)

Applicability: ALL

Syntax: `pslw=<value>`

Description: Global parameter that adjusts the line width of PostScript plots.

Values: 0 (narrowest) to 100 (widest) line width.

Related: `pl` Plot spectra (C)
`pshr` PostScript High Resolution plotting control (P)

pssl Plot Arrayed Numbers (C)

Syntax: `pssl(<options>)`

Description: Plots a label for each element in a set of stacked spectra. The label is an integer value from 1 up to the number of spectra in the display.

Arguments: `options` can be any of the following:

- 'all' is a keyword to display all of the spectra.
- 'int' is a keyword to display only the integral, independently of the value of the parameter `intmod`
- 'top' or 'side' are keywords that cause the spectrum to be displayed either above or at the left edge, respectively, of a contour plot. This assumes that the parameters `sc`, `wc`, `sc2`, and `wc2` are those used to position the contour plot.
- 'dodc' is a keyword for all spectra to be drift corrected independently.
- 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'black', and 'white' are keywords that select a color.
- 'pen1', 'pen2', 'pen2' ... are keywords that pens.
- 'nopars' — prevents the display commands from drawing the parameters at the bottom of the graphics screen.
- 'custom' — uses the parameters `shownumx` (x position) and `shownumy` (y position), counting from bottom left of every spectrum.
- 'reverse' — rotate the text by 90° - useful if the arrayed parameter values are long with respect to the width of the individual sub-spectra.
- 'value' — The values of up to two simultaneous arrays are displayed. Diagonal arrays are allowed. The second parameter is shown in different color). The name of the arrayed parameter(s) is also shown. If used on a one-dimensional array representation of a 2D spectrum, `ni` and `phase` (in case of phase sensitive 2Ds) parameters are shown.
- 'list=xxx' produces a display of the values contained in the arrayed parameter `xxx`.
- 'format=yyy' uses the format `yyy` to control the plot of each label. See the `write` command for information about formats.

Examples: `pssl`
`pssl('top','left')`
`pssl('value','format=%3.1f')`

See also: *NMR Spectroscopy User Guide*

Related: `dssl` Label a display of stacked spectra (M)
`write` Write formatted text to a device (C)

p_{text} Print out a text file (M)

Syntax: `ptext(file)`

Description: Prints out a text file.

Arguments: `file` is the name of the text file.

Examples: `ptext(' /vnmr/maclib/ptext')`
`ptext(curexp+' /dept.out')`

See also: *NMR Spectroscopy User Guide*

Related: `curexp` Current experiment directory (P)
`dtext` Display a text file in the graphics window (C)
`lookup` Look up words and lines from a text file (C)
`pltext` Plot a text file (C)
`text` Display text or set new text for current experiment (C)
`textvi` Edit text file of current experiment (M)
`vi` Edit text file with `vi` text editor (C)

p_{tspec3d} Region-selective 3D processing (P)

Description: Sets whether region-selective 3D processing occurs. If `ptspec3d` does not exist, it is created by the macro `par3d`. `ptspec3d` is functional at this time only for the f_3 dimension. If `ptspec3d`= 'ynn', only the currently displayed region of f_3 is retained as non-zero values after the f_3 transform in the 3D FT. A larger f_3 region may be kept to ensure that the number of hypercomplex f_3 points is a power of 2; but that portion of the f_3 spectrum that is retained outside of the currently displayed region contains only zeroes. This 3D utility can reduce the fully transformed 3D data size by factors of 2 to 4, especially in some of the triple resonance experiments.

Values: A three-character string such as 'nnn', 'nny', 'nyn', etc. The default is 'nnn'. The first character refers to the f_3 dimension (`sw`, `np`, `fn`); the second character, to the f_1 dimension (`sw1`, `ni`, `fn1`); and the third character, to the f_2 dimension (`sw2`, `ni2`, `fn2`). Each character may take one of two values: 'n' for no region-selective processing in the relevant dimension, or 'y' for region-selective processing in the relevant dimension.

See also: *NMR Spectroscopy User Guide*

Related: `fiddc3d` 3D time-domain dc correction (P)
`fn` Fourier number in directly detected dimension (P)
`fn1` Fourier number in 1st indirectly detected dimension (P)
`fn2` Fourier number in 2nd indirectly detected dimension (P)
`ft3d` Perform a 3D Fourier transform (M)
`ni` Number of increments in 1st indirectly detected dimension (P)
`ni2` Number of increments in 2nd indirectly detected dimension (P)
`np` Number of data points (P)
`ntype3d` N-type peak selection in f_1 or f_2 (P)
`par3d` Create 3D acquisition, processing, display parameters (C)
`specdc3d` 3D spectral drift correction (P)

<code>sw</code>	Spectral width in directly detected dimension (P)
<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)
<code>sw2</code>	Spectral width in 2nd indirectly detected dimension (P)

ptsval **PTS frequency synthesizer value (P)**

Description: Configuration parameter for the frequency of the PTS synthesizer on each channel. Every broadband system is equipped with a PTS frequency synthesizer as part of broadband frequency generation. The frequency of the unit is marked on its front panel. The value is set for each channel using the Synthesizer label in the Spectrometer Configuration window.

Values: 0 (Not Present choice in Spectrometer Configuration window); 160, 200, 250, 320, 500, 620, 1000 (PTS 160, PTS 200, PTS 250, PTS 320, PTS 500, PTS 620, PTS 1000 choices in Spectrometer Configuration window, respectively).

See also: *VnmrJ Installation and Administration*.

Related:	<code>config</code>	Display current configuration and possibly change it (M)
	<code>latch</code>	Frequency synthesizer latching (P)
	<code>overrange</code>	Frequency synthesizer overrange (P)

pulseinfo **Shaped pulse information for calibration (M)**

Syntax: `pulseinfo<(shape,pulse_width<,reference_power>)>
:width,power`

Description: Returns or prints a table with the bandwidth and predicted pulse power settings for a given pulse shape. No parameter settings are changed. The necessary data is contained in the file `shapeinfo` in the system `shapelib` subdirectory.

Arguments: `shape` is the name of the pulse shape. The default is the system interactively prompts the operator for the name of the shape and the duration of the pulse and then prints a table containing the bandwidth of that pulse and the predicted pulse power settings.

`pulse_width` is the duration of the pulse, in μ s.

`reference_power` is a value, in dB, for power calculations. The default is 55. This value replaces the assumption used for power calculation that `pw90` is set for a `tpwr` of 55.

`width` returns the bandwidth of that pulse, in Hz.

`power` returns the predicted 90° pulse power settings.

Examples: `pulseinfo('gauss',1000):bw,pwr`

See also: *User Programming*

Related:	<code>bandinfo</code>	Shaped pulse information for calibration (M)
	<code>pw90</code>	90° pulse width (P)
	<code>tpwr</code>	Observe transmitter power level with linear amplifiers (P)

pulsetool **RF pulse shape analysis (U)**

Syntax: `pulsetool <-shape filepath>`

Description: Enables examination of shaped rf pulses. It is started from a UNIX window.

Arguments: The optional `-shape filepath` specifies the name of an rf pulse template file that is displayed when `pulsetool` is started.

Examples: `pulsetool`
`pulsetool -shape /vnmr/shapelib/sinc.RF`

See also: *NMR Spectroscopy User Guide*

purge Remove macro from memory (C)

Syntax: `purge<(file)>`

Description: Removes one or more macros from memory, freeing extra memory space.

Arguments: `file` is the name of a macro file to be removed from memory. The default is to remove all macros that have been loaded into memory.

CAUTION: The `purge` command with no arguments should never be called from a macro. The `purge` command with an argument should never be called by the macro being purged.

Examples: `purge`
`purge('_sw')`

See also: *User Programming*

Related: `macroload` Load a macro into memory (C)

puttxt Put text file into a data file (C)

Syntax: `puttxt(file)`

Description: Copies text from current experiment into a data file.

Arguments: `file` is the name of a data file (i.e., a directory with a `.fid` or `.par` suffix). Do not include the suffix in the name provided to `file`.

Examples: `puttxt('mydata')`

See also: *NMR Spectroscopy User Guide*

Related: `gettext` Get text file from another file (C)

putwave Write a wave into Pbox.inp file (M)

Syntax: `putwave(sh,bw,pw,ofs,st,ph,fla,trev,d1,d2,d0)`

Description: Sets up a single excitation band in the `Pbox.inp` file. An unlimited number of waves can be combined by reapplying `putwave`.

Arguments: 1 to 11 wave parameters in the following predefined order:

`sh` is the name of a shape file.

`bw` is the bandwidth, in Hz.

`pw` is the pulsewidth, in sec.

`ofs` is the offset, in Hz.

`st` is a number specifying the spin status: 0 for Mz, or 1 for Mxy.

`ph` is the phase (or phase cycle, see `wavelib/supercycles`).

`fla` is the flip angle. Note that `fla` can override the default flip angle.

`trev` concerns time reversal. It can be used to cancel time reversal if spin status (`st`) is set to 1 for Mxy.

`d1` is the delay, in sec, prior the pulse.

`d2` is the delay, in sec, after the pulse.

`d0` is a delay or command prior to `d1`. If `d0=a`, the wave is appended to the previous wave.

Examples: `putwave('eburp1')`
`putwave('GARP',12000.0)`
`putwave('esnobl',600,-1248.2,1,90.0,'n','n',0.001)`

P

See also: *NMR Spectroscopy User Guide*

Related: **pbox** Pulse shaping software (U)
setwave Write a wave definition string into the Pbox.inp file (M)

pw Enter pulse width pw in degrees (C)

Syntax: `pw(flip_angle, <90_pulse_width>)`

Description: Calculates the flip time, in μs , given a desired flip angle and 90° pulse. The value is entered into the parameter **pw**.

Arguments: **flip_angle** is the desired flip angle, in degrees.
90_pulse_width is the 90° pulse length, in μs . The default is the value of parameter **pw90**, if it exists.

Examples: `pw(30)`
`pw(90, 12.8)`

See also: *NMR Spectroscopy User Guide*

Related: **ernst** Calculate the Ernst angle pulse (C)
pw Pulse width (P)
pw90 90° pulse width (P)

pw Pulse width (P)

Description: Length of the final pulse in the standard two-pulse sequence. In “normal” 1D experiments with a single pulse per transient, this length is the observe pulse width.

Values: 0, 0.1 μs to 8190 sec, smallest value possible is 0.1 μs , finest increment possible is 12.5 ns.

See also: *NMR Spectroscopy User Guide*

Related: **p1** First pulse width (P)
pw Enter pulse width parameter pw in degrees (C)

pw90 90° pulse width (P)

Description: Length of the 90° pulse. **pw90** is not used by pulse sequences directly, but is used by a number of commands to assist in setting up special experiments. **pw90** is also used by certain output programs to be able to print the value of the pulse width in degrees instead of microseconds. Note that this parameter must be updated by the user and is not automatically determined or magically correct under all circumstances.

Values: 0, 0.1 μs to 8190 sec, smallest value possible is 0.1 μs , finest increment possible is 12.5 ns.

See also: *NMR Spectroscopy User Guide*

Related: **AC1S-AC11S** Autocalibration macros (M)
pw Enter pulse width parameter pw in degrees (C)

pwd Display current working directory (C)

Syntax: `pwd<:directory>`

Description: Displays the path of the current working directory.

Arguments: **directory** is a string variable with the path of the current directory.

Examples: `pwd:$name`

See also: *NMR Spectroscopy User Guide*

Related: `cd` Change working directory (C)
`dir` List files in current directory (C)
`lf` List files in current directory (C)
`ls` List files in current directory (C)

pwpat Shape of refocusing pulse (P)

Applicability: Systems with imaging capabilities.

Description: Specifies the shape of the refocusing pulse `pw` in imaging experiments

Values: 'hard', 'sinc', 'gauss', 'sech', 'sine', or any shape resident in the system pulse shape library or libraries.

See also: *VnmrJ Imaging NMR*

Related: `plpat` Shape of an excitation pulse (P)
`pw` Pulse width (P)

pwr Set power mode in directly detected dimension (C)

Description: Selects the power spectra display mode by setting `dmg` = 'pwr'. In the *power mode*, each real point in the displayed spectrum is calculated as the sum of the squares of the real and imaginary points comprising each respective complex data point. All information, including noise, is positive and the relationship between signal and noise is non-linear.

For multidimensional data, `pwr` has no effect on data prior to the second Fourier transform. If `pmode` = 'full', `pwr` acts in concert with the commands `ph1`, `av1` or `pwr1` to yield the resultant contour display for the 2D data.

See also: *NMR Spectroscopy User Guide*

Related: `av` Set abs. value mode in directly detected dimension (C)
`av1` Set abs. value mode in 1st indirectly detected dimension (C)
`dmg` Data display mode in directly detected dimension (P)
`ft` Fourier transform 1D data (C)
`ft1d` Fourier transform along f_2 dimension (C)
`ft2d` Fourier transform 2D data (C)
`pa` Set phase angle mode in directly detected dimension (C)
`pa1` Set phase angle mode in 1st indirectly detected dimension (C)
`ph` Set phased mode in directly detected dimension (C)
`ph1` Set phased mode in 1st indirectly detected dimension (C)
`pmode` Processing mode for 2D data (P)
`pwr1` Set power mode in 1st indirectly detected dimension (C)
`pwr2` Set power mode in 2nd indirectly detected dimension (C)
`wft` Weight and Fourier transform 1D data (C)
`wft1d` Weight and Fourier transform f_2 of 2D data (M)
`wft2d` Weight and Fourier transform 2D data (M)

pwr1 Set power mode in 1st indirectly detected dimension (C)

Description: Selects the power spectra display mode along the first indirectly detected dimension by setting `dmg1` = 'pwr1'. If the parameter `dmg1` does not exist, `pwr1` creates it and sets it to 'pwr1'. In the *power mode*, each real point in the displayed trace is calculated as the sum of the squares of the real and imaginary points comprising each respective complex data point. For hypercomplex data, the real-real and imaginary-real points from each respective hypercomplex data

point are used in the summation. In this mode, all information, including noise, is positive and the relationship between signal and noise is non-linear.

The `pwr1` command is only needed if mixed-mode display is desired. If the parameter `dmg1` does not exist or is set to the null string, the display mode along the first indirectly detected dimension defaults to the display mode of the directly detected dimension (characterized by the parameter `dmg`). For the contour display of multidimensional data, the result of `pwr1` is the same as for traces, provided that `pmode='partial'` or `pmode=''`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dmg1</code>	Data display mode in 1st indirectly detected dimension (P)
	<code>pa</code>	Set phase angle mode in directly detected dimension (C)
	<code>pa1</code>	Set phase angle mode in 1st indirectly detected dimension (C)
	<code>pmode</code>	Processing mode for 2D data (P)
	<code>pwr</code>	Set power mode in directly detected dimension (C)
	<code>pwr2</code>	Set power mode in 2nd indirectly detected dimension (C)

pwr2

Set power mode in 2nd indirectly detected dimension (C)

Description: Selects the power spectra display mode along the second indirectly detected dimension by setting `dmg2='pwr2'`. If `dmg2` does not exist or is set to the null string, `pwr2` will create `dmg2` and set it equal to `'pwr2'`. In the *power mode*, all information, including noise, is positive and the relationship between signal and noise is non-linear. Each real point in the displayed trace is calculated as the sum of the squares of the real and imaginary points comprising each respective complex data point. For hypercomplex data, the real-real and imaginary-real points from each respective hypercomplex data point are used in the summation.

The `pwr2` command is only needed if mixed-mode display is desired. If the parameter `dmg2` does not exist or is set to the null string, the display mode along the second indirectly detected dimension defaults to the display mode of the directly detected dimension (characterized by the parameter `dmg`). For the contour display of multidimensional data, the result of `pwr2` is the same as for traces, provided that `pmode='partial'` or `pmode=''`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>av2</code>	Set abs. value mode in 2nd indirectly detected dimension (C)
	<code>dmg2</code>	Data display mode in 2nd indirectly detected dimension (P)
	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>ft2d</code>	Fourier transform 2D data (C)
	<code>ph2</code>	Set phased mode in 2nd indirectly detected dimension (C)
	<code>pmode</code>	Processing mode for 2D data (P)
	<code>pwr</code>	Set power mode in directly detected dimension (C)

pwsadj

Adjust pulse interval time (M)

Applicability: Systems with waveform generators.

Syntax: `pwsadj(shape_file,pulse_parameter)`

Description: Adjusts the pulse interval time so that the pulse interval for the specified shape is an integral multiple of 100 ns. This ensures there is no time truncation error in executing the shaped pulse by waveform generators.

Arguments: `shape_file` is a file name of a shaped pulse file. The name can be specified with or without the `.RF` file extension. `pwsadj` first looks for the file name specified by `shape_file` in the user's `shapelib` directory. If the file

specified is not found there, `pwsadj` then looks in the system `shapelib` directory.

`pulse_parameter` is a string containing the adjusted pulse interval time.

Examples: `pwsadj('pulse12','pulseparam')`

See also: *User Programming*

Related: `dmfadj` Adjust decoupler tip-angle resolution time (M)
`dmf2adj` Adjust second decoupler tip-angle resolution time (M)

pxcal Decoupler pulse calibration (M)

Description: Provides an interactive method of selecting the decoupler (first, second, or third) and the nucleus (^{13}C , ^{15}N , or ^{31}P) to calibrate. The `pxcal` pulse sequence determines the pulse width characteristics of the probe's decoupler channel(s) in indirect detection or triple resonance experiments. `pxcal` can also be used to determine the rf field homogeneity of the decoupler.

The parameter `px1` is arrayed to calibrate the 90° pulse width on the first decoupler. If a second decoupler is present, the parameter `px2` is arrayed to calibrate the 90° pulse width on that decoupler. If a third decoupler is present, the parameter `px3` is arrayed to calibrate the 90° pulse width on that decoupler. Other parameters include: `jC13` is the ^{13}C - ^1H coupling, constant, `jN15` is the ^{15}N - ^1H coupling constant, `jP31` is the ^{31}P - ^1H coupling constant, and `jname` is a selected calibration nucleus.

See also: *System Administration*

pxbss Bloch-Siegert shift correction during Pbox pulse generation (P)

Description: A flag to enable or disable Bloch-Siegert shift correction during the creation of Pbox pulses.

Values: 'y' enable Bloch-Siegert shift correction
'n' disable Bloch-Siegert shift correction
Default value is 'y'.

See also: *NMR Spectroscopy User Guide*

Related: `htfrq1` Hadamard frequency list in `ni` (P)

pxrep Flag to set the level of Pbox reports (P)

Description: A flag to set the level of Pbox debug messages displayed at the start of acquisition.

Values: 'y' shows all Pbox reports.
'h' shows the Hadamard matrix.
'n' shows no reports.
Default value is 'nnn'.

See also: *NMR Spectroscopy User Guide*

Related: `htfrq1` Hadamard frequency list in `ni` (P)

pxset Assign Pbox calibration data to experimental parameters (M)

Syntax: `pxset<(file.ext)>`

Description: Retrieves experimental settings from a file and assigns them to corresponding experimental parameters using a dialog form. If no file name is provided, `pxset` extracts data from the `Pbox.cal` file that contains the output data of the last created waveform

P

Arguments: `file.ext` is the name of a shape or pattern file.

Examples: `pxset`
`pxset('Pbox.RF')`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)
[pboxget](#) Extract Pbox calibration data (M)

pxshape Generates a single-band shape file (M)

Syntax: `pxshape('sh bw/pw ofs st ph fla trev \`
`d1 d2 d0', name, disp)`

Description: Generates a single-band waveform based on wave definition provided as a single string of wave parameters.

Arguments: A single string of 1 to 12 wave parameters in predefined order. Note that a single quote is required at the start and the end of the entire string, but no single quotes are required surrounding characters and strings inside the entire string.

`sh` is the name of a shape file.

`bw/pw` is either the bandwidth, in Hz, or the pulsewidth, in sec.

`ofs` is the offset, in Hz.

`st` is a number specifying the spin status: 0 for Mz, or 1 for Mxy.

`ph` is the phase (or phase cycle, see `wavelib/supercycles`).

`fla` is the flip angle. Note that `fla` can override the default flip angle.

`trev` is a time reversal. This can be used to cancel time reversal if spin status (`st`) is set to 1 for Mxy.

`d1` is the delay, in sec, prior the pulse.

`d2` is the delay, in sec, after the pulse.

`d0` is a delay or command prior to `d1`. If `d0=a`, the wave is appended to the previous wave.

`name` is the output file name. An extension is optional and can be used to override an internally defined shape type.

`disp` is the shape is displayed by default in the graphics window. If `disp` is set to 'n', the shape is not displayed.

Examples: `pxshape('eburp1', 'myshape.RF')`
`pxshape('GARP 12000.0', 'shape2', 'y')`
`pxshape('esnob 600.0 -1248.2 n 180.0 n n 0.001', 'xxx')`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

Pxsim Simulate Bloch profile for a shaped pulse (U)

Syntax: `Pxsim file <simtime <num_steps <add/sub>>>`

Description: Used by the `dprofile` macro to simulate a Bloch profile for a shaped pulse. `Pxsim` extracts the information necessary for simulation from the shape header. Only shape files containing this information can be processed.

Arguments: `file` is the name of a shape or pattern file including an `.RF` or `.DEC` extension. `Pxsim` searches for the file in the user's `shapelib` (`~/vnmrsys/shapelib`), and if not found there, it searches in the system `shapelib` (`vnmr/shapelib`).

`simtime` is the maximum simulation time (in sec) that can be provided.

`num_steps` is the number of steps in the profile.

`add/sub` is add (a) or subtract (s) from the previous simulation.

Examples: `Pxsim myshape.RF`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

Pxspy Create shape definition using Fourier coefficients (U)

Syntax: `Pxspy file`

Description: An interactive program that converts shaped pulse files into a Fourier series and produces an output file `pbox.cf` in the user's `shapelib` (`~/vnmrsys/shapelib`), which can be used to create a wave definition file in the `wavelib` directory. `Pxspy` can also be used to convert hard pulse decoupling sequences into soft (“cool”) decoupling waveforms. The resulting Fourier coefficients can depend on the number of points in the waveform.

Arguments: `file` is the name of a shape or pattern file, including an `.RF`, `.DEC`, or `.GRD` extension. The name can be given as a relative name, absolute name, or as a simple name (i.e., with a path). If given as a simple name, `Pxspy` searches for the file in the user's `shapelib` (`~/vnmrsys/shapelib`), and then if not found there, it searches in the system `shapelib` (`vnmr/shapelib`).

Examples: `Pxspy myshape.RF`
`Pxspy /vnmr/shapelib/myshape.RF`
`Pxspy ~vnmrsys/shapelib/myshape.RF`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

Q

qcomp	Longer dead time for longer ring down (P)
QKexp	Set up quick experiment (M)
qtune	Tune probe using swept-tune graphical tool (C)
?	Display the value of an individual parameter)

qcomp Longer dead time for longer ring down (P)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Global parameter to handle longer ring down times following the rf pulse. This is only active if `dsp= 'i'` or if `dsp= 'r'` and `fsq= 'y'`. The dead time is calculated by the software and the DSP parameters are appropriately adjusted for flat baseline and good phase properties. If it is necessary to use a user specified delay, create the `prealfa` parameter. `qcomp` is not effective in explicit acquisition experiments. Not compatible with `srof2`.

Values: `qcomp= 'y'` triggers a longer dead time before the receiver is gated on for the acquisition.

Related: `prealfa` Specify a delay for longer ring down (P)
`dsp` Type of DSP for data acquisition (P)

QKexp Set up quick experiment (M)

Syntax: `QKexp (arguments)`

Description: Set up parameters for quick experiment for a chained acquisition. Multiple arguments can be given to define the chain. Default parameter values are used by the macro and or the probe file is used.

Examples: `QKexp ( ' PROTON ' , ' COSY ' , ' HMQC ' )`
`QKexp ( ' PROTON ' , ' CARBON ' , ' HETCOR ' , ' gCOSY ' )`

qtune Tune probe using swept-tune graphical tool (C)

Syntax: `qtune< (gain<, power>) >`

Description: Displays a real-time graph showing reflected power versus frequency for tuning probes. If the acquisition system has been recently rebooted, enter `su` before running `qtune`. Refer to the manual *NMR Spectroscopy User Guide* for a detailed description of this tool.

Arguments: `gain` specifies the gain value, typically 20 to 50. The default is 50.
`power` specifies the power value, typically 60 to 70. The default is 60.

Examples: `qtune`
`qtune (20)`
`qtune (38, 65)`

See also: *NMR Spectroscopy User Guide*

Related: `tugain` Amount of receiver gain used by `qtune` (P)
`su` Submit a setup experiment to acquisition (M)
`tune` Assign frequencies (C)

Display the value of an individual parameter (C)

Syntax: `parameter_name< [index] >?`

Description: The question mark displays the current numerical or string value of a parameter when the parameter name is followed by a question mark. No change is made to the value of the parameter. To display an individual element of an parameter array, provide the index in square brackets (e.g., `nt [3] ?` might display “`nt [3] =2`”)

Certain parameters can be “turned off” by setting the parameter to 'n'. The display of a parameter that is turned off will be the phrase “Not Used” followed by the actual value in parentheses. For example, if `lb` is set to 1.5 and then set to 'n', entering `lb?` will display `lb= Not Used (1.5)`. Such a parameter can be “turned on” by setting it to 'y'. It will then have its prior value.

To show a parameter’s array of values or learn about its attributes, use the `display` command.

Arguments: `index` is the integer for a selected member of an arrayed parameter.

Examples: `lb?`
`sw?`
`pw [2] ?`

See also: *NMR Spectroscopy User Guide*

Related: `display` Display parameters and their attributes (C)
`getvalue` Get value of a parameter in a tree (C)

R

<code>r</code>	Recall display parameter set (M)
<code>r(n)</code>	Recall some display parameters (C)
<code>r1-r7</code>	Real-value storage for macros (P)
<code>ra</code>	Resume acquisition stopped with sa command (C)
<code>rcvrwt</code>	Weighting for different receivers (P)
<code>react</code>	Recover from error conditions during werr processing (M)
<code>readallshims</code>	Read all shims from hardware (M)
<code>readbrutape</code>	Read Bruker data files from 9-track tape (U)
<code>readfile</code>	Read the contents of a text file into two parameters (C)
<code>readhw</code>	Read current values of acquisition hardware (C)
<code>readlk</code>	Read current lock level (C)
<code>readparam</code>	Read one of more parameters from a file (C)
<code>readultra</code>	Read shim coil setting for Ultra•nmr shim system (M)
<code>real</code>	Create a real variable without a value (C)
<code>recon_all</code>	Reconstruct images from 2D MRI fid data (C)
<code>record</code>	Record keyboard entries as a macro (M)
<code>redor1</code>	Set up parameters for REDOR1 pulse sequence (M)
<code>redosy</code>	Restore 2D DOSY display from sub experiment (M)
<code>reff1</code>	Reference f2 Indirect Dimension from Observe Dimension (M)
<code>reff2</code>	Reference f2 Indirect Dimension from Observe Dimension (M)
<code>reffrq</code>	Reference frequency of reference line (P)
<code>reffrq1</code>	Reference freq. of reference line in 1st indirect dimension (P)
<code>reffrq2</code>	Reference freq. of reference line in 2nd indirect dimension (P)
<code>refpos</code>	Position of reference frequency (P)
<code>refpos1</code>	Position of reference frequency in 1st indirect dimension (P)
<code>refpos2</code>	Position of reference frequency in 2nd indirect dimension (P)
<code>refsource1</code>	Center frequency in 1st indirect dimension (P)
<code>refsource2</code>	Center frequency in 2nd indirect dimension (P)
<code>region</code>	Divide spectrum into regions (C)
<code>relayh</code>	Set up parameters for RELAYH pulse sequence (M)
<code>rename</code>	Move and/or rename a file (C)
<code>reqparcheck</code>	Flag which enables/disables required parameters (P)
<code>reqparclear</code>	Clears the parameters in required parameter list (M)
<code>reqparlist</code>	List of required parameters (P)
<code>reqpartest</code>	Tests whether required parameters are set (M)
<code>resetf3</code>	Reset parameters after a partial 3D Fourier transform (M)
<code>resetplotter</code>	Reset plotter to system plotter (M)
<code>resolv</code>	Set resolution enhancement parameters (M)
<code>restorenuctable</code>	Calculate and (Re-)store accurate nuctable (M)
<code>resume</code>	Resume paused acquisition queue (C)
<code>return</code>	Terminate execution of a macro (C)
<code>rev</code>	System software revision level (P)
<code>revdate</code>	System software preparation date (P)

R

rfband	RF band in use (P)
rfblk	Reverse FID block (C)
rfchannel	Independent control of rf channel selection (P)
rfchtype	Type of rf channel (P)
rfdata	Reverse FID data (C)
rfl	Reference peak position in directly detected dimension (P)
rfl1	Reference peak position in 1st indirectly detected dimension (P)
rfl2	Reference peak position in 2nd indirectly detected dimension (P)
rfp	Reference peak frequency in directly detected dimension (P)
rfp1	Reference peak freq. in 1st indirectly detected dimension (P)
rfp2	Reference peak freq. in 2nd indirectly detected dimension (P)
rftrace	Reverse FID trace (C)
rftype	Type of rf generation (P)
rfwg	RF waveform generator (P)
right	Set display limits to right half of screen (C)
rights	Determine an operator's specified right (C)
rintput	Input data for a regression analysis (M)
rl	Set reference line in directly detected dimension (M)
rl1	Set reference line in 1st indirectly detected dimension (M)
rl2	Set reference line in 2nd indirectly detected dimension (M)
rm	Delete file (C)
rmdir	Remove directory (C)
rmsAddData	Add transformed data files with weighting (U)
Roesy	Convert the parameter to a ROESY experiment (M)
Roesy1d	Convert the parameter set to a Roesy1d experiment (M)
rof1	Receiver gating time preceding pulse (P)
rof2	Receiver gating time following pulse (P)
rof3	Receiver gating time following T/R switch (P)
rotate	Rotate 2D data (C)
rotorsync	Rotor synchronization (P)
rp	Zero-order phase in directly detected dimension (P)
rp1	Zero-order phase in 1st indirectly detected dimension (P)
rp2	Zero-order phase in 2nd indirectly detected dimension (P)
rt	Retrieve FIDs (M)
rtcmx	Return Spinsight data into current experiment (C)
rtp	Retrieve parameters (M)
rts	Retrieve shim coil settings (C)
rttmp	Retrieve experiment data from experiment subfile (M)
rtv	Retrieve individual parameters (C)
rtx	Retrieve parameters based on rtx rules (C)

r Recall display parameter set (M)

Syntax: (1) rset_number
(2) r(set_number)

Description: Recalls the parameters **sp**, **wp**, **sp1**, **wp1**, **sp2**, **wp2**, **sc**, **wc**, **sc2**, **wc2**, **ho**, **vo**, **vs**, and **ai/nm** of a selected display parameter set. Not recalled are phase

parameters, drift correction parameters, integral reset parameters, and reference parameters. This allows, for example, saving a set of display parameters, adjusting the phase or drift correction, and later recalling the display parameters without undoing the new phase or drift correction.

Arguments: `set_number` is the number, from 1 to 9, of a display parameter set.

Examples: `r2`
`r(3)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>ai</code>	Select absolute intensity mode (C)
	<code>fr</code>	Full recall of a display parameter set (M)
	<code>ho</code>	Horizontal offset (P)
	<code>nm</code>	Select normalized intensity mode (C)
	<code>s</code>	Save display parameters as a set (M)
	<code>sc</code>	Start of chart (P)
	<code>sc2</code>	Start of chart in second direction (P)
	<code>sp</code>	Start of plot in directly detected dimension (P)
	<code>sp1</code>	Start of plot in 1st indirectly detected dimension (P)
	<code>sp2</code>	Start of plot in 2nd indirectly detected dimension (P)
	<code>vo</code>	Vertical offset (P)
	<code>vs</code>	Vertical scale (P)
	<code>wc</code>	Width of chart (P)
	<code>wc2</code>	Width of chart in second direction (P)
	<code>wp</code>	Width of plot in directly detected dimension (P)
	<code>wp1</code>	Width of plot in 1st indirectly detected dimension (P)
	<code>wp2</code>	Width of plot in 2nd indirectly detected dimension (P)

r(n) Recall some display parameters (C)

Applicability: All

Syntax: `r(n<, noupdate>)`

Description: `r(n)` recalls only the following parameters: `sp`, `wp`, `sp1`, `wp1`, `sp2`, `wp2`, `sc`, `wc`, `sc2`, `wc2`, `ho`, `vo`, `vs`, and `ai/nm`.

`noupdate` — as a second argument prevents the automatic update of interactive programs.

Arguments: `n=1 to 9`

See also: *User Programming*

Related:	<code>fr(n)</code>	Recall all the parameters of the specified display parameter set (C)
	<code>s(n)</code>	Save a copy of the current values of all display parameters (C)

r1-r7 Real-value storage for macros (P)

Description: The seven parameters `r1`, `r2`, `r3`, `r4`, `r5`, `r6`, and `r7` are available in each experiment for macros to store a real value.

See also: *User Programming*

Related:	<code>dgs</code>	Display group of special/automation parameters (M)
	<code>n1, n2, n3</code>	Name storage for macros (P)

ra Resume acquisition stopped with sa command (C)

Description: Resumes an experiment acquisition that was stopped with the `sa` command. `ra` is not permitted after any parameters have been brought into the stopped

experiment with the `rt` or `rtp` macros. The parameters `dp` and `np` may not be altered.

`ra` applies to the experiment that you are joined to at the time the command is entered. If experiment 1 has been previously stopped with `sa`, you must be joined to experiment 1 for `ra` to resume that acquisition. If you are in experiment 2, entering `ra` has no effect on experiment 1.

If an experiment has been stopped with `sa`, you can increase the number of transients `nt` and resume the acquisition with `ra`. You cannot, however, increase `nt` and enter `ra` if the experiment had completed in a normal fashion (i.e., it was not stopped with `sa`).

Note that the completion time and remaining time shown in the Acquisition Status window are not accurate after `ra` is executed.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dp</code>	Double precision (P)
	<code>np</code>	Number of data points (P)
	<code>nt</code>	Number of transients (P)
	<code>rt</code>	Retrieve FID (M)
	<code>rtp</code>	Retrieve parameters (M)
	<code>sa</code>	Stop acquisition (C)

rcvrwt Weighting for different receivers (P)

Applicability: Systems with multiple receivers.

Description: An array of real numbers giving weighting factors to use when combining multiple receiver data. The *i*'th array element is used to weight data from the *i*'th receiver. Applying a weight factor is like increasing the gain of the receiver by the same factor (but the weights are specified as numerical factors rather than in dB).

Examples: `rcvrwt=10,12,8`

react Recover from error conditions during werr processing (M)

Syntax: `react<('wait')>`

Description: When an acquisition error occurs, any action specified by the `werr` parameter is executed. The `react` macro is a prototype for handling these errors. This macro can be invoked for error handling by setting `werr='react'`. The `acqstatus` parameter is provided so that `react` can determine which specific error has occurred.

Arguments: `'wait'` is a keyword for a special type of error handling during an automation run. The `react` macro always uses the `'next'` option when it calls the command `au`. Under certain conditions, it is also appropriate to use the `'wait'` option. `react` checks to see if an argument was passed to it; that is, `werr='werr(\ 'wait\ ')` to determine whether to use the `'wait'` option of `au`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>acqstatus</code>	Acquisition status (P)
	<code>au</code>	Submit experiment to acquisition and process data (C)
	<code>werr</code>	Specify action when error occurs (C)
	<code>werr</code>	When error (P)

readallshims Read all shims from hardware (M)

Description: Reads all shims from the hardware and sets the values into the shim parameters in the current parameter tree. The shims used depend on the [shimset](#) configuration. For the shim set on the Ultra•nmr shim system, `readallshims` is active only if hardware-to-software shim communication is enabled.

See also: *NMR Spectroscopy User Guide*

Related: [load](#) Load status of displayed shims (P)
[readhw](#) Read current values of acquisition hardware (C)
[setallshims](#) Set all shims into hardware (M)
[sethw](#) Set values for hardware in acquisition system (C)
[shimset](#) Type of shim set (P)
[su](#) Submit a setup experiment to acquisition (M)

readbrutape Read Bruker data files from 9-track tape (U)

Syntax: (From UNIX) `readbrutape file <number_skipped>`

Description: A shell script that reads one file from a Bruker tape into a UNIX file with the name specified. Bruker tapes are likely to be made at 1600 bpi, although 1600 bpi is not a requirement.

Arguments: `file` is the name of the file read into UNIX. For identification, the `.bru` extension is added to the file name.

`number_skipped` is the number of files skipped and *includes* the header file (which is assumed to be the first file on the tape). The default is the script reads the first file after the header file. If `number_skipped` equals 0, there is no rewinding and the first file (or the next file) on the tape is read.

See also: *NMR Spectroscopy User Guide*

Related: [convertbru](#) Convert Bruker data (M,U)

readfile Read the contents of a text file into two parameters (C)

Examples: `readfile (path, par1, par2, <,cmpstr <,tree> >):num`

Description: `readfile` reads the contents of a file and puts the contents into two supplied parameters. The first word on each line in the file is placed in the first parameter. The remainder of the line is placed in the second parameter. An optional fourth argument specifies a string which is used to match the first word of the line. For example, if the file contained:

```
H1pw 10
H1pwr 55
C13pw 14
C13pwr 50
```

and the comparison string was set to `H1`, only the lines starting with `H1` would be put into the parameters. Namely, `H1pw` and `H1pwr`.

Arguments: `path` is the path name of the file to read.

`par1` is the name of the parameter to hold the first word of the line.

`par2` is the name of the parameter to hold the remainder of each line.

`cmpstr` is the optional comparison string for matching the first word.

`tree` is an optional parameter to select the `tree` for `par1` and `par2`. The possibilities are `current`, `global`, and `local`. `Current` is the default. `Local` is used if the parameters are `$macro` parameters. If `tree` is used, the `cmpstr` must also be supplied. If `cmpstr` is `' '`, then it is ignored.

The `par1` and `par2` parameters must already exist. If `par1` or `par2` are defined as a real parameter, as opposed to a string parameter, then if the value does not have a number as the first word, a zero will be assigned.

`num` will be set to the number of items in the arrayed parameters `par1` and `par2`.

Lines that only contain white space are not added to the parameters. Lines that start with a `#` are not added to the parameters. Lines which start with a `#` can be used as comment lines. If a line only contains a single word, that word is put into the first parameter. The corresponding array element of the second parameter will be set to an empty string. The `readfile` will return the number of lines added to the parameters.

Examples: Examples using a prototype file containing the following:

```
# A readfile test case
# Proton values
H1pw 10
H1pwr 55
# Carbon values
C13pw 14
C13pwr 50
H1macro ft f full aph vsadj
End
```

```
readfile(systemdir+'/probes/testcase','attr','vals')
```

This sets the `attr` and `vals` parameters to arrays of six strings.

```
attr='H1pw','H1pwr','C13pw','C13pwr','H1macro','End'
vals='10','55','14','50','ft f full aph vsadj',''
```

```
readfile(systemdir+'/probes/
testcase','attr','vals','H1')
```

This sets the `attr` and `vals` parameters to arrays of three strings.

```
attr='H1pw','H1pwr','H1macro'
vals='10','55','ft f full aph vsadj'
```

The `readfile` command might be used in conjunction with the `teststr` command. The `teststr` command can be used to search an arrayed parameter to determine the index of a specified element.

For example,

```
teststr(attr,'H1pwr'):$e
vals[$e] will be the value of 'H1Pwr'
```

readhw

Read current values of acquisition hardware (C)

Syntax: `readhw("param1","param2",...)<:r1,r2,...>`
`readhw("keyword"):$res1,...`

Description: Returns or displays the current values of the lock system parameters `lockpower`, `lockgain`, `lockphase`, `lock`, `temp`, `loc`, and `z0`.

The values of the shims can also be obtained. The particular shims that can be read depends upon the type of shim hardware present in the system. See the description of `shimset` for a list of the shim names for each type of shim hardware.

Shim DACs read by `readhw`:

- Axial shim: `z1`, `z2`, `z3`, `z4`, `z1c`, `z2c`
- Non-axial shims: `x1`, `y1`, `xz`, `yz`, `xy`, `x2y2`, `x3`, `y3`
- Special Oxford magnets shims: `z5`, `xz2`, `yz2`, `zx2y2`, `zxy`

Arguments: `param1`, `param2`, ... parameter to read — maximum of 10 parameters.

`r1, r2, . . .` Vnmr variables hold the returned results

no variables supplied — results are displayed in the text panel

Keywords:

`loc` —sample changer location.

`temp` — returns the sample temperature, controller status, and set point.
Results are displayed in the text panel if no variables are supplied

<i>Returned value</i>	<i>Status</i>
0	Regulation off
1	Regulated
2	Not regulated
3	No controller

`status` — returns the systems status as an integer. The returned values are:

<i>Returned value</i>	<i>Status</i>
10	IDLE
15	PARSE
16	PREP
17	SYNCED
20	ACQUIRE
25	PAD
30	VTWAIT
40	SPINWAIT
50	AGAIN
60	ALOCK
61	AFINDRES
62	APOWER
63	APHASE
70	SHIMMING
80	SMPCHANGE
81	RETRIEVSMP
82	LOADSMP
90	INTERACTIVE
100	TUNING
0	INACTIVE

Error messages

-1	Available on spectrometer only (i.e. system = 'datastation')
-2	acquisition not active (acquisition communication programs are not running try running <code>su acqproc</code>).
-7	console powered down or not connected

Results are displayed in the text panel if no variables are supplied.

`readhw` cannot be used when an acquisition is in progress or when `acqi` is connected to the acquisition system.

Arguments: `param1, param2, . . .` are the names of the parameters to be read.
`value1, value2, . . .` are return variables to store the settings of the parameters specified. The default is to display the setting in the status window.

R

Examples: `readhw('z1c','z2c','z1','z2')`
`readhw('z1c','z2c','z1','z2'):r1,r2,r3,r4`
`readhw('temp'):$t sets $t`

See also: *NMR Spectroscopy User Guide*

Related: `lockgain` Lock gain (P)
`lockphase` Lock phase (P)
`lockpower` Lock power (P)
`readallshims` Read all shims from hardware (M)
`sethw` Set values for hardware in the acquisition system (C)
`shimset` Type of shim set (P)

readlk Read current lock level (C)

Syntax: `readlk<:lock_level>`

Description: Returns the same information as would be displayed on the digital lock display using the manual shimming window. `readlk` can be used in developing automatic shimming methods such as shimming via grid searching. It *cannot* be used during acquisition or manual shimming.

Arguments: `lock_level` returns the current lock level.

Examples: `readlk`
`readlk:$level1`

See also: *User Programming*

Related: `alock` Automatic lock status (P)

readparam Read one of more parameters from a file (C)

Syntax: `readparam(file,parlist[,tree[,type]]) -`

Description: The `readparam` command will read one or more parameters from a specified file. The first argument is the name of the file. The second argument is a list of the names of the parameters to be read. It is a string parameter and the names can be separated either by a space or a comma. If a parameter in the list is not present in the file being read, no error is generated. The optional third argument is the tree into which the parameters are read. The variable trees are 'current', 'global', 'processed' and 'systemglobal'. The optional fourth argument controls the behavior of the `readparam` command. The options are 'read', 'replace', and 'add'. The default type is 'read'.

Examples: In order to specify the type, the tree must also be specified. The behaviors are best illustrated with specific examples. Lets say that there is a temporary file containing only the parameters a and b. We are going to use the `readparam` command to read parameters into a current tree which contains the parameters a and c but does not contain the parameters b and d. This can be summarized as:

Parameters in mypar: a=1 b=2

Initial parameters in current tree: a=4 c=8 (b and d do not exist)

`readparam(curexp+'/mypar','a b c d','current','read')`

Parameter in a current tree is replaced with parameter from mypar. Parameter b in current tree is read in from mypar Parameter c in current tree is unaltered Parameter d in current tree still does not exist. Final parameters in current tree: a=1 b=2 c=8 (d does not exist).

`readparam(curexp+'/mypar','a b c d','current','replace')`

Parameter in a current tree is replaced with parameter from mypar. Parameter b in current tree still does not exist. Parameter c in current tree is deleted.

Parameter d in current tree still does not exist. Final parameters in current tree: a=1 (b c and d do not exist).

```
readparam(curexp+'/mypar','a b c d','current','add')
```

Parameter in a current tree is unaltered. Parameter b in current tree is read in from mypar. Parameter c in current tree is unaltered. Parameter d in current tree still does not exist. Final parameters in current tree: a=4 b=2 c=8 (d does not exist).

This command may be used to read temporary values which have been saved with the writeparam command.

More Examples:

```
readparam(curexp+'/mypar','in')
```

reads the parameter in from the file mypar in the current experiment directory.

```
readparam(curexp+'/mypar','sw ct np','processed')
```

reads the parameters sw, ct, and np into the processed tree from the file mypar in the current experiment directory.

readultra Read shim coil setting for Ultra•nmr shim system (M)

Applicability: Systems with the Ultra•nmr shim system.

Syntax: `readultra<(file_number)>`

Description: Reads shim set files for a Ultra•nmr shim system from a Sun floppy disk into VnmrJ. The floppy disk for Ultra•nmr contains up to 63 shim sets named file1.dac to file63.dac.

Arguments: `file_number` is the number of the shim set file, from 1 to 63. The default is to read all of the shim set files.

Examples: `readultra`
`readultra(6)`

See also: *NMR Spectroscopy User Guide*

Related: `shimset` Type of shim set (P)
`svs` Save shim coil settings (C)

real Create a real variable without a value (C)

Syntax: `real(variable)`

Description: Creates a real variable without a value.

Arguments: `variable` is the name of the variable to be created.

Examples: `real('realval1')`

See also: *User Programming*

Related: `create` Create a new parameter in a parameter tree (C)
`string` Create a string variable (C)

recon_all Reconstruct images from 2D MRI fid data (C)

Applicability: Imaging Systems

Syntax: `recon_all(acqstring,<pc option>)`
or
`recon_all(acqstring,<image directory>,<pc option>)`
or
`recon_all`

Description: Produces 2D images (in `fdf` format) from FID data acquired with most 2D imaging sequence, including `sems`, `gems`, `fsems`, and `epi`.

Supported features:

- Compressed/Standard/Arrayed experiments supported (relevant VNMR parameter: `seqcon`)
- Capable of running concurrently with acquisition (set `acqstring` to `acq` after first `wnt`; empty or dummy string initially).
- Disable image display (relevant parameter: `recondisplay`. Create in processed tree as a real variable and set it to 0)
- Display every N images (relevant parameter: `recondisplay`. Create in processed tree as a real variable and set it to N)
- DC removal (relevant parameter: `dcrmv`)
- Image shifting (relevant VNMR parameter: `lsfrq`, `lsfrql`)
- Multi-shot/sorting (relevant parameters: `petable`, `etl`, and/or `nseg`)
- Multi-slice (interleaved) acquisitions (relevant VNMR parameter: `ns`)
- Separate output from multiple receivers (relevant VNMR parameter: `rcvrout`, a string. Set to `i`, will yield either raw- (if VNMR parameter `raw` is set) or image-domain magnitude and phase images for separate coils)
- Multi-echo imaging support (`sems`, `epi`) (relevant VNMR parameter: `ne`)
- Multiple receiver data (magnitude sum) (relevant parameter: `rcvrs`)
- Weighting (through VnmrJ panel selections) (relevant parameter: `ftproc`)
- Zero filling (through VnmrJ panel selections) (relevant parameters: `fn` and/or `fn1`)
- Output magnitude and/or phase raw data components. (relevant (optional) parameter: `raw`. Create in processed tree as a string which can be set to 'm' (magnitude), 'p' (phase), or 'b' (both))
- Partial k-space conjugation. Relevant parameters are `fract_kx` and `fract_ky`, which denote the number of points/echoes acquired beyond the intended N/2. Example: `nv=80`, `fract_ky=16` results in the central 32 echoes used as a correction map prior to conjugate synthesis. Resulting image has 128 ($2 \times (80-16)$) lines in the phase encoded direction.
- Phase correction (relevant parameters: `image`, `epi_pc`). Implemented for `epi` sequences. Phase of transformed imaging data (`image=1`) is corrected by phase of transformed reference data (`image=0`). Accepted values for `pc_option` in command string or for the optional parameter `epi_pc` are:
 POINTWISE (the default; direct use of the phase of profile)
 LINEAR (1st order fit of phase of profile)
 QUADRATIC (2nd order fit of phase of profile)
 CENTER_PAIR (even/odd pair at center of echo train used for all even/odd echoes)
 PAIRWISE (even/odd pair phase differences along echo train used)
 6.FIRST_PAIR (1st and 2nd echoes used for even/odd correction)
- Navigator Echo correction. Requires acquisition of *echo train* data (`fsems`, `epi`), some of which are not phase encoded. Adjusts phase of

encoded echoes according to the phase of navigator echoes of the same echo train, relative to the first such navigator echo. Relevant parameters are:

- `navigator` (can be string set to 'y' or 'n', or array of integers giving navigator echo positions within the echo train (i.e., `navigator=1,2`).)
- `nav_type` (optional; string, set to 'off' to disable correction or 'POINTWISE' (default)).

Order of operation per echo in block:

1. DC removal
2. echo reversal if necessary
3. raw data output if requested
4. windowing if necessary
5. read direction Fourier transform
6. phase correction if necessary
7. sorting if necessary

Order of operation per slice:

1. navigator correction if necessary
2. windowing in phase direction if necessary
3. partial Fourier correction if necessary
4. phase direction Fourier transform
5. accumulation of multi-receiver data
6. write `fdf` output file

Arguments:

<code>acqstring</code>	Set to 'acq' to indicate concurrent reconstruction; performs no initialization. Any other value can be used for retrospective reconstruction or the first pass through concurrent reconstruction (initialization is performed).
<code>pc option</code>	Optional argument to specify phase correction method (see description of phase correction below).
<code>image directory</code>	Optional argument to specify the directory which will contain produced <code>fdf</code> files.
<code>NB</code>	<code>recon_all</code> accesses parameters in the PROCESSED tree for control of some features. It is in the PROCESSED tree that variables should be created and/or modified for effectiveness with <code>recon_all</code> .
<code>Input/Output</code>	<code>recon_all</code> reads the FID file in the <code>acqfil</code> subdirectory of the current experiment, and creates <code>fdf</code> files that are written to the <code>recon</code> subdirectory of the current experiment when run in standalone mode, or to the study tree when run in study mode. If raw data output is selected, the resulting <code>fdf</code> files are written to the <code>rawmag</code> or <code>rawphs</code> subdirectory of the current experiment. If phase images are optionally generated, the resulting <code>fdf</code> files are written to the <code>reconphs</code> subdirectory of the current experiment's directory.

Examples: `recon_all('', '/usr/home/myimages')`
`recon_all('', '/usr/home/myimages', 'CENTERPAIR')`
`recon_all('ignorethis', 'LINEAR')`
`recon_all('acq')`

See also: *VnmrJ Imaging User's Guide*

R

record Record keyboard entries as a macro (M)

Syntax: `record<(file|'off')>`

Description: Records keyboard entries and stores the entries as a MAGICAL macro in the user's `maclib` directory. To start recording keyboard entries, enter `record`. You are prompted for a macro name (you can also give the name as an argument to `record`). The command line prompt then becomes "Command?" to indicate that the `record` macro is active. Type the MAGICAL commands to be recorded on the keyboard. Function keys can be included by entering F1 to F8 for function keys 1 to 8, respectively. Enter `off` or `record('off')` to finish the recording.

Arguments: `file` is the name of the macro file in which the entries are saved. The default is that the user is prompted for a file name. If the macro file name already exists, the user is asked if the file should be overwritten.

'`off`' is a keyword to stop recording the entries.

Examples: `record`
`record('mymacro')`
`record('off')`

See also: *User Programming*

redor1 Set up parameters for REDOR1 pulse sequence (M)

Applicability: Three-channel systems with a triple-tuned MAS solids probe.

Description: Sets up a parameter set, obtained with `XPOLAR1`, for REDOR (rotational echo double-resonance) experiment.

See also: *User Guide: Solid-State NMR*

Related: `xpolar1` Set up parameters for XPOLAR1 pulse sequence (M)

redosy Restore 2D DOSY display from sub experiment (M)

Description: Restores the previous 2D DOSY display (if one exists) by recalling the data stored by the `dosy` macro in the file `subexp/dosy2Ddisplay` in the current experiment. `undosy` and `redosy` enable easy switching between the 1D DOSY data (spectra as a function of `gzlv1`) and the 2D DOSY display (signal as a function of frequency and diffusion coefficient).

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)
`undosy` Restore original 1D NMR data from subexperiment (M)

reff1 Reference f1 Indirect Dimension from Observe Dimension (M)

Syntax: `reff1<(refsource1)>`

Description: Macro uses the ratio of the Ξ values for the relevant nuclei from `refsource1` or the reference source specified to determine the reference frequency in the f1 indirect dimension directly from the reference frequency in the observe dimension using the formula:

$$\text{reffrq1} = (\text{refrq} / \Xi[\text{tn}]) * \Xi[\text{nucf1}]$$

$$\text{rfp1} = 0$$

$$\text{rf11} = \text{sw1}/2 - (\text{frq}[\text{f1}] - \text{reffrq1}) * 1e6$$

Ξ is the normalized frequency such that the ^1H signal from TMS is 100.00 MHz.

Referencing in the observe dimension using `setref` and this method is same as using `setref1` (apart from minor round-off errors).

Referencing the observe dimension to an internal reference standard as proposed by IUPAC references all dimensions to that single reference signal and not the lock as with `setref`, `setref1`, and `setref2`.

Limitations: the macro works with data recalled from an archive or acquired on an other system provided the data was acquired using VNMR6.1C or newer.

Referencing is based on `nuctables/nuctabrefBio` if `bioref='y'` (global or local). Setting `bioref='n'` (global or local) or if the flag does not exist the standard IUPAC / organic chemistry referencing (`nuctables/nuctabref`) is used.

See `/vnmr/nuctables/nuctabref`.

Arguments: No argument — reference source is determined from `refsource1`. If the relevant parameter is missing, the macro tries to determine the (indirect) reference source from the `axis` parameter.

'`sfrq`', '`dfrq`', '`dfrq2`', '`dfrq3`', or '`dfrq4`' as a reference source

Examples: `reff1 reff1('sfrq')`

Related:	<code>reff2</code>	Reference f2 Indirect Dimension from Observe Dimension (M)
	<code>setref</code>	Set Frequency Referencing for Proton Spectra (M)
	<code>setref1</code>	Set Frequency Referencing for f1 Evolution Dimension (M)
	<code>setref2</code>	Set Frequency Referencing for f2 Evolution Dimension (M)
	<code>mref</code>	Set Referencing Based on Spectrum from the same sample (M)
	<code>bioref</code>	Flag for Bio-NMR Referencing (P)

reff2 Reference f2 Indirect Dimension from Observe Dimension (M)

Syntax: `reff2<(refsource2)>`

Description: Macros uses the ratio of the Ξ values for the relevant nuclei from `refsource1` or the reference source specified to determine the reference frequency in the f1 indirect dimension directly from the reference frequency in the observe dimension using the formula:

$$\text{reffrq1} = (\text{reffrq} / \Xi[\text{tn}]) * \Xi[\text{nucf1}]$$

$$\text{rfp1} = 0$$

$$\text{rfl1} = \text{sw1}/2 - (\text{frq}[\text{f1}] - \text{reffrq1}) * 1e6$$

Ξ is the normalized frequency such that the ^1H signal from TMS is 100.00 MHz.

Referencing in the observe dimension using `setref` and this method is same as using `setref1` (apart from minor round-off errors).

Referencing the observe dimension to an internal reference standard as proposed by IUPAC references all dimensions to that single reference signal and not the lock as with `setref`, `setref1`, and `setref2`.

Limitations: the macro works with data recalled from an archive or acquired on an other system provided the data was acquired using VNMR6.1C or newer.

Referencing is based on `nuctables/nuctabrefBio` if `bioref='y'` (global or local). Setting `bioref='n'` (global or local) or if the flag does not exist the standard IUPAC / organic chemistry referencing (`nuctables/nuctabref`) is used.

See `/vnmr/nuctables/nuctabref`.

Arguments: No argument — reference source is determined from `refsource2`. If the relevant parameter is missing, the macro tries to determine the (indirect) reference source from the `axis` parameter.

'`sfrq`', '`dfrq`', '`dfrq2`', '`dfrq3`', or '`dfrq4`' as a reference source

Examples: `reff2('dfrq3')`

Related:	<code>reffl</code>	Reference f2 Indirect Dimension from Observe Dimension (M)
	<code>setref</code>	Set Frequency Referencing for Proton Spectra (M)
	<code>setref1</code>	Set Frequency Referencing for f1 Evolution Dimension (M)
	<code>setref2</code>	Set Frequency Referencing for f2 Evolution Dimension (M)
	<code>mref</code>	Set Referencing Based on Spectrum from the same sample (M)
	<code>bioref</code>	Flag for Bio-NMR Referencing (P)

reffrq Reference frequency of reference line (P)

Description: Reference frequency, in MHz, of the reference line. This parameter is set by the `rl` macro. By defining `reffrq` as the conversion factor between Hz and ppm using the `unit` command, ppm calculations can be made.

If referencing is on (i.e., `refpos` is not set to 'n'), the `go`, `ga`, and `au` macros calculate values of `rfl` and `rfp` based on `reffrq` and `refpos`. If referencing is off, `go`, `ga`, and `au` set `reffreq` to `sfrq`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (M)
	<code>crl</code>	Clear reference line in directly detected dimension (M)
	<code>ga</code>	Submit experiment to acquisition and FT the result (M)
	<code>go</code>	Submit experiment to acquisition (M)
	<code>reffrq1</code>	Ref. frequency of reference line in 1st indirect dimension (P)
	<code>reffrq2</code>	Ref. frequency of reference line in 2nd indirect dimension (P)
	<code>refpos</code>	Position of reference frequency (P)
	<code>rfl</code>	Reference peak position in directly detected dimension (P)
	<code>rfp</code>	Reference peak frequency in directly detected dimension (P)
	<code>rl</code>	Set reference line in directly detected dimension (M)
	<code>sfrq</code>	Transmitter frequency of observe nucleus (P)
	<code>unit</code>	Define conversion units (C)

reffrq1 Reference freq. of reference line in 1st indirect dimension (P)

Description: Reference frequency, in MHz, of the reference line in the first indirect dimension of a nD experiment. This parameter should be used as the conversion factor between hertz and ppm in the first indirect dimension.

See also: *NMR Spectroscopy User Guide*

Related:	<code>crl1</code>	Clear reference line in 1st indirectly detected dimension (M)
	<code>reffrq</code>	Reference frequency of reference line (P)
	<code>refpos1</code>	Position of reference frequency in 1st indirect dimension (P)

reffrq2 Reference freq. of reference line in 2nd indirect dimension (P)

Description: Reference frequency, in MHz, of the reference line in the second indirect dimension of a 2D experiment. This parameter should be used as the conversion factor between hertz and ppm in the second indirect dimension.

See also: *NMR Spectroscopy User Guide*

Related:	<code>crl2</code>	Clear reference line in 2nd indirectly detected dimension (M)
	<code>reffrq</code>	Reference frequency of reference line (P)
	<code>refpos2</code>	Position of reference frequency in 2nd indirect dimension (P)

refpos Position of reference frequency (P)

Description: Position of reference frequency, set by the `setref` and `rl` macros. Setting `refpos='n'` indicates that referencing has been turned off. The `crl` macro turns referencing off.

Values: Because all spectra are (by definition) referenced to a frequency at 0 ppm, `refpos` is either 0 or “not used”.

See also: *NMR Spectroscopy User Guide*

Related:

<code>crl</code>	Clear reference line in directly detected dimension (M)
<code>reffrq</code>	Reference frequency of reference line (P)
<code>refpos1</code>	Position of reference frequency in 1st indirect dimension (P)
<code>refpos2</code>	Position of reference frequency in 2nd indirect dimension (P)
<code>rl</code>	Set reference line indirectly detected dimension (M)
<code>setref</code>	Set frequency referencing (M)

refpos1 Position of reference frequency in 1st indirect dimension (P)

Description: Position of reference frequency in the first indirect dimension of a nD experiment, set by `setref1` and `rl1` macros. Setting `refpos1='n'` indicates that f1 referencing has been turned off. The `crl1` macro turns f1 referencing off.

Values: Because all spectra are (by definition) referenced to a frequency at 0 ppm, `refpos1` is either 0 or “not used”.

See also: *NMR Spectroscopy User Guide*

Related:

<code>crl1</code>	Clear reference line in 1st indirectly detected dimension (M)
<code>reffrq1</code>	Ref. frequency of reference line in 1st indirect dimension (P)
<code>refpos</code>	Position of reference frequency (P)
<code>rl1</code>	Set reference line in 1st indirect dimension (M)
<code>setref1</code>	Set frequency referencing for 1st indirectly detected dimension (M)

refpos2 Position of reference frequency in 2nd indirect dimension (P)

Description: Position of reference frequency in the second indirect dimension of a 3D experiment, set by `setref2` and `rl2` macros. Setting `refpos2='n'` indicates that f2 referencing has been turned off in 3D spectra. The `crl2` macro turns f2 referencing off.

Values: Because all spectra are (by definition) referenced to a frequency at 0 ppm, `refpos2` is either 0 or “not used”.

See also: *NMR Spectroscopy User Guide*

Related:

<code>crl2</code>	Clear reference line in 2nd indirectly detected dimension (M)
<code>reffrq2</code>	Ref. frequency of reference line in 2nd indirect dimension (P)
<code>refpos</code>	Position of reference frequency (P)
<code>rl2</code>	Set reference line in 2nd indirect dimension (M)
<code>setref2</code>	Set frequency referencing for 2nd indirectly detected dimension (M)

refsource1 Center frequency in 1st indirect dimension (P)

Description: Holds a parameter name to be used as the center frequency in the first indirect dimension of 2D experiments. If `refsource1` does not exist, the default is `'sfrq'`.

For 2D experiments, the second dimension may be related to `sfrq` if it is a homonuclear experiment. The second dimension may also be related to `dfrq`

if it is a heteronuclear experiment. `refsource1` would then be set as `refsource1='sfrq'` and `refsource1='dfrq'`, respectively.

See also: *NMR Spectroscopy User Guide*

Related: `dfrq` Transmitter frequency of first decoupler (P)
`refsource2` Center frequency in 2nd indirect frequency (P)
`sfrq` Transmitter frequency of observe nucleus (P)

refsource2 Center frequency in 2nd indirect dimension (P)

Description: Holds a parameter name to be used as the center frequency in the second indirect dimension. `refsource2` is analogous to `refsource1`

See also: *NMR Spectroscopy User Guide*

Related: `refsource1` Center frequency in 1st indirect dimension (P)

region Divide spectrum into regions (C)

Syntax: `region<(tail_length,relative_number,threshold,
number_points,tail_size)>:<number_regions >`

Description: Breaks a spectrum up into regions containing peaks.

Arguments: `tail_length` is the length from 0.0 to `sw`, in Hz, that is added to the start and end of each calculated peak region; default value is `sw/10`. The default value is used if a negative number is entered for this argument. If the addition of these wings would cause overlap between adjacent regions, the wings are reduced until the regions no longer overlap.

`relative_number` is a number that, in combination with other factors, governs the relative number of regions to be found. The default is 12, which is used if 0 is entered for this argument. `relative_number` is used as part of a test to determine whether two spectral areas containing peaks are close enough together to be represented as a single region. There are no strict rules that associate the value of `relative_number` to the total number of regions that will be found. In general, increasing this number decreases the number of regions that will be found and increases the size of an individual region. A value of 1 would give more regions; a value of 100 would give fewer regions.

`threshold` is a sensitivity factor used to decide if a data point is large enough, relative to the noise level, to qualify it as part of a peak. The default value is 0.6, which is used if 0 is entered for this argument. Smaller values of `threshold` make peak selection more sensitive; larger values make peak selection less sensitive.

`number_points` governs the number of successive data points, normally from 7 to 40, that must qualify as part of a peak (see the description of `threshold` above) in order for that spectral area to be considered a real peak. The default value is a function of `fn`, `sw`, weighting functions, and other values. The default is used if 0 is entered for this argument. For carbon spectra with large spectral windows, experimental peaks often contain only one or two data points. Adjust `number_points` to 1 or 2 in those cases.

`tail_size` is a number that, in combination with `relative_number` and other factors, governs whether two spectral areas that contain peaks are close enough together to be represented as a single region. The default value is used if 0 is entered for this argument.

`number_regions` is the total number of regions determined by `region`.

Examples: `region`
`region:$1`
`region(50,0,1)`
`region(-1,0,0,2):r1`

See also: *NMR Spectroscopy User Guide*

Related: **fn** Fourier number in directly detection dimension (P)
sw Spectral width in directly detected dimension (P)

relayh Set up parameters for RELAYH pulse sequence (M)

Description: Sets up parameters for absolute-value COSY, or a single or double RELAY-COSY pulse sequence.

See also: *NMR Spectroscopy User Guide*

Related: **Cosy** Set up parameters for COSY pulse sequence (M)
cosyps Set up parameters for phase-sensitive COSY (M)
Dqcosy Set up parameters for double quantum filtered COSY (M)

rename Move and/or rename a file (C)

Syntax: `rename(from_file,to_file)`

Description: Renames and/or moves a file or directory. `rename` is identical in function to the command **mv**.

Arguments: `from_file` is the name of the file to be moved to renamed.
`to_file` is the name of the file after moving or renaming it. If the `from_file` argument has an extension such as `.fid` or `.par`, be sure the `to_file` argument has the same extension.

Examples: `rename('/home/vnmr1/vnmrsys/seqlib/d2pul',
'/vnmr/seqlib/d2pul')`

See also: *NMR Spectroscopy User Guide*

Related: **copy** Copy a file (C)
cp Copy a file (C)
delete Delete a file, parameter directory, or FID directory (C)
mv Move and/or rename a file (C)
rm Delete file (C)

reqparcheck Flag which enables/disables required parameters (P)

Syntax: `reqparcheck= 'y' or 'n'`

Description:

Description: The parameter `reqparcheck` is a flag with the possible values of 'y' or 'n'. Only if it is set to 'y' are actual parameters compared to the file. If it is set to 'n', `reqpartest` will always return 0.

Values: 'y' or 'n', indicating whether required parameters are to be checked.

Related: **callacq** Utility macro to call Acq command (M)
reqparlist List of required parameters (P)
reqparclear Clears the parameters in required parameter list (M)
reqpartest Tests whether required parameters are set (M)

reqparclear Clears the parameters in required parameter list (M)

Syntax: `reqparclear`

Description: Clears the parameters listed in `reqparlist`. If for some reason `reqparlist` has been destroyed, then this macro exits without a message. The parameter is cleared on

the current tree, if it exists there, or on the global tree, if it exists there. If it exists in neither place, a message is printed and the routine moves on to the next parameter in reqparlist.

The definition of "clear" is that real parameters are turned "off" and string parameters are set to the empty string "".

There is a known issue with this macro, which due to its obscurity will remain as "user beware." The issue is that if a parameter of the same name exists in both the 'global' and 'current' trees, and if that parameter is part of reqparlist, then it will be cleared in the 'current' tree but not in the global tree. Users should just not be doing this.

Also note that while this macro checks for reqparlist="", if it is an array and any element in the array is "" then it assumes "" is a parameter and reports a "does not exist" message.

Related: `callacq` Utility macro to call Acq command (M)
`reqparcheck` Flag which enables/disables required parameters (P)
`reqparlist` List of required parameters (P)
`reqpartest` Tests whether required parameters are set (M)

reqparlist List of required parameters (P)

Description: The parameter reqparlist holds the parameter names. It is an array of strings. It will not array the experiment.

Related: `callacq` Utility macro to call Acq command (M)
`gettoken` Utility macro to separate a string into tokens (M)
`reqparcheck` Flag which enables/disables required parameters (P)
`reqparclear` Clears the parameters in required parameter list (M)
`reqpartest` Tests whether required parameters are set (M)

reqpartest Tests whether required parameters are set (M)

Syntax: `reqpartest<('showtext' | 'showgui'<, callback_string)>>`

Description: If the parameter reqparcheck='y', then this macro examines the list of parameter names in reqparlist and if all of them exist and are properly set, returns 0. Properly set is defined as a non- empty string for string parameters, or the active bit set (parameter is 'on') for real parameters.

This macro also checks the string which is the concatenation of autoname + globalauto + sqname for any parameters in that string. Parameters in this string are delimited by \$.

For convenience, this macro will return different values depending on the specific non-true condition, as defined in the following table (X is "don't care").

All parameters exist	T	X	F	T	F
All parameters set	T	X	T	F	F
reqparcheck='y'	'T	F	T	T	T
return value	0	-1	1	2	3

Also note that the non-existence of either reqparcheck or reqparlist is equivalent to reqparcheck not set to 'y'.

Parameters are checked in the current tree first for existence, and if that parameter exists there, then that tree is checked for whether it is set. If it does

not exist in the current tree, then the global tree is checked. If and only if it exists in neither tree is it considered to not exist.

If the argument to this macro is 'showtext' then if one or more parameters do not exist or are not properly set, then they are listed on the alphanumeric (text) screen.

If the argument to this macro is 'showgui', then an entry popup is displayed for both creation (of non-existing parameters) and value entry. The return value is not affected by the fact that the values are now being entered - in other words, the return value is to be interpreted as 'did not exist' or 'was not set' prior to running the macro.

The comprehensive list to check is `reqparlist+autoname+globalauto+sqname`. Some duplicates may occur, and this macro checks and eliminates duplicates.

The argument `callback_string` is an optional argument that gets passed onto VnmrJ, and then gets passed back to `vnmrbg` when the required parameters entry popup closes. VnmrJ and `vnmrbg` are not otherwise synchronized, so this allows for re-entrance.

Arguments: 'showgui' | 'showtext'

'showgui' displays an entry popup in the required parameter is not set;

'show text' displays information about the required parameters in the text window

`callback_string` — optional callback to `vnmrbg` from VnmrJ (ignored in 'showtext' option)

See also: *VnmrJ User Programming*

Related:	<code>callacq</code>	Utility macro to call Acq command (M)
	<code>reqparcheck</code>	Flag which enables/disables required parameters (P)
	<code>reqparclear</code>	Clears the parameters in required parameter list (M)

resetf3

Reset parameters after a partial 3D Fourier transform (M)

Description: Restores the acquisition parameter `sw`, the processing parameter `fn`, and the display parameters `sp`, `wp`, `rfl`, and `rfp` in the 3D parameter set, which are read into VnmrJ by either the `select` command or the `dplane` or `dproj` macros. These parameters were modified due to the selection of regional f_3 processing (`ptspec3d = 'ynn'`). The original value for each of these parameters is stored in the parameter `$sv`, where `$` represents `sw`, `fn`, `sp`, `wp`, `rfl`, or `rfp` (e.g., `swsv`).

If a 2D plane into VnmrJ is retrieved from a 3D transformed data set that was processed with regional f_3 processing, `resetf3` must be run before executing `ft3d` in that particular VnmrJ environment.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dplane</code>	Display a 3D plane (M)
	<code>dproj</code>	Display a 3D plane projection (M)
	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>ft3d</code>	Perform a 3D Fourier transform (M)
	<code>ptspec3d</code>	Region-selective 3D processing (P)
	<code>rfl</code>	Ref. peak position in directly detected dimension (P)
	<code>rfp</code>	Ref. peak frequency in directly detected dimension (P)
	<code>select</code>	Select a spectrum or 2D plane without displaying it (C)
	<code>sp</code>	Start of plot (P)
	<code>sw</code>	Spectral width in directly detected dimension (P)

`vnmrjcmd()` Commands to invoke the GUI popup (C)
`wp` Width of plot (P)

resetplotter Reset plotter to system plotter (M)

Description: Command to reset a (temporarily chosen) plotter back to the system plotter `sysplotter`. Command is called by all `plotfile/plotpreview` and `plot/autoplot` buttons on plot panels.

resolv Set resolution enhancement parameters (M)

Syntax: `resolv<(a,b)>`

Description: Calculates a default resolution enhancement function, setting up `lb` and `gf` based on the acquisition time `at`. “Zero-filling” is also accomplished, if possible, by making `fn` $\geq 2 * np$.

Arguments: `a` sets a value of `lb` using `lb = -0.318 / (a * sw)`. The default for `a` is 0.1.
`b` sets a value of `gf` using `gf = b * sw`. The default for `b` is 0.3.

Examples: `resolv`
`resolv(.2, .4)`

See also: *NMR Spectroscopy User Guide*

Related: `at` Acquisition time (P)
`fn` Fourier number in directly detected dimension (P)
`gf` Gaussian function in directly detected dimension (P)
`lb` Line broadening in directly detected dimension (P)
`np` Number of data points (P)
`sw` Spectral width in directly detected dimension (P)

restorenuctable Calculate & store accurate nuctable for current system (M)

Syntax: `restorenuctable`

Description: The `setref` contribution is a generic nucleus table, `/vnmr/nuctables/nuctable`, based on a standard proton frequency of 1000.0 MHz. All standard nucleus tables in the `/vnmr/nuctables` are symbolic links pointing to a generic table.

The `restorenuctable` is used to replace the standard links with specific links that to files containing proper and accurately calculated nucleus tables. Problems arising with custom macros and third party software that are not aware of the symbolic links pointing to a generic table can be fixed using this macro.

Commands and utilities that do not scale nuctable entries to the actual proton frequency (as they should) will work better than with the standard tables.

Limitations: `restorenuctable` is not compatible with `qtune` and certain commands in current software.

Examples: `restorenuctable`

Related: `nuctable` Display nucleus table for a given H1 frequency (M)

resume Resume paused acquisition queue (C)

Description: Enables continuing submitting experiments to the acquisition system. For experiments initiated with the command `au('wait')`, the acquisition is paused during the time of data processing in order to prevent the acquisition

from submitting new experiments that might be queued. `resume` then allows the data processing macro to initiate another acquisition with `au('next')`, which is then performed immediately instead of at the end of the queue.

See also: *NMR Spectroscopy User Guide*

Related: `au` Submit experiment to acquisition and process data (C)

return Terminate execution of a macro (C)

Syntax: `return<(expression1, expression2, ...) >`

Description: Terminates the execution of a macro and optionally returns values to another calling macro. This is usually used after testing some condition. `return` is used only in macros and not entered from the keyboard.

Arguments: `expression1, expression2, ...` are return values to another calling macro.

See also: *User Programming*

Related: `abort` Terminate action of calling macro and all higher macros (C)

rev System software revision level (P)

Description: Stores a string identifying the VnmrJ software version for the system. This parameter is not be entered by the user, but can be examined by entering `rev?`.

See also: *VnmrJ Installation and Administration*

Related: `revdate` System software preparation date (P)

revdate System software preparation date (P)

Description: Stores a string identifying the date the current VnmrJ software version was prepared. This parameter is not be entered by the user, but can be examined by entering `revdate?`.

See also: *VnmrJ Installation and Administration*

Related: `rev` System software revision level (P)

rfband RF band in use (P)

Description: Indicates which rf band of the amplifier is in use for each channel.

Values: A string, such as 'hlc', in which the first channel is determined by the first character, the second channel is determined by the second character, and so forth. The following values are available for each channel:

'h' indicates the high rf band is in use on the channel.

'l' indicates the low rf band is in use on the channel.

'c' indicates the system software will calculate whether to use the high band or the low band for the channel.

See also: *NMR Spectroscopy User Guide*

rfblk Reverse FID block (C)

Syntax: `rfblk(<src_expno>, src_blk_no, dest_expno, dest_blk_no)`

Description: Reverses and copies data from a source FID block specified by `src_blk_no` to a destination FID block specified by `dest_expno` and `dest_blk_no`,

using memory-mapped input and output. The file header determines the size and type of data to reverse.

`rfblk` searches for the source and destination FID file in the directory `$vnmruser/expN/acqfil`; `N` is the requested experiment number or the current experiment number. If the FID file is not open, `rfblk` opens the file, copies the data, and closes the file. If a number of blocks need to be copied, explicitly opening and closing the files with the commands `mfopen` and `mfclose` can significantly speed up the data reformatting process.

`rfblk` can also be used to append blocks of data to a FID file by specifying that the `dest_blk_no` is greater than the number of blocks in a file.

Be aware that `rfblk` can modify data returned to an experiment with the `rt` command. To avoid modification, enter the following sequence of commands before running `rfblk`:

```
cp(curexp+'/acqfil/fid',curexp+'/acqfil/fidtmp')
rm(curexp+'/acqfil/fid')
mv(curexp+'/acqfil/fidtmp',curexp+'/acqfil/fid')
```

Arguments: `src_expno` specifies the experiment number of the source FID file. The default is the FID file of the current experiment.

`src_blk_no` specifies the source block of data to be copied. Block numbers run from 1 to the number of blocks in a file.

`dest_expno` specifies the experiment number of the destination FID file.

`dest_blk_no` specifies the destination block to send the copied data.

Examples: `rfblk(1,2,1)` reverses and copies block 1 from the current experiment to block 1 of experiment 2.

See also: *User Programming*

Related:	<code>mfbld</code>	Move FID block (C)
	<code>mfclose</code>	Memory map close FID file (C)
	<code>mfddata</code>	Move FID data (C)
	<code>mfopen</code>	Memory map open FID file (C)
	<code>mftrace</code>	Move FID trace (C)
	<code>rfdata</code>	Reverse FID data (C)
	<code>rftrace</code>	Reverse FID trace (C)

rfchannel Independent control of rf channel selection (P)

Description: Gives override capability over the selection of rf channels. `rfchannel` does not normally exist but can be created by a user with the command `create('rfchannel','flag')`.

The control of each rf channel is built around a collection of parameters and pulse sequence statements. The frequency of channel 1 is set by `sfrq` and `tof`, its power by `tpwr` and `tpwrf`. The first decoupler uses the corresponding parameters `dfrq`, `dof`, `dpwr`, and `dpwrf`, respectively. Furthermore, the decoupler can have modulation modes specified with the parameters `dmf`, `dm`, `dmm`, `dres`, and `dseq`. The second decoupler has the same set of parameters as the first decoupler and they are distinguished by appending a 2 to each name. That is, the names are `dfrq2`, `dof2`, `dpwr2`, `dpwrf2`, `dmf2`, `dm2`, `dmm2`, `dres2`, and `dseq2`. The third decoupler would use parameters with a 3 appended: `dfrq3`, `dof3`, `dpwr3`, `dpwrf3`, `dmf3`, `dm3`, `dmm3`, `dres3`, and `dseq3`. The `rfchannel` parameter provides a mechanism to override the default parameter usage.

Values: A string of one to four characters in which the position of each character identifies the rf channel controlled.

- The first character selects which rf channel (1 to 4) the parameters **sfrq**, **tof**, **tpwr**, etc. control. The first character also identifies the rf channel used as the receiver.
- The second character selects which rf channel (1 to 4) the parameters **dfrq**, **dof**, **dpwr**, etc. control.
- The third character maps the parameter set **dfrq2**, **dof2**, **dpwr2**, etc. to an rf channel (1 to 4).
- The fourth character maps **dfrq3**, **dof3**, **dpwr3**, etc. to an rf channel (1 to 4).

For example, `rfchannel='132'` would exchange control of the second and third rf channels from the default parameter usage.

The number of characters in the `rfchannel` parameter must match the number of real rf channels (defined by the parameter **numrfch**) and each rf channel must be selected by the parameter.

Besides remapping the parameters to different rf channels, pulse sequence statements are also remapped. For example, if `rfchannel='132'`, then statements `decpulse`, `decshaped_pulse`, `decoffset`, `decpower`, `decspinlock`, and so on are applied on rf channel 3 and `dec2pulse`, `dec2shaped_pulse`, and so on are applied on rf channel 2.

An obvious use for this remapping is on systems with the decoupler set to U+ H1 Only in the Spectrometer Configuration window. On these systems, if multinuclear pulses are needed and ¹H needs to be observed, the parameter sets that assume a dual-broadband system can be used and the parameters remapped by setting `rfchannel='21'`. However, internal logic checks if the first decoupler is set to U+ H1 Only, **tn** is set to 'H1', and **dn** is not set to 'H1'. If these settings are the case, the parameter mapping for rf channels 1 and 2 is exchanged automatically.

See also: *NMR Spectroscopy User Guide; User Programming*

Related:	create	Create new parameter in parameter tree (C)
	dfrq	Transmitter frequency for first decoupler (P)
	dm	Decoupler mode for first decoupler (P)
	dmf	Decoupler modulation frequency for first decoupler (P)
	dmm	Decoupler modulation mode for first decoupler (P)
	dn	Nucleus for first decoupler (P)
	dof	Frequency offset for first decoupler (P)
	dpwr	Power level for first decoupler with linear amplifier (P)
	dpwrf	First decoupler fine power (P)
	dres	Tip-angle resolution for first decoupler (P)
	dseq	Decoupler sequence for first decoupler (P)
	numrfch	Number of rf channels (P)
	sfrq	Transmitter frequency for observe nucleus (P)
	tn	Nucleus for observe transmitter (P)
	tof	Frequency offset for observe transmitter (P)
	tpwr	Observe transmitter power level with linear amplifiers (P)
	tpwrf	Observe transmitter fine power (P)

rfchtype **Type of rf channel (P)**

Description: Configuration parameter for type of rf on each channel. The value for a channel is set using the Type of RF label in the Spectrometer Configuration window. Pulse sequence programs check `rfchtype` to determine if indirect detection should be used for some experiments. Indirect detection occurs automatically if the decoupler is set to U+ H1 Only in the Spectrometer Configuration window, **tn** is set to 'H1', and **dn** is not set to 'H1'.

Values: The values of `rfchtype` parallel the `rfdtype` values. The only distinction is that the setting for `rfdtype` is 'd' on the U+ Direct Synthesis and U+ H1 Only entries.

'U+ Direct Synthesis' is the setting for a system with direct synthesis (U+ Direct Synthesis in the Spectrometer Configuration window).

'U+ H1 Only' is a fixed-frequency proton system (U+ H1 Only in Spectrometer Configuration window).

'Deuterium Decoupler' is the setting for a system deuterium decoupler channel.

'Direct Synthesis' is the setting for direct synthesis (Direct Synthesis in the Spectrometer Configuration window).

'Broadband' is the setting for broadband (Broadband in the Spectrometer Configuration window).

'Fixed Frequency' is the setting for fixed frequency (Fixed Frequency in the Spectrometer Configuration window).

'SIS Modulator' is the setting for imaging modulator (SIS Modulator in the Spectrometer Configuration window).

See also: *VnmrJ Installation and Administration*

Related:	<code>config</code>	Display current configuration and possibly change it (M)
	<code>dn</code>	Nucleus for first decoupler (P)
	<code>rfdtype</code>	Type of rf generation (P)
	<code>tn</code>	Nucleus for observe transmitter (P)

rfdata

Reverse FID data (C)

Syntax: `rfdata(<src_expno,>src_blk_no,src_start_loc, \`
`dest_expno,dest_blk_no,dest_start_loc,num_points)`

Description: Reverses and copies data specified by `src_start_loc` from a FID block specified by `src_blk_no` to a destination location specified by `dest_expno`, `dest_blk_no`, and `dest_start_loc`, using memory-mapped input and output. The data point locations and the `num_points` to be reversed are specified by data points corresponding to the `np` parameter, not bytes or complex points; however, when reversing the data, `rfdata` looks at the file header to determine the size and type of data to reverse.

`rfdata` searches for the source and destination FID file in the directory `$vnmruser/expN/acqfil`; N is the requested experiment number or the current experiment number. If the FID file is not open, `rfdata` opens the file, copies the data, and closes the file. If a number of blocks need to be copied, explicitly opening and closing the files with the commands `mfopen` and `mfclose` can significantly speed up the data reformatting process.

Be aware that `rfdata` can modify data returned to an experiment with the `rt` command. To avoid modification, enter the following sequence of commands before running `rfdata`:

```
cp(curexp+'/acqfil/fid',curexp+'/acqfil/fidtmp')
rm(curexp+'/acqfil/fid')
mv(curexp+'/acqfil/fidtmp',curexp+'/acqfil/fid')
```

Arguments: `src_expno` specifies the experiment number of the source FID file. The default is the FID file of the current experiment.

`src_blk_no` specifies the source block of data to be copied. Block numbers run from 1 to the number of blocks in a file.

`src_start_loc` specifies the starting data location within the specified block to copy the data. Data locations start from 0 and are specified as data points corresponding to the `np` parameter.

`dest_expno` specifies the experiment number of the destination FID file.
`dest_blk_no` specifies the destination block to send the copied data.
`dest_start_loc` specifies the starting data destination location within the specified block to send the copied data.

Examples: `rfdata(1,0,2,1,(nv-1)*np,np)` copies and reverses `np` points of data from the starting location 0 of block 1 of the current experiment to the data location `(nv-1)*np` of block 1 of experiment 2.

See also: *User Programming*

Related:	<code>mfbldk</code>	Move FID block (C)
	<code>mfcldse</code>	Memory map close FID file (C)
	<code>mfdldt</code>	Move FID data (C)
	<code>mfdpen</code>	Memory map open FID file (C)
	<code>mfdtrce</code>	Move FID trace (C)
	<code>rfblk</code>	Reverse FID block (C)
	<code>rftrce</code>	Reverse FID trace (C)

rf1 Reference peak position in directly detected dimension (P)

Description: Actual position of the reference line in the spectrum (i.e., the distance from the right edge of the spectrum to the reference line). If there is no reference line in the spectrum, `rf1` can be used to enter the frequency where the reference line would appear if the line were present in the spectrum.

Values: Number, in Hz.

See also: *NMR Spectroscopy User Guide*

Related:	<code>rf11</code>	Reference peak position in 1st indirectly detected dimension (P)
	<code>rf12</code>	Reference peak position in 2nd indirectly detected dimension (P)
	<code>rfp</code>	Reference peak frequency in directly detected dimension (P)

rf11 Reference peak position in 1st indirectly detected dimension (P)

Description: Analogous to the `rf1` parameter except that `rf11` applies to the first indirectly detected dimension of a multidimensional data set. `rf11` can either be set manually or be adjusted automatically when the macro `rl1` is used to assign a reference line.

Values: Number, in Hz.

See also: *NMR Spectroscopy User Guide*

Related:	<code>rf1</code>	Reference peak position in directly detected dimension (P)
	<code>rf12</code>	Reference peak position in 2nd indirectly detected dimension (P)
	<code>rfp1</code>	Reference peak frequency in 1st indirectly detected dimension (P)

rf12 Reference peak position in 2nd indirectly detected dimension (P)

Description: Analogous to the `rf1` parameter except that `rf12` applies to the second indirectly detected dimension of a multidimensional data set. `rf12` can either be set manually or be adjusted automatically when the macro `rl2` is used to assign a reference line.

Values: Number, in Hz.

See also: *NMR Spectroscopy User Guide*

Related:	<code>rf1</code>	Reference peak position in directly detected position (P)
	<code>rf11</code>	Reference peak position in 1st indirectly detected dimension (P)
	<code>rfp2</code>	Reference peak frequency in 2nd indirectly detected dimension (P)

R

rfp	Reference peak frequency in directly detected dimension (P)

Description: Sets the frequency to be assigned to the reference line in the spectrum. `rfp` is always stored in Hz, but can be entered in ppm by using the `p` suffix (e.g., `rfp=2.1p`).

Values: Number, in Hz.

See also: *NMR Spectroscopy User Guide*

Related:	rf1	Reference peak position in directly detected dimension (P)
	rfp1	Ref. peak frequency in 1st indirectly detected dimension (P)
	rfp2	Ref. peak frequency in 2nd indirectly detected dimension (P)
	rl	Set reference line in directly detected dimension (M)

rfp1 **Reference peak freq. in 1st indirectly detected dimension (P)**

Description: Analogous to the `rfp` parameter except that `rfp1` applies to the first indirectly detected dimension of a multidimensional data set. `rfp1` can either be set manually or be assigned a value when `rll` is called with an argument (e.g., `rll(7.2p)` assigns the value of 7.2 ppm to `rfp1`).

Values: Number, in Hz.

See also: *NMR Spectroscopy User Guide*

Related:	rfl1	Ref. peak position in 1st indirectly detected dimension (P)
	rfp	Ref. peak frequency in directly detected dimension (P)
	rfp2	Ref. peak frequency in 2nd indirectly detected dimension (P)
	rl1	Set reference line in 1st indirectly detected dimension (M)

rfp2	Reference peak freq. in 2nd indirectly detected dimension (P)
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
15	15
16	16
17	17
18	18
19	19
20	20
21	21
22	22
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80	80
81	81
82	82
83	83
84	84
85	85
86	86
87	87
88	88
89	89
90	90
91	91
92	92
93	93
94	94
95	95
96	96
97	97
98	98
99	99
100	100

Description: Analogous to the `rfp` parameter except that `rfp2` applies to the second indirectly detected dimension of a multidimensional data set. `rfp2` can be set manually or be assigned a value when `rl2` is called with an argument. For example, entering `rl2 (7.2p)` assigns the value of 7.2 ppm to `rfp2`.

Values: Number, in Hz.

See also: *NMR Spectroscopy User Guide*

Related:	rf12	Reference peak position in 2nd indirectly detected dimension (P)
	rfp	Reference peak frequency in directly detected dimension (P)
	rfp1	Reference peak frequency in 1st indirectly detected dimension (P)
	r12	Set reference line in 2nd indirectly detected dimension (C)

rftrace Reverse FID trace (C)

Syntax: `rftrace(<src_expno,src_blk_no,src_trace_no, \`
`dest_expno,<dest blk no,dest trace no)`

Description: Reverses and copies FID traces specified by `src_trace_no` from a FID block specified by `src_blk_no` to a destination location specified by `dest_expno`, `dest_blk_no`, and `dest_trace_no`, using memory-mapped input and output. The file header determines the size and type of data to be reversed.

`rftrace` searches for the source and destination FID file in the directory `$vnmruser/expN/acqfil`; `N` is the requested experiment number or the current experiment number. If the FID file is not open, `rftrace` opens the file, copies the data, and closes the file. If a number of blocks need to be copied, explicitly opening and closing the files with the commands `mfopen` and `mfclose` can significantly speed up the data reformatting process.

You cannot use `rftrace` to append data to a FID file. Its purpose is for moving around data.

Be aware that `rftrace` can modify data returned to an experiment with the `rt` command. To avoid modification, enter the following sequence of commands before running `rftrace`:

```
cp(curexp+' /acqfil/fid', curexp+' /acqfil/fidtmp')
rm(curexp+' /acqfil/fid')
mv(curexp+' /acqfil/fidtmp', curexp+' /acqfil/fid')
```

Arguments: `src_expno` specifies the experiment number of the source FID file. The default is the FID file of the current experiment.

`src_blk_no` specifies the source block of data to be copied. Block numbers run from 1 to the number of blocks in a file.

`src_trace_no` specifies the source trace of data within the specified block to be copied. Trace numbers run from 1 to number of traces in a file.

`dest_expno` specifies the experiment number of the destination FID file.

`dest_blk_no` specifies the destination block to send the copied data.

`src_trace_no` specifies the destination trace of data within the specified block to be copied. Trace numbers run from 1 to the number of traces in a file.

Examples: `rftrace(1,1,2,1,nv)` copies and reverses trace 1 from block 1 of the current experiment to trace `nv` of block 1 of experiment 2.

See also: *User Programming*

Related:	<code>mfblk</code>	Move FID block (C)
	<code>mfclose</code>	Memory map close FID file (C)
	<code>mfdata</code>	Move FID data (C)
	<code>mfopen</code>	Memory map open FID file (C)
	<code>mftrace</code>	Move FID trace (C)
	<code>rfblk</code>	Reverse FID block (C)
	<code>rfdata</code>	Reverse FID data (C)

rftype **Type of rf generation (P)**

Description: Configuration parameter for type of rf generation on each rf channel. On other systems, the value is set using the Type of RF label in the Spectrometer Configuration window.

Values: The values of `rftype` parallel the `rfchtype` values. The setting for `rftype` is 'd' on the entries U+ Direct Synthesis and U+ H1 Only.

'd' is the setting for a system with direct synthesis (U+ Direct Synthesis in the Spectrometer Configuration window) or a fixed-frequency proton system (U+ H1 Only in Spectrometer Configuration window).

'l' is the setting for a deuterium decoupler channel.

'c' is the setting for direct synthesis (Direct Synthesis in the Spectrometer Configuration window).

'b' is the setting for broadband (Broadband in the Spectrometer Configuration window).

'a' is the setting for fixed frequency (Fixed Frequency in the Spectrometer Configuration window).

'm' is the setting for imaging modulator (SIS Modulator in the Spectrometer Configuration window).

See also: *VnmrJ Installation and Administration*

Related:	<code>config</code>	Display current configuration and possibly change it (M)
	<code>rfchtype</code>	Type of rf channel (P)

R

rfwg RF waveform generator (P)

Description: Configuration parameter for whether a waveform generator board is present or not on the current rf channel. The value for each channel is set using the Waveform Generator label in the Spectrometer Configuration window.

Values: 'n' is setting for no waveform generator board on the channel (Not Present choice in Spectrometer Configuration window).

'y' is setting for a waveform generation board on the channel (Present choice in Spectrometer Configuration window).

See also: *VnmrJ Installation and Administration*

Related: [config](#) Display current configuration and possibly change it (M)

right Set display limits to right half of screen (C)

Description: Sets the horizontal control parameters, [sc](#) and [wc](#), to produce a display (and subsequent plot) in the right portion of the screen (and page). For 2D data, space is left for the scales.

See also: *NMR Spectroscopy User Guide*

Related: [center](#) Set display limits for center of screen (C)
[full](#) Set display limits for a full screen (C)
[fullt](#) Set display limits for full screen with room for traces (C)
[left](#) Set display limits for left half of screen (C)
[sc](#) Start of chart (P)
[wc](#) Width of chart (P)

rights Determine an operator's specified right (C)

Applicability: Walkup

Syntax: `rights('right'<,'errval'><:$ret>`

Description: The rights program queries the rights database to determine if the current operator has the specified right. This command is used by the interface designer to determine if and how certain options are presented. An operator does not typically use this command. The system administrator sets (restricts) the rights for an operator using VnmrJ administrator interface. By default, the rights command grants any requested right. Rights requested that are not in the rights database are granted. Granting a right means that the rights program returns a 1 to the calling macro.

Arguments: `right` — a specific operator right, not case sensitive.

- 1 is returned by the command if the specified `right` is granted or the `right` is not in the rights data base
- 0 is default value returned by the command if the `right` is both in the database and the operator does not have the specified right.

`errval` — optional argument specifying return value if a right is both in the database and the operator does not have the specified right.

`$ret` — variable holding the return value from the `right` command.

Examples: `rights('prioritySample',-1):$ok`

Sets `$ok` to -1 if the `prioritySample` right is not granted. A value of 1 is returned if the `prioritySample` is granted. Returning either a 0 or -1 if a right is not granted lets the interface designer choose to show or gray out a control.

See also: *VnmrJ Installation and Administration* and *VnmrJ Walkup* manuals.

rinput **Input data for a regression analysis (M)**

Description: Formats data for regression analysis and places the data into the file `regression.inp`. The program is interactive. If a `regression.inp` already exists, `rinput` starts by asking if you want to overwrite the file. Type `y` and press the Return key. It then asks for an x-axis title and a y-axis title. Enter the titles as asked (for no title, simply press Return). Next, `rinput` asks you to input the data in pairs. Separate each pair of values with a blank and press Return after the second value. At the end of the data set, press Return in response to the request for data. If you have another data set, type `y` and press Return to the question and then type in the data when it is asked for.

See also: *NMR Spectroscopy User Guide; User Programming*

Related: `expl` Display exponential or polynomial curves (C)
`poly0` Find mean of data in the file `regression.inp` (C)

r1 **Set reference line in directly detected dimension (M)**

Syntax: `r1<(frequency)>`

Description: Sets the direct dimension reference line, taking into account any frequency scaling with the `scalesw` parameter.

Arguments: `frequency` is a value, in Hz, to assign to the reference line. The default is the cursor position `cr`. To enter the value in ppm, add a `p` suffix.

Examples: `r1`
`r1(0)`
`r1(7.2p)`

See also: *NMR Spectroscopy User Guide*

Related: `cr` Current cursor position in directly detected dimension (P)
`cr1` Clear ref. line in directly detected dimension (C)
`reffrq` Reference frequency of the reference line (P)
`r11` Set ref. line in 1st indirectly detected dimension (M)
`r12` Set ref. line in 2nd indirectly detected dimension (M)
`scalesw` Scale spectral width in directly detected dimension (P)

r11 **Set reference line in 1st indirectly detected dimension (M)**

Syntax: `r11<(frequency)>`

Description: Sets the first indirect dimension reference line, taking into account any frequency scaling with the `scalesw1` parameter.

Arguments: `frequency` is a value, in Hz, to assign to the reference line. The default is the cursor position `cr1`. You can enter the suffixes `p`, `d`, or `k` to mean ppm, decoupler ppm, and kilo, respectively. These suffixes are exactly equivalent to using `*sfrq`, `*dfrq`, and `*1000`. Thus, if you are doing a 2D experiment in which the indirect axis is determined by the decoupler channel, you might enter, for example, `r11(10d)`, which is equivalent to `r11(10*dfrq)`.

Examples: `r11`
`r11(0)`
`r11(7.2p)`

See also: *NMR Spectroscopy User Guide*

Related: `cr1` Cursor position in 1st indirectly detected dimension (P)
`cr11` Clear ref. line in 1st indirectly detected dimension (M)
`dfrq` Transmitter frequency of first decoupler (P)
`refpos2` Position of reference frequency in 2nd indirect dimension (P)

R

<code>r1</code>	Set ref. line in directly detected dimension (M)
<code>r12</code>	Set ref. line in 2nd indirectly detected dimension (M)
<code>scalesw1</code>	Scale spectral width in 1st indirectly detected dimension (P)
<code>sfrq</code>	Transmitter frequency of observe nucleus (P)

r12 **Set reference line in 2nd indirectly detected dimension (M)**

Syntax: `r12<(frequency)>`

Description: Sets the second indirect dimension reference line, taking into account any frequency scaling with the `scalesw2` parameter.

Arguments: `frequency` is a value, in Hz, to assign to the reference line. The default is the cursor position `cr2`. You can enter the suffixes `p`, `d`, or `k` to mean ppm, decoupler ppm, and kilo, respectively. These suffixes are exactly equivalent to using `*sfrq`, `*dfrq`, and `*1000`. Because there is no suffix for the second decoupler (i.e., the third channel), to reference the third axis using `r12` you might enter (e.g., `r12(45*dfrq2)`).

Examples: `r12`
`r12(0)`
`r12(7.2p)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>cr2</code>	Cursor position in 2nd indirectly detected dimension (P)
	<code>crl</code>	Clear ref. line in directly detected dimension (C)
	<code>crl1</code>	Clear ref. line in 1st indirectly detected dimension (C)
	<code>crl2</code>	Clear ref. line in 2nd indirectly detected dimension (C)
	<code>dfrq</code>	Transmitter frequency of first decoupler (P)
	<code>dfrq2</code>	Transmitter frequency of second decoupler (P)
	<code>r1</code>	Set ref. line in directly detected dimension (M)
	<code>r11</code>	Set ref. line in 1st indirectly detected dimension (M)
	<code>scalesw2</code>	Scale spectral width in 2nd indirectly detected dimension (P)
	<code>sfrq</code>	Transmitter frequency of observe nucleus (P)

rm **Delete file (C)**

Syntax: `rm(file1<,file2,...>)`

Description: Removes one or more files from the file system, functioning like the UNIX command of the same name. Because it allows wildcard characters (`*` and `?`) in the command argument and recursive file deletion with the `-r` option, `rm` is very powerful. But it can be quite dangerous—without warning important files can be inadvertently deleted, even by experienced users. **Using `rm` to delete files in VnmrJ is not recommended.** The `delete` command is provided as a safer alternative.

Arguments: `file1, file2, ...` are names of files to delete.

See also: *NMR Spectroscopy User Guide*

Related:	<code>delete</code>	Delete a file, parameter directory, or FID directory (C)
	<code>delexp</code>	Delete an experiment (C)
	<code>exists</code>	Determine if a parameter, file, or macro exists (C)
	<code>mv</code>	Move and/or rename a file (C)
	<code>rename</code>	Move and/or rename a file (C)

rmdir **Remove directory (C)**

Syntax: `rmdir(directory)`

Description: Removes one or more empty directories (i.e., directories without files).

Arguments: `directory` is the name of the directory to be removed.

Examples: `rmdir( '/home/dan/temp' )`

See also: *NMR Spectroscopy User Guide*

Related:	<code>delete</code>	Delete a file, parameter directory, or FID directory (C)
	<code>dir</code>	List files in current directory (C)
	<code>lf</code>	List files in current directory (C)
	<code>ls</code>	List files in current directory (C)
	<code>mkdir</code>	Create new directory (C)

rmsAddData Add transformed data files with weighting (U)

Applicability: Systems with multiple receivers.

Description: This command is not normally executed directly by the user.

Roesy Convert the parameter to a ROESY experiment (M)

Description: Convert the parameter to a rotating frame Overhauser effect spectroscopy (ROESY) experiment.

Roesy1d Convert the parameter set to a Roesy1d experiment (M)

Description: Convert the parameter set to a 1D rotating frame Overhauser effect spectroscopy (Roesy1D) experiment.

See also: *NMR Spectroscopy User Guide*

Related:	<code>Proton</code>	Set up parameters for ^1H experiment (M).
	<code>sel1d</code>	Selective 1D protocols to set up (M).

rof1 Receiver gating time preceding pulse (P)

Description: Sets the period of time in most pulse sequences when the receiver is gated off before each pulse. This allows the amplifier to fully turn on before the start of the pulse. Systems are configured with linear amplifiers that are normally “blanked” to give the best possible signal-to-noise (i.e., the amplifiers are turned off when the receiver is turned on). The $^1\text{H}/^{19}\text{F}$ amplifiers have a short turn-on time, usually 1 to 5 μs following the removal of blanking by turning the receiver off. The low-frequency amplifier modules have a longer turn-on time, about 40 to 60 μs .

Values: Typically 2-5 microseconds.

See also: *NMR Spectroscopy User Guide*

Related:	<code>rof2</code>	Receiver gating time following pulse (P)

rof2 Receiver gating time following pulse (P)

Description: Sets the time after the final pulse in each pulse sequence that the receiver is gated off before acquisition begins. If “pulse breakthrough” effects are seen (a spike in the beginning of the FID), increasing `rof2` can reduce or eliminate the problem, particularly for low-frequency nuclei.

Values: Typically 10 microseconds.

R

See also: *NMR Spectroscopy User Guide*

Related: `rofl` Receiver gating time preceding pulse (P)
`setlp0` Set parameters for zero linear phase (M)

rofl3 Receiver gating time following T/R switch (P)

Description: Sets the time when the receiver is gated on following the T/R switch during the pulse. This allows for the elimination of pulse artifacts during the acquisition period.

rotate Rotate 2D data (C)

Syntax: `rotate<(number_degrees)>`

Description: Rotates a 2D spectrum. Both complex and hypercomplex 2D data will work.

Arguments: `number_degrees` is the amount of counter-clockwise rotation, in degrees. The default is 45.

See also: *NMR Spectroscopy User Guide*

Related: `foldcc` Fold INADEQUATE data about 2-quantum axis (C)
`foldj` Fold J-resolved 2D spectrum about $f1=0$ axis (C)
`foldt` Fold COSY-like spectrum along diagonal axis (C)

rotorsync Rotor synchronization (P)

Applicability: Systems with the solids rotor synchronization module.

Description: Configuration parameter that identifies if the system has the optional solids rotor synchronization module. The value of `rotorsync` is set using the Rotor Synchronization label in the Spectrometer Configuration window. Rotor synchronization requires either the Acquisition Controller board (Part No. 969204) or the Pulse Sequence Controller board (Part No. 992560) in the system.

Values: 1 is setting that system has solids rotor synchronization (Present choice in the Spectrometer Configuration window).

0 is setting that system does not have solid rotor synchronization (Not Present choice in the Spectrometer Configuration window).

See also: *VnmrJ Installation and Administration*

Related: `config` Display current configuration and possibly change it (M)

rp Zero-order phase in directly detected dimension (P)

Description: Specifies the right phase-correction angles along the directly detected dimension according to

$$\text{absorption spectrum}(\omega) = \text{real channel}(\omega) * \sin \theta + \text{imaginary channel}(\omega) * \cos \theta$$

where the phase angle θ is a function of frequency:

$$\theta = \text{rp} + (\omega - \omega_0) * \text{lp}$$

ω_0 is defined as the right end of the spectrum. This dimension is referred to as the f_2 dimension in 2D data sets, f_3 dimension in 3D data sets, and so on.

Values: -360 to +360, in degrees.

See also: *NMR Spectroscopy User Guide*

Related:	<code>aph</code>	Automatic phase adjustment of spectra (C)
	<code>aph0</code>	Automatic phase of zero-order term (C)
	<code>lp</code>	First-order phase in directly detected dimension (P)
	<code>rp1</code>	Zero-order phase in 1st indirectly detected dimension (P)
	<code>rp2</code>	Zero-order phase in 2nd indirectly detected dimension (P)
	<code>setlp0</code>	Set parameters for zero linear phase (M)

rp1 Zero-order phase in 1st indirectly detected dimension (P)

Description: Specifies the right phase parameter along the first indirectly detected dimension, in degrees, for the f_1 dimension of a multidimensional data set during the process of phase-sensitive 2D transformation.

See also: *NMR Spectroscopy User Guide*

Related:	<code>lp1</code>	First-order phase in 1st indirectly detected dimension (P)
	<code>rp</code>	Zero-order phase in directly detected dimension (P)
	<code>rp2</code>	Zero-order phase in 2nd indirectly detected dimension (P)

rp2 Zero-order phase in 2nd indirectly detected dimension (P)

Description: Controls the zero-order phase constant along the second indirectly detected dimension during a `ds`, `dconi`, or equivalent display operation on the 2D data or a 1D trace therein. This dimension is often referred to as the f_2 dimension.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dconi</code>	Interactive 2D contour display (C)
	<code>ds</code>	Display a spectrum (C)
	<code>lp2</code>	First-order phase in 2nd indirectly detected dimension (P)
	<code>rp</code>	Zero order phase in directly detected dimension (P)

rt Retrieve FIDs (M)

Syntax: `rt<(file<,'nolog'>)>`

Description: Retrieves FIDs from a file into the current experiment.

The `rt` macro does not copy the FID into the experiment. Instead, it links access to the original FID from the experiment. Most of the time, this behavior is desired, because the FID file is seldom changed. By making a link, disk space is also conserved. However, if the FID file in the experiment is written to, the data in the original file is also written to. It is best to make a copy of a FID file before altering it. The `makefid` command alters the FID file. The manual entry for `makefid` gives details on how to make a copy of the FID.

As another somewhat subtle point, because the FID in the experiment is a link to another .fid file, if that .fid file is removed, the link from the experiment may be gone. If you expect the FID in the experiment to be there, even if you delete the .fid file from where it was retrieved using `rt`, you should explicitly copy the file into the experiment.

Arguments: `file` is the name of the file that, with the suffix `.fid` added, contains the FIDs to be retrieved. The default is that the system prompts for the name (in that case, the name can be given without single quotes). If `file.fid` does not exist and `file.par` does, `rt` retrieves the parameters from `file.par`.

'nolog' is a keyword specifying that the log file is not to be retrieved.

Examples: `rt`
`rt('/vnmr/fidlib/fid1d')`

See also: *NMR Spectroscopy User Guide*

Related: **fixpar** Correct parameter characteristics in experiment (M)
makefid Make a FID element using numeric text input (C)
rtp Retrieve parameters (M)
rtv Retrieve individual parameters (C)
svf Save FIDs in current experiment (M)

rtcmx Return Spinsight data into current experiment (C)

Syntax: `rtcmx<(file)>`

Description: Retrieves Spinsight data into the current experiment.

Arguments: `file` is the name of the file. The default is that the macro prompts for the file name.

Alternate: Load button in the **files** program.

Examples: `rtcmx`
`rtcmx('redor.data')`

See also: *NMR Spectroscopy User Guide*

Related: **files** Interactively handle files (C)

rtp Retrieve parameters (M)

Syntax: `rtp<(file)>`

Description: Retrieves parameters from a file into the current experiment.

Arguments: `file` is the name of the file that, with the suffix `.par` added, contains the parameters to be retrieved;. The default is that the system prompts for the name (in that case, the name can be given without single quotes). If `file.par` does not exist and `file.fid` does, `rtp` retrieves the parameters only from `file.fid`.

Examples: `rtp`
`rtp('/vnmr/stdpar/P31')`

See also: *NMR Spectroscopy User Guide*

Related: **fixpar** Correct parameter characteristics in experiment (M)
rt Retrieve FIDs (M)
rtv Retrieve individual parameters (C)
svp Save parameters from current experiment (M)

rts Retrieve shim coil settings (C)

Syntax: `rts(file)<:status>`

Description: Locates a preexisting file of shim settings and copies the settings into the current parameter set of the current experiment and sets `load='y'` to facilitate subsequent loading of shims with **su** (or related commands or macros). If the shim file is not found, `rts` displays the file names it tried.

The `rts` command returns shims from a `.fid` file or a `.par` file, selecting the shim parameters from the parameters stored there.

Arguments: `file` — the name of a file containing the shim coil settings to be retrieved. If the file name is an absolute path, `rts` uses it with no modifications. Otherwise, `rts` searches the applications directories.

`status` — the return variable with one of the following values after `rts` finishes searching for the shim coil settings file:

- 0 indicates that `rts` failed to find requested file.
- 1 indicates that `rts` found the requested file, either as an absolute path or in the `shims` directory of the first application directory.
- ≥ 2 indicates that `rts` found the requested file in `shims` subdirectory of the second, third, or later application directory.

Examples: `rts('acetone')`
`rts('bb10mm'):r1`

See also: *NMR Spectroscopy User Guide*

Related: `load` Load status of displayed shims (P)
`su` Submit a setup experiment to acquisition (M)
`svs` Save shim coil settings (C)

rttmp Retrieve experiment data from experiment subfile (M)

Syntax: `rttmp(file)`

Description: Retrieves experiment data—parameters, FID, and transformed spectrum—from the file specified in a subdirectory inside `curexp+ '/subexp'`.

Arguments: `file` is the name of the subfile from which to retrieve the experiment data.

Examples: `rttmp('H1')`
`rttmp('cosy')`

See also: *NMR Spectroscopy User Guide*

Related: `cptmp` Copy experiment data into experiment subfile (M)
`curexp` Current experiment directory (P)
`svtmp` Move experiment data into experiment subfile (M)

rtv Retrieve individual parameters (C)

Syntax: `rtv<(file,par1<,index1<,par2,index2...>>>>><:val>`
`rtv('paramaster','noabort','parameter'):$pm`

Description: Retrieves one or more parameters from a parameter file. The file might have been made with `svf` or `svp` or `sd` commands, or it might be from another experiment. If no return argument is added, the parameters are copied into the experiment's current tree. If the parameter does not already exist in the current tree, it is created. If the returned parameter is an array, the entire array is returned.

`rtv` returns values into the macro if a return argument is added. This form of `rtv` command, in which values are passed only to macro variables, avoids the creation of additional parameters in the experiment's current tree.

Arguments: `file` — name of the directory or a parameter file. If the supplied value for `file` is a directory (with or without the `.fid` or `.par` extension), the parameters are retrieved from the `procpa` file in that directory. If the supplied value does not correspond to a directory but rather is a parameter file, that file is used. The default is that `rtv` prompts for a file name. In that case, the file name can be given without single quotes.

`par1,index1,par2,index2,...` — name and array index of one or more parameters to be retrieved. The default for each array index argument is the first index. Including the array index for a parameter is only useful when returning values to the macro through a return argument.

`val` — return argument for values to return to the macro. If the requested parameter do not exist in the parameter file, `rtv` will abort.

`noabort` — keyword option must follow the `'parmaster'` keyword and precede the `parameter` argument. This option applies to a single parameter. Command does not abort if the requested parameter does not exist.

`parmaster` — filename of the parameter set.

`parameter` — the parameter name.

Executing `rtv` without macro return values causes the `fixpar` macro run. The macro `fixpar` is not executed if return values are requested. `rtv` will prompt for a file name if the command is executed without an argument. The filename given in response to the prompt does not require single quotes.

In LC-NMR, `rt` will retrieve the `lcdata` (and `drunlog`) files if these files were saved along with the NMR data by using `svf`.

Examples: `rtv`
`rtv('/vnmr/parlib/cosy.par', 'phase')`
`rtv('/vnmr/parlib/cosy.par', 'noabort', 'phase')`

See also: *NMR Spectroscopy User Guide* and *User Programming* manuals

Related: `rt` Retrieve FIDs (M)
`rtp` Retrieve parameters (M)
`sd` Set first decoupler frequency to cursor position (M)
`svf` Save FIDs in current experiment (M)
`svp` Save parameters from current experiment (M)

rtx Retrieve parameters based on rtx rules (C)

Syntax: `rtx(filename <, tree <, keyword1 <, keyword2 >>>)`

Description: The `rtx` command retrieves parameters from `filename`, based on the setting of the `P_LOCK` protection bit and using the rules below.

Arguments: `tree` is `'current'`, `'processed'`, `'global'`, or `'systemglobal'`.
`keyword1` may be `'keep'` or `'rt'`. The default is `'keep'`.
`keyword2` may be `'clear'` or `'noclear'`. The default is `'clear'`.
`keyword2` determines if the `P_LOCK` bit is cleared after `rtx` is executed.

Truth table for `rtx`.

<i>Status of P_LOCK bit in current exp</i>	<i>Status of P_LOCK bit in filename</i>	<i>keyword1</i>	<i>result</i>
on	on	keep or rt	do not rt
on	off	keep or rt	do not rt
off	on	keep or rt	do rt
off	off	keep	do not rt
off	off	rt	do rt
<no parameter>	on	keep or rt	do rt
<no parameter>	off	keep	do not rt
<no parameter>	off	rt	do rt

See also: *NMR Spectroscopy User Guide*

Related: `execpars` Set up the exec parameters (M)
`rtp` Retrieve parameters (M)

S

s	Save display parameters as a set (M)
s(n)	Save display parameters (C)
s2pul	Set up parameters for standard two-pulse sequence (M)
sa	Stop acquisition (C)
sample	Submit change sample, Autoshim experiment to acquisition (M)
samplename	Sample name (P)
save	Save data (M)
savefile	Base file name for saving files (P)
saveglobal	Save selected parameters from global tree (P)
sb	Sinebell constant in directly detected dimension (P)
sb1	Sinebell constant in 1st indirectly detected dimension (P)
sb2	Sinebell constant in 2nd indirectly detected dimension (P)
sbs	Sinebell shift in directly detected dimension (P)
sbs1	Sinebell shift in 1st indirectly detected dimension (P)
sbs2	Sinebell shift in 2nd indirectly detected dimension (P)
sc	Start of chart (P)
sc2	Start of chart in second direction (P)
scalelimits	Set limits for scales in regression (M)
scalesw	Set scaling factor for multipulse experiments (M)
scalesw	Scale spectral width in directly detected dimension (P)
scalesw1	Set f_1 scaling factor for 2D multipulse experiments (M)
scalesw1	Scale spectral width in 1st indirectly detected dimension (P)
scalesw2	Scale spectral width in 2nd indirectly detected dimension (P)
sd	Set first decoupler frequency to cursor position (M)
sd2	Set second decoupler frequency to cursor position (M)
sd3	Set third decoupler frequency to cursor position (M)
sda	Set first decoupler frequency array (M)
sd2a	Set second decoupler frequency array (M)
sd3a	Set third decoupler frequency array (M)
sdp	Show diffusion projection (M)
selld	Apptype macro for Selective 1D experiments
select	Select spectrum, FID, trace, or 2D plane without display (C)
selex	Defines excitation band (M)
selexcit	Set up PFG selective excitation pulse sequence (M)
selexHT	Set up a selective Hadamard experiment (M)
send2vnmr	Send a command to VnmrJ (U)
seqfil	Pulse sequence name (P)
seggen	Initiate compilation of user's pulse sequence (M,U)
serverport	Returns the VnmrJ network listening port value (C)
set2D	General setup for 2D experiments (M)
set2d	General setup for 2D experiments (M)
set3dproc	Set 3D processing (C)
setallshims	Set all shims into hardware (M)

S

<code>setcolor</code>	Set colors for graphics window and for plotters (C)
<code>setdecpars</code>	Set decoupler parameter values from probe file (M)
<code>setdec2pars</code>	Set decoupler 2 parameter values from probe file (M)
<code>setdgroup</code>	Set the Dgroup of a parameter in a tree (C)
<code>setenumeral</code>	Set values of a string parameter in a tree (C)
<code>setether</code>	Connect or reconnect host computer to Ethernet (U)
<code>setexport</code>	Set parameter bits for use with protocols (M)
<code>setfrq</code>	Set frequency of rf channels (C)
<code>setgauss</code>	Set a Gaussian fraction for lineshape (M)
<code>setgcal</code>	Set the gradient calibration constant (M)
<code>setgcoil</code>	Assign sysgcoil configuration parameter (M)
<code>setgrid</code>	Divide graphics window into rows and columns (C)
<code>setgroup</code>	Set group of a parameter in a tree (C)
<code>sethtfrq1</code>	Set a Hadamard frequency list from a line list ((M)
<code>sethw</code>	Set values for hardware in acquisition system (C)
<code>setint</code>	Set value of an integral (M)
<code>setlimit</code>	Set limits of a parameter in a tree (C)
<code>setlk</code>	Set up lock parameters (M)
<code>setlockfreq</code>	Set lock frequency (M)
<code>setLP</code>	Set up linear prediction in the direct dimension (M)
<code>setLP1</code>	Set F1 linear prediction parameters (M)
<code>setlp0</code>	Set parameters for zero linear phase (M)
<code>setnoether</code>	Disconnect host computer from Ethernet (U)
<code>setoffset</code>	Calculate offset frequency for given nucleus and ppm (M)
<code>setparams</code>	Write parameter to current probe file (M)
<code>setpen</code>	Set maximum number of HP plotter pens (M)
<code>setplotdev</code>	Return characteristics of a named plotter (C)
<code>setpower</code>	Set power and pulsewidth for a given γB_1 value (M)
<code>setprotect</code>	Set protection mode of a parameter (C)
<code>setrc</code>	Set receiver constants (M)
<code>setref</code>	Set frequency referencing (M)
<code>setref1</code>	Set freq. referencing for 1st indirectly detected dimension (M)
<code>setref2</code>	Set freq. referencing for 2nd indirect detected dimension (M)
<code>setscout</code>	Set up a scout run (M)
<code>setssfilter</code>	Set ss1sfrq to the frequencies of each suppressed solvents (M)
<code>setsw</code>	Set spectral width (M)
<code>setsw1</code>	Set spectral width in evolution dimension (M)
<code>setsw2</code>	Set spectral width in 2nd evolution dimension (M)
<code>setselfrqc</code>	Set selective frequency and width (M)
<code>setselinv</code>	Set up selective inversion (M)
<code>settclddefault</code>	Select default display templates for pulse sequence (M)
<code>settune</code>	Opens the Auto Tune Setup dialog (M)
<code>settype</code>	Change type of a parameter (C)
<code>setup</code>	Set up parameters for basic experiments (M)
<code>setup_dosy</code>	Set up gradient levels for DOSY experiments (M)
<code>setvalue</code>	Set value of any parameter in a tree (C)
<code>setwave</code>	Write a wave definition string into Pbox.inp file (M)

<code>setwin</code>	Activate selected window (C)
<code>sf</code>	Start of FID (P)
<code>sf1</code>	Start of interferogram in 1st indirectly detected dimension (P)
<code>sf2</code>	Start of interferogram in 2nd indirectly detected dimension (P)
<code>sfrq</code>	Transmitter frequency of observe nucleus (P)
<code>sh2pul</code>	Set up for a shaped observe excitation sequence (M)
<code>shdec</code>	Set up for shaped observe excitation sequence (M)
<code>shell</code>	Start a UNIX shell (C)
<code>shelli</code>	Start an interactive UNIX shell (C)
<code>shim</code>	Submit an Autoshim experiment to acquisition (C)
<code>shimset</code>	Type of shim set (P)
<code>showconfig</code>	Show system configuration settings (M)
<code>showconsole</code>	Show console configuration parameters (U)
<code>showfit</code>	Display numerical results of deconvolution (M)
<code>showloginbox</code>	Shows operator login dialog (M)
<code>shownumx</code>	x position counting from bottom left of every spectrum (P)
<code>shownumy</code>	y position counting from bottom left of every spectrum (P)
<code>showoriginal</code>	Restore first 2D spectrum in 3D DOSY experiment (M)
<code>showplotter</code>	Show list of currently defined plotters and printers (M)
<code>showplotq</code>	Display plot jobs in plot queue (M)
<code>showprintq</code>	Display print jobs in print queue (M)
<code>showprotunegui</code>	Show the graphical interface while tuning (P)
<code>showrfmon</code>	Show RF Monitor Button in Hardware Bar (P)
<code>showstat</code>	Display information about status of acquisition (M,U)
<code>sin</code>	Find sine value of an angle (C)
<code>sine</code>	Find values for a sine window function (M)
<code>sinebell</code>	Select default parameters for sinebell weighting (M)
<code>sinesq</code>	Find values for a sine-squared window function (M)
<code>size</code>	Returns the number of elements in an arrayed parameter (O)
<code>slfreq</code>	Measured line frequencies (P)
<code>slw</code>	Spin simulation linewidth (P)
<code>smaxf</code>	Maximum frequency of any transition (P)
<code>sminf</code>	Minimum frequency of any transition (P)
<code>smsport</code>	Sample Management System serial port connection (P)
<code>sn</code>	Signal-to-noise ratio (P)
<code>solppm</code>	Return ppm and peak width of solvent resonances (M)
<code>solvent</code>	Lock solvent (P)
<code>solvinfo</code>	Retrieve information from solvent table (C)
<code>sort</code>	Sort real values of a parameter (M)
<code>sp</code>	Start of plot in directly detected dimension (P)
<code>sp1</code>	Start of plot in 1st indirectly detected dimension (P)
<code>sp2</code>	Start of plot in 2nd indirectly detected dimension (P)
<code>spadd</code>	Add current spectrum to add/subtract experiment (C)
<code>spcfrq</code>	Display frequencies of rf channels (M)
<code>specdc3d</code>	3D spectral drift correction (P)
<code>spin</code>	Submit a spin setup experiment to acquisition (C)
<code>spin</code>	Sample spin rate (P)

S

<code>spincad</code>	Run SpinCAD program (C)
<code>spingen</code>	Compile SpinCAD pulse sequence *C)
<code>spinll</code>	Set up a slfreq array (M)
<code>spinner</code>	Open the Spinner Control window (C)
<code>spins</code>	Perform spin simulation calculation (C)
<code>split</code>	Split difference between two cursors (M)
<code>spintype</code>	Spinner Type ((P)
<code>spmax</code>	Take the maximum of two spectra (C)
<code>spmin</code>	Take minimum of two spectra in add/subtract experiment (C)
<code>spsm</code>	Enter spin system (M)
<code>spsub</code>	Subtract current spectrum from add/subtract experiment (C)
<code>sqcosine</code>	Set up unshifted cosine-squared window function (M)
<code>sqdir</code>	Study queue directory (P)
<code>sqend</code>	End a study queue (M)
<code>sqexp</code>	Load experiment from protocol (M)
<code>sqfilemenu</code>	Study queue file menu commands (M)
<code>sqmode</code>	Study queue mode (P)
<code>sqname</code>	Study queue parameter template (P)
<code>sqpars</code>	Create study queue parameters for imaging (M)
<code>sqprotocol</code>	Macro to create protocols (M)
<code>sqreset</code>	Reset study queue parameters for imaging (M)
<code>sqr</code>	Return square root of a real number (O)
<code>sqsavestudy</code>	Macro to save study parameters for imaging (M)
<code>qsinebell</code>	Set up unshifted sinebell-squared window function (M)
<code>srate</code>	Spinning rate for magic angle spinning (P)
<code>sread</code>	Read converted data into VnmrJ (C)
<code>srof2</code>	Calculate exact rof2 value for Cold Probes (M)
<code>ss</code>	Steady-state transients (P)
<code>ssecho</code>	Set up solid-state echo pulse sequence (M)
<code>ssecho1</code>	Set up parameters for SSECHO1 pulse sequence (M)
<code>ssfilter</code>	Full bandwidth of digital filter to yield a filtered FID (P)
<code>sslsfrq</code>	Center of solvent-suppressed region of spectrum (P)
<code>ssntaps</code>	Number of coefficients in digital filter (P)
<code>ssorder</code>	Order of polynomial to fit digitally filtered FID (P)
<code>stack</code>	Stacking mode for processing and plotting arrayed spectra (M)
<code>stackmode</code>	Stacking control for processing arrayed 1D spectra (P)
<code>startq</code>	Start a chained study queue (M)
<code>status</code>	Display status of sample changer (C,U)
<code>stdld</code>	Apptype macro for Standard 1D experiments (M)
<code>stdshm</code>	Interactively create a method string for autoshimming (M)
<code>sth</code>	Minimum intensity threshold (P)
<code>string</code>	Create a string variable (C)
<code>strtext</code>	Starting point for LP data extension in np dimension (P)
<code>strtext1</code>	Starting point for LP data extension in ni dimension (P)
<code>strtext2</code>	Starting point for LP data extension in ni2 dimension (P)
<code>strtlp</code>	Starting point for LP calculation in np dimension (P)
<code>strtlp1</code>	Starting point for LP calculation in ni dimension (P)

strtlp2	Starting point for LP calculation in ni2 dimension (P)
studyid	Study identification (P)
studypar	Study parameters (P)
studystatus	Study status (P)
studytime	Study time (P)
su	Submit a setup experiment to acquisition (M)
sub	Subtract current FID from add/subtract experiment (C)
substr	Select a substring from a string (C)
suselfrq	Select peak, continue selective excitation experiment (M)
svdat	Save data (C)
svf	Save FIDs in current experiment (M)
svfdf	Save FID data in FDF format (M)
svfdir	Directory for non-study data (P)
svfname	Filename parameter template for non-study data ((P)
Svfname	Create path for data storage (C)
svp	Save parameters from current experiment (M)
svs	Save shim coil settings (C)
svs	Spin simulation vertical scale (P)
svtmp	Move experiment data into experiment subfile (M)
sw	Spectral width in directly detected dimension (P)
sw1	Spectral width in 1st indirectly detected dimension (P)
sw2	Spectral width in 2nd indirectly detected dimension (P)
sw3	Spectral width in 3rd indirectly detected dimension (P)
sysgcoil	System gradient coil (P)
system	System type (P)
systemdir	VnmrJ system directory (P)

s Save display parameters as a set (M)

Syntax: (1) `sset_number`
(2) `s (set_number)`

Description: Saves a copy of the current values of all display parameters. The set is data-independent because the parameters that govern a display (**sp**, **wp**, **vs**, etc.) are saved but no data is saved.

Arguments: `set_number` is number of the display parameter set to be saved.

Examples: `s2`
`s (3)`

See also: *NMR Spectroscopy User Guide*

Related: **fr** Full recall of display parameter set (M)
r Recall display parameter set (M)

s (n) Save display parameters (C)

Applicability: All

Syntax: `s (n<, noupdate>)`

Description: Saves a copy of the current values of all display parameters as display parameter set `n` in the current experiment

noupdate as second argument prevents the automatic update of interactive programs.

Arguments: `n=1 to 9`

Related: `fr(n)` Recall all the parameters of the specified display parameter set (C)
`r(n)` Recalls limited number of display parameters)

s2pul Set up parameters for standard two-pulse sequence (M)

Description: Converts the current experiment to an experiment suitable for the standard two-pulse sequence (S2PUL).

See also: *NMR Spectroscopy User Guide*

sa Stop acquisition (C)

Syntax: `sa<(option|number)>`

Description: Stops an experiment that has been submitted to acquisition. If experiment is active, it is stopped. Data is retained. `sa` applies to the experiment that you are joined to at the time the `sa` command is entered. Thus, if experiment 1 is active, you must be joined to experiment 1 for `sa` to stop that acquisition. If you are in experiment 2, entering `sa` has no effect on experiment 1.

When experiments are queued, the behavior of `sa` is more complex. If an experiment is active in `exp1` and queued in `exp2`, entering `sa` from `exp1` stops that experiment and immediately begins acquisition on `exp2`. Entering `sa` from `exp2`, on the other hand, removes `exp2` from the queue, without affecting the active experiment 1.

Entering `sa` from an experiment that is not active or queued has no effect.

Arguments: `option` is one of the following:

- `'eos'`, `'ct'`, `'scan'` are keywords to stop at the next `ct`.
- `'eob'`, `'bs'` are keywords to stop at the next block size.
- `'eof'`, `'nt'`, `'fid'` are keywords to stop at the next complete FID.
- `'eoc'`, `'il'` are keywords to stop at next complete `il` cycle (i.e., the latest block size that has been completed for all FIDs in interleave cycle).

`number` is an integer number to stop at the next `ct`, where the value of `ct` is a multiple of `number`. This is useful when you want to complete a phasecycle before stopping.

Examples: `sa`
`sa('ct')`
`sa(4)`

See also: *NMR Spectroscopy User Guide*

Related: `bs` Block size (P)
`ct` Completed transients (P)
`il` Interleave arrayed and 2D experiments (P)
`nt` Number of transients (P)
`ra` Resume acquisition stopped with `sa` command (C)

sample Submit change sample, Autoshim experiment to acquisition (M)

Applicability: Systems with a sample changer.

Description: Performs the combined operations `change`, `spin`, `lock`, and `shim`, making it a convenient setup command for a new sample.

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (C)
	<code>change</code>	Submit a change sample experiment to acquisition (M)
	<code>ga</code>	Submit experiment to acquisition and FT the result (C)
	<code>go</code>	Submit experiment to acquisition (C)
	<code>lock</code>	Submit an Autolock experiment to acquisition (C)
	<code>shim</code>	Submit an Autoshim experiment to acquisition (C)
	<code>spin</code>	Submit a spin setup experiment to acquisition (C)
	<code>su</code>	Submit a setup experiment to acquisition (M)

samplename **Sample name (P)**

Description: Specifies the name of the sample. It is saved with a liquids study.

See also: *NMR Spectroscopy User Guide*, *VnmrJ Walkup*

Related:	<code>cgsavestudy</code>	Macro to save study queue parameters (M)
	<code>notebook</code>	Notebook name (P)
	<code>page</code>	Name of page (P)
	<code>studypar</code>	Study parameters (P)

save **Save data (M)**

Description: Macro to save data. In a study, it uses `sqdir` and `autoname` to construct the data filename. If not in a study, it uses `svfdir` and `svfname` to construct the data filename.

See also: *NMR Spectroscopy User Guide*, *VnmrJ Walkup*

Related:	<code>acquire</code>	Acquire data (M)
	<code>autoname</code>	Create path for data storage (C)
	<code>autoname</code>	Prefix for automation data file (P)
	<code>sqdir</code>	Study queue directory (P)
	<code>svfdir</code>	Directory for non-study data (P)
	<code>Svfname</code>	Create path for data storage (C)
	<code>svfname</code>	Filename parameter template for non-study data ((P)

savefile **Base file name for saving files (P)**

Applicability: Systems with LC-NMR accessory.

Description: Contains the base file name using the format `savefile.001`, `savefile.002`, etc., to which a series of FIDs or data sets are saved. If `savefile` does not exist, the `parlc` macro can create it.

See also: *NMR Spectroscopy User Guide*

Related:	<code>parlc</code>	Create LC-NMR parameters (M)

saveglobal **Save selected parameters from global tree (P)**

Description: Saves an array of parameter names from the global or systemglobal tree. Whenever `go` is executed, the parameters listed are saved in the current tree with an underscore (`_`) appended. These parameters are copied back into the global tree (without the underscore) whenever processing by `wbs`, `wnt`, `wexp`, or `werr` occurs.

See also: *NMR Spectroscopy User Guide*

Related:	<code>go</code>	Submit experiment to acquisition (C)
	<code>loc</code>	Location of sample in tray (P)

sb Sinebell constant in directly detected dimension (P)

Description: Applies a sinebell constant along the directly detected dimension. This dimension is often referred to as the f_2 dimension in 2D data sets, the f_3 dimension in 3D data sets, etc.

Values: A positive value applies a sinebell of the form $\sin\left(\frac{t \cdot \pi}{2 \cdot sb}\right)$
 A negative value applies a squared sinebell function of form $\sin^2\left(\frac{t \cdot \pi}{2 \cdot sb}\right)$
 sb is given in seconds. Typical value is sb = 'n'.

See also: *NMR Spectroscopy User Guide*

Related:

sb1	Sinebell constant in 1st indirectly detected dimension (P)
sb2	Sinebell constant in 2nd indirectly detected dimension (P)
sbs	Sinebell shift constant in directly detected dimension (P)
sine	Find values for a sine window function (M)
sinebell	Select default parameters for sinebell weighting (M)
sinesq	Find values for a sine squared window function (M)

sb1 Sinebell constant in 1st indirectly detected dimension (P)

Description: Applies a sinebell constant along the first indirectly detected dimension. This dimension is often referred to as the f_1 dimension in multidimensional data sets. sb1 works analogously to the parameter sb. The “conventional” parameters, such as lb and gf, operate on the detected FIDs, while this “2D” parameter is used during processing of the interferograms.

Values: A positive value applies a sinebell of the form $\sin\left(\frac{t \cdot \pi}{2 \cdot sb1}\right)$
 A negative value applies a squared sinebell function of form $\sin^2\left(\frac{t \cdot \pi}{2 \cdot sb1}\right)$
 sb1 is given in seconds. Typical value is sb1 = 'n'.

See also: *NMR Spectroscopy User Guide*

Related:

sb	Sinebell constant in the directly detected dimension (P)
sb2	Sinebell constant in 2nd indirectly detected dimension (P)

sb2 Sinebell constant in 2nd indirectly detected dimension (P)

Description: Applies a sinebell constant along the second indirectly detected dimension. This dimension is often referred to as the f_2 dimension in multidimensional data sets. sb2 works analogously to the parameter sb. The value of sb2 can be set with wti on the 2D interferogram data.

Values: A positive value applies a sinebell of the form $\sin\left(\frac{t \cdot \pi}{2 \cdot sb2}\right)$
 A negative value applies a squared sinebell function of form $\sin^2\left(\frac{t \cdot \pi}{2 \cdot sb2}\right)$
 sb2 is given in seconds. Typical value is sb2 = 'n'.

See also: *NMR Spectroscopy User Guide*

Related:

sb	Sinebell constant in directly detected dimension (P)
sb1	Sinebell constant in 1st indirectly detected dimension (P)
wti	Interactive weighting (C)

sbs Sinebell shift in directly detected dimension (P)

Description: Working in combination with the parameter sb, sbs allows shifting the origin of the sinebell function along the directly detected dimension. This dimension is often referred to as the f_2 dimension in 2D data sets, the f_3 dimension in 3D data sets, etc.

Values: The origin is shifted according to the formula $\sin\left(\frac{(t - sbs) \cdot \pi}{2 \cdot sb}\right)$

The square of this function is applied if `sb` is negative. `sbs` is given in seconds. The typical value is `sbs='n'`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>sb</code>	Sinebell constant in directly detected dimension (P)
	<code>sbs1</code>	Sinebell shift in 1st indirectly detected dimension (P)
	<code>sbs2</code>	Sinebell shift in 2nd indirectly detected dimension (P)
	<code>sine</code>	Find values for a sine window function (M)
	<code>sinesq</code>	Find values for a sine squared window function (M)

sbs1 Sinebell shift in 1st indirectly detected dimension (P)

Description: Working in combination with the parameter `sb1`, `sbs1` allows shifting the origin of the sinebell function along the first indirectly detected dimension. This dimension is often referred to as the f_1 dimension in multidimensional data sets. `sbs1` works analogously to parameter `sbs`. The “conventional” parameters, such as `lb` and `gf`, operate on the detected FIDs, while this “2D” parameter is used during processing of the interferograms.

Values: The origin is shifted according to the form $\sin\left(\frac{(t - sbs1) \cdot \pi}{2 \cdot sb1}\right)$. The square of this function is applied if `sb1` is negative. `sbs1` is given in seconds. The typical value is `sbs1='n'`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>sb1</code>	Sinebell constant in 1st indirectly detected dimension (P)
	<code>sbs</code>	Sinebell shift constant in directly detected dimension (P)
	<code>sb2</code>	Sinebell constant in 2nd indirectly detected dimension (P)

sbs2 Sinebell shift in 2nd indirectly detected dimension (P)

Description: Working in combination with the parameter `sb2`, `sbs2` allows shifting the origin of the sinebell function along the second indirectly detected dimension. This dimension is often referred to as the f_2 dimension in multidimensional data sets. `sbs2` works analogously to parameter `sbs`. `sbs2` can be set with `wti` on the 2D interferogram data.

Values: The origin is shifted according to the formula $\sin\left(\frac{(t - sbs2) \cdot \pi}{2 \cdot sb2}\right)$. The square of this function is applied if `sb2` is negative. `sbs2` is given in seconds. The typical value is `sbs2='n'`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>sbs</code>	Sinebell shift constant in directly detected dimension (P)
	<code>sb2</code>	Sinebell constant in 2nd indirectly detected dimension (P)
	<code>wti</code>	Interactive weighting (C)

sc Start of chart (P)

Description: Positions of the start of the plotting position (the “chart”) with respect to the right edge of the plotter.

Values: 0 to `wcmax`, in mm

See also: *NMR Spectroscopy User Guide*

Related:	<code>sc2</code>	Start of chart in second direction (P)
	<code>wc</code>	Width of chart (P)
	<code>wcmax</code>	Maximum width of chart (P)

S

sc2 Start of chart in second direction (P)

Description: Controls the start of plotting position of the second axis (or y axis) of a 2D contour plot. The parameter **wc2** controls the width of the chart.

Values: 0 to **wc2max**, in mm.

See also: *NMR Spectroscopy User Guide*

Related: **sc** Start of chart (P)
wc2 Width of chart in second direction (P)
wc2max Maximum width of chart in second direction (P)

scalelimits Set limits for scales in regression (M)

Syntax: `scalelimits(x_start,x_end,y_start,y_end)`

Description: Causes the command **expl**, which is used by regression to display data, to use typed-in scale limits. The limits are retained as long as an **expl** display is retained.

Arguments: **x_start,x_end,y_start,y_end** are x-axis and y-axis starting and ending limits. The default is that **scalelimits** prompts for the limits.

See also: *NMR Spectroscopy User Guide, User Programming*

Related: **autoscale** Resume autoscaling after limits set by **scalelimits** (M)
expl Display exponential or polynomial curves (C)

scalesw Set scaling factor for multipulse experiments (M)

Description: Sets the spectral width scaling factor for the multipulse sequences set up by macros **br24** and **mrev8**. The value of the scaling factor is stored in the parameter **scalesw**.

See also: *User Guide: solid-State NMR*

Related: **br24** Set up BR24 multiple pulse experiment (M)
mrev8 Set up MREV8 multiple pulse experiment (M)
scalesw Scale spectral width in directly detected dimension (P)
scalesw1 Set f_1 scaling factor for 2D multipulse experiments (M)

scalesw Scale spectral width in directly detected dimension (P)

Description: Adjusts the frequency scale dimension used with the parameter sets in the sequences set up by the **br24**, **mrev8**, **ssecho**, and **xpolar1** macros. If **scalesw** is active, the labels for the frequency scales includes the letters **sc** in parentheses. A scaled frequency can be referenced using the **r1** macro.

Values: 'n', number greater than 0.0

See also: *User Guide: Solid-State NMR*

Related: **br24** Set up BR24 multiple pulse experiment (M)
mrev8 Set up MREV8 multiple pulse experiment (M)
r1 Set reference line (M)
scalesw Set scaling factor for multipulse experiments (M)
scalesw1 Scale spectral width in 1st indirectly detected dimension (P)
scalesw2 Scale spectral width in 2nd indirectly detected dimension (P)
ssecho Set up solid-state echo pulse sequence (M)
xpolar1 Set up parameters for XPOLAR1 pulse sequence (M)

scalesw1 Set f_1 scaling factor for 2D multipulse experiments (M)

Description: Sets the f_1 spectral width scaling factor for the multipulse sequences set up by the **br24** and **mrev8** macros. The value of the scaling factor is stored in the parameter **scalesw1**.

See also: *User Guide: Solid-State NMR*

Related: **br24** Set up BR-24 multiple pulse experiment (M)
mrev8 Set up MREV8 multiple pulse experiment (M)
scalesw1 Scale spectral width in 1st indirectly detected dimension (P)

scalesw1 Scale spectral width in 1st indirectly detected dimension (P)

Description: Analogous to the **scalesw** parameter except that **scalesw1** applies to first indirectly detected dimension of a multidimensional data set. A scaled frequency along this dimension can be referenced using the **r11** macro.

Values: 'n', number greater than 0.0

See also: *User Guide: Solid-State NMR*

Related: **r11** Set reference line in 1st indirectly detected dimension (M)
scalesw Scale spectral width in directly detected dimension (P)
scalesw1 Set f_1 scaling factor for 2D multipulse experiments (M)
scalesw2 Scale spectral width in 2nd indirectly detected dimension (P)

scalesw2 Scale spectral width in 2nd indirectly detected dimension (P)

Description: Analogous to the **scalesw** parameter except **scalesw2** applies to second indirectly detected dimension of a multidimensional data set. A scaled frequency along this dimension can be referenced using the **r12** macro.

Values: 'n', number greater than 0.0

See also: *User Guide: Solid-State NMR*

Related: **r12** Set reference line in 2nd indirectly detected dimension (M)
scalesw Set scaling factor for multipulse experiments (M)
scalesw1 Set f_1 scaling factor for 2D multipulse experiments (M)

sd Set first decoupler frequency to cursor position (M)

Description: Sets the first decoupler frequency offset parameter **dof** to place the first decoupler at the cursor position in the spectrum. This works only if the transmitter nucleus and first decoupler nucleus are the same (**tn=dn**).

See also: *NMR Spectroscopy User Guide*

Related: **dof** Frequency offset for first decoupler (P)
dn Nucleus of first decoupler (P)
sd2 Set second decoupler frequency to cursor position (M)
sd3 Set third decoupler frequency to cursor position (M)
sda Set first decoupler frequency array (M)
tn Nucleus for observe transmitter (P)

sd2 Set second decoupler frequency to cursor position (M)

Applicability: Systems with a second decoupler.

Description: Sets the second decouple frequency offset parameter **dof2** to place the second decoupler at the cursor position in the spectrum. This works only if the transmitter nucleus and second decoupler nucleus are the same (**tn=dn2**).

See also: *NMR Spectroscopy User Guide*

Related:	dn2	Nucleus for second decoupler (P)
	dof2	Frequency offset for second decoupler (P)
	sd	Set first decoupler frequency to cursor position (M)
	sd2a	Set second decoupler frequency array (M)
	tn	Nucleus for observe transmitter (P)

sd3 Set third decoupler frequency to cursor position (M)

Applicability: Systems with a third decoupler.

Description: Sets the third decoupler frequency offset parameter **dof3** to place the third decoupler at the cursor position in the spectrum. This works only if the transmitter nucleus and third decoupler nucleus are the same (**tn=dn3**).

See also: *NMR Spectroscopy User Guide*

Related:	dn3	Nucleus for third decoupler (P)
	dof3	Frequency offset for third decoupler (P)
	sd	Set first decoupler frequency to cursor position (M)
	sd3a	Set third decoupler frequency array (M)
	tn	Nucleus for observe transmitter (P)

sda Set first decoupler frequency array (M)

Description: Sets up an array of offset values for the first decoupler, using **sd** for the first decoupler position and **sda** for subsequent positions. This works only if the transmitter nucleus and first decoupler nucleus are the same (**tn=dn**).

See also: *NMR Spectroscopy User Guide*

Related:	dn	Nucleus for first decoupler (P)
	sd	Set first decoupler frequency to cursor position (M)
	sd2a	Set frequency array for second decoupler (M)
	sd3a	Set frequency array for third decoupler (M)
	tn	Nucleus for observe transmitter (P)

sd2a Set second decoupler frequency array (M)

Applicability: Systems with a second decoupler.

Description: Sets up an array of offset values for the second decoupler, using **sd2** for the first position and **sd2a** for subsequent positions. This works only if the transmitter nucleus and second decoupler nucleus are the same (**tn=dn2**).

See also: *NMR Spectroscopy User Guide*

Related:	dn2	Nucleus for second decoupler (P)
	sd2	Set second decoupler frequency to cursor position (M)
	sda	Set first decoupler frequency array (M)
	tn	Nucleus for observe transmitter (P)

sd3a Set third decoupler frequency array (M)

Applicability: Systems with a third decoupler.

Description: Sets up an array of offset values for the third decoupler, using **sd3** for the first position and **sd3a** for subsequent positions. This works only if the transmitter nucleus and third decoupler nucleus are the same (**tn=dn3**).

See also: *NMR Spectroscopy User Guide*

Related: **dn2** Nucleus for third decoupler (P)
sd3 Set third decoupler frequency to cursor position (M)
sda Set first decoupler frequency array (M)
tn Nucleus for observe transmitter (P)

sdp Show diffusion projection (M)

Description: Displays projection onto diffusion axis using the **dsp** facility. Use with 2D or 3D DOSY data after DOSY analysis. The unit of the resulting axis is D (10^{-10} m²/sec). Because **sdp** overwrites the parameters in the current experiment, use it in only an experiment in which it is okay for existing data to be overwritten.

See also: *NMR Spectroscopy User Guide*

Related: **dosy** Process DOSY experiments (M)

sel1d Apptype macro for Selective 1D experiments (M)

Description: Perform the actions for Selective 1D protocols to set up, process, and plot experiments.

Examples: **sel1d('setup')** – execute sel1d experimental setup
sel1d('process') – execute sel1d processing
sel1d('plot') – execute sel1d plotting

Related: **apptype** Application type (p)
execpars Set up the exec parameters (M)

select Select spectrum, FID, trace, or 2D plane without display (C)

Syntax: (1) **select**<('next' | 'prev' | selection) ><:index>
 (2) **select**<(<'f1f3' | 'f2f3' | 'f1f2'><, 'proj'>
 <, 'next' | 'prev' | plane>) ><:index>

Description: Directs future actions to apply to a particular spectrum or FID in a 1D array, to a trace in 2D (syntax 1), or to a particular 2D plane from a 3D data set (syntax 2). If **select** is called with no arguments, it returns the current index. When VnmrJ is first booted up, **select** is in 1D mode. **select** enters the 2D mode if any of the keywords 'f1f3', 'f2f3', 'f1f2', or 'proj' are present in the argument list. Entering the **ds** and **jexp** commands set **select** back in the 1D mode.

Arguments: For 1D operations (syntax 1):

- 'next' is keyword to increment by 1 the 1D spectrum or trace index.
- 'prev' is keyword to decrement by 1 the 1D spectrum or trace index.
- selection is a number selecting a 1D spectrum, FID, or trace.
- index returns the number of the current 1D spectrum, FID, or trace.

For selecting various 2D planes of a 3D data set (syntax 2):

- 'f1f3', 'f2f3', and 'f1f2' are types of 2D planes. The parameters **plane** and **index2** serve to indicate the exact 2D plane that is currently viewable by VnmrJ. Note that **index2** cannot be entered from the keyboard (i.e., you cannot select a new 2D plane by changing the value of **index2**); you must use the **select** command instead.
- 'proj' is keyword to use the 2D projection whose plane type is determined by the parameter **plane**.

- 'next' is keyword to increment the parameter `index2` to its next value and sets up VnmrJ to be ready to display the 2D plane whose number is the new `index2` value.
- 'prev' performs analogously except that `index2` is decremented.
- `plane` is a number selecting the plane.
- `index` returns the number of the current plane.

Examples: `select('next')`
`select(2):r1`
`select('f1f3')`

See also: *NMR Spectroscopy User Guide, User Programming*

Related: `arraydim` Dimension of experiment (P)
`ds` Display a spectrum (C)
`index2` Projection or 3D plane index selected (P)
`jexp` Join existing experiment (C)
`plane` Currently displayed 3D plane type (P)

selex **Defines excitation band (M)**

Syntax: `selex<(sh<,pw<,st<,ph<,fla<,trev>>>>>)>`

Description: Defines the excitation band from the position of cursors in the graphics window and reports them to user. It also sets `r1` to excitation bandwidth and `r2` to offset. `selex` is part of the Pbox software environment and uses the Pbox macros `pbox_bw` and `putwave`.

Arguments: `sh` is the name of a shape file.
`pw` is the pulsewidth, in sec.
`st` is the spin status: 0 for excitation, 0.5 for refocusing, or 1 for de-excitation.
`ph` is the phase (or phase cycle, see `wavelib/supercycles`).
`fla` is the flip angle.
`trev` is the time reversal. This argument can be used to cancel time reversal introduced by setting the spin status (`st`) to 1 for de-excitation.

Examples: `selex`
`selex('esnob',0.0,1,90.0)`

See also: *NMR Spectroscopy User Guide*

Related: `Pbox` Pulse shaping software (U)

selexcit **Set up PFG selective excitation pulse sequence (M)**

Applicability: Systems with a pulsed field gradient module.

Description: Prepares an experiment for PFG (pulsed field gradient) selective excitation, with presaturation option.

See also: *NMR Spectroscopy User Guide*

selexHT **Set up a selective Hadamard experiment (M)**

Description: Sets up parameters for a selective shaped pulse Hadamard-encoded test experiment.

See also: *NMR Spectroscopy User Guide*

Related: `htofs1` Hadamard offset in `ni` (P)
`fn1` Fourier number in 1st indirectly detected dimension (P)

<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
<code>ft2d</code>	Fourier transform 2D data (C)
<code>sethtfrql</code>	Set Hadamard frequency list from a line list (M)

send2vnmr Send a command to VnmrJ (U)

Syntax: `send2Vnmr $vnmruser/.talk command`

Description: Sends a command from UNIX to VnmrJ using the port number stored in the `$vnmruser/.talk` file. This file is created when the macro `listenon` is entered on the VnmrJ command line.

Arguments: `command` is any character string (commands, macros, or if statements) normally typed into the VnmrJ command line.

Examples: `send2Vnmr $vnmruser/.talk dg`

See also: *User Programming*

Related: `bootup` Macro executed automatically when VnmrJ activated (M)
`listenon` Enable receipt of messages from `send2Vnmr` (M)
`listenoff` Disable receipt of messages from `send2Vnmr` (M)

seqfil Pulse sequence name (P)

Description: Identifies the name of the pulse sequence to be used. The value of `seqfil` is displayed on the top line of the screen after the “Seq:” label. Macros used to set up new pulse sequences, such as `Dept` and `Apt`, automatically change the `seqfil` parameter.

See also: *NMR Spectroscopy User Guide*

Related: `pslabel` Pulse sequence label (P)

seqgen Initiate compilation of user's pulse sequence (M,U)

Syntax: (From VnmrJ) `seqgen(<-static,>file<.c>)`
(From UNIX) `seqgen <-static> file<.c> <file1,...>`

Description: Begins compilation of a user pulse sequence. When used from VnmrJ, the macro `seqgen` calls the UNIX shellscript `seqgen`, which can also be called directly from UNIX, as shown above. The `seqgen` shellscript then calls the compilation makefile `seqgenmake`, located in the directory `/vnmr/acqbin`.

The specified pulse sequence can be located in `~/vnmrsys/psglib` or in `/vnmr/psglib`. If two files with the same name exist in these two directories, the local directory (`~/vnmrsys/psglib`) takes precedence. For sequences in `/vnmr/psglib`, `seqgen` first copies the file into the local directory `~/vnmrsys/psglib` and then compiles it there; the resulting executable is then placed in `~/vnmrsys/seqlib`. A copy of the pulse sequence is also copied into the `seqlib` directory along with the executable. As it is running, `seqgen` reports where it found the specified sequence(s).

`seqgen` uses library files (object modules) found in `/vnmr/lib`. If `setuserpsg` and `psggen` has been run, the library files in the local directory `~/vnmrsys/psg` take precedence of those in `/vnmr/lib`.

Error messages are written into the file `file.errors`, where `file` is the name of the pulse sequence in `psglib` in which compilation is performed.

Note that `seqgen` not only accepts file names with and without extensions, but also accepts files specified with wildcards and complex paths (`seqgen` strips the directory part, and `seqgen /vnmr/psglib/apt` will compile `~/vnmrsys/psglib/atp.c` if it exists).

Arguments: `-static` is a keyword for `seqgen` to use static rather than dynamic binding. Static binding results in larger executables in `seqlib` (several hundred Kbytes), but these sequences execute slightly faster (i.e., the `go` command). While insignificant generally, faster execution is helpful in some special applications such as the Scout Scan™ mode of LC-NMR, where the time spent on the `go` command becomes critical. Static binding results in a fixed-size time gain, regardless of the number of increments; for large multidimensional experiments, the speed difference is not noticeable.

`file` is the file name of a standard two-pulse sequence.

`.c` is the extension on the file name.

`file1, file2, ...` are the names of files containing more sequences.

Examples: (From VnmrJ) `seqgen ('/vnmr/psglib/*.c')`
 (From UNIX) `seqgen /vnmr/psglib/*.c`
 (From UNIX) `seqgen apt dept noesy`
 (From UNIX) `seqgen -static lcld`

See also: *User Programming*

serverport Returns the VnmrJ network listening port value (C)

Applicability: VnmrJ

Syntax: `serverport`

Description: The `serverport` command returns the port number when VnmrJ opens a network port (socket) for other programs to send it network messages. See the `write('net', ...)` command for an example on how to use this port number.

Related: `write`

Write formatted text to a device (C)

set2D General setup for 2D experiments (M)

Syntax: `set2D<(F2_dig_res<, F1_dig_res>)>`

Description: Similar to `set2d` but does not execute `par2d` and does not make `sw1`, `rf11`, and `rfp1` decisions based on `tn=dn` condition.

Arguments: `F2_dig_res` is the f_2 digital resolution desired, in Hz/pt. Default is 6.

`F1_dig_res` is the f_1 digital resolution desired, in Hz/pt. Default is 12.

Related:	<code>rf11</code>	Reference peak position in 1st indirectly detected dimension (P)
	<code>rfp1</code>	Reference peak frequency in 1st indirectly detected dimension (P)
	<code>set2d</code>	General setup for 2D experiments (M)
	<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)

set2d General setup for 2D experiments (M)

Syntax: `set2d(experiment<, F2_dig_res<, F1_dig_res>>)`

Description: Runs the macro `par2d` to create new parameters needed for 2D experiments, then selects starting values for a number of parameters. The `set2d` macro is “internal” and not normally typed directly by the user.

Arguments: `experiment` is the name of a 2D experiment (e.g., 'noesy').

`F2_dig_res` is the f_2 digital resolution desired, in Hz/pt.

`F1_dig_res` is the f_1 digital resolution desired, in Hz/pt.

Examples: `set2d('cosyps')`
`set2d('hetcor',16)`
`set2d('het2dj',16,(2*sw1)/fn1)`

See also: *NMR Spectroscopy User Guide*

Related: `par2d` Create 2D acquisition parameters (M)

set3dproc Set 3D processing (C)

Syntax: `set3dproc(<'nocoef'><,directory>)>`

Description: Creates the file `procdat` that contains binary 3D information used by `ft3d` in processing the 3D FID data. It also creates the 3D parameter set `procp3d` that is used by the `select` command to display the 2D planes from the 3D transformed data. `set3dproc` can only create the proper 3D coefficient file if the parameters `phase` and `phase2` are used to generate States-Haberkorn (hypercomplex) or TPPI data along the t_1 and t_2 dimensions.

`set3dproc` creates the coefficient file for the following five values of `array` (where SH is States-Haberkorn):

- if `array=''` (null string), type of 3D data is TPPI(t_1) – TPPI(t_2)
- if `array='phase'`, type of 3D data is SH(t_1) – TPPI(t_2)
- if `array='phase2'`, type of 3D data is SH(t_2) – TPPI(t_1)
- if `array='phase2,phase'`, type of 3D data is SH(t_1) – SH(t_2)

If `array` is set to some other value, `set3dproc` cannot create the 3D coefficient file and an error is reported within VnmrJ.

Arguments: `'nocoef'` is a keyword that the 3D coefficient file `coef` is not to be created.
`directory` is the name of the directory for `procdat` and `procp3d`. The default is the subdirectory `info` in the directory `curexp`.

Examples: `set3dproc`
`set3dproc('nocoef','curexp/info3d')`

See also: *NMR Spectroscopy User Guide*

Related: `array` Parameter order and precedence (P)
`ft3d` Perform a 3D Fourier transform (M,U)
`phase` Phase selection (P)
`phase2` Phase selection for 3D acquisition (P)
`select` Select a spectrum or 2D plane without displaying it (C)
`wfft3` Process f_3 dimension during 3D acquisition (M)

setallshims Set all shims into hardware (M)

Description: Sets shims from the current parameter tree into hardware. `setallshims` is equivalent to entering `load='y'su` but without setting all the hardware parameters normally set by `su` (temperature, decoupling, transmitter initialization, etc.). The shims used depend on the `shimset` configuration. For the shim set on the Ultra•nmr shim system, `setallshims` is active only if hardware-to-software shim communication is enabled.

See also: *NMR Spectroscopy User Guide*

Related: `load` Load status of displayed shims (P)
`readallshims` Read all shims from hardware (M)
`readhw` Read current values of acquisition hardware (C)
`sethw` Set values for hardware in acquisition system (C)

<code>shimset</code>	Type of shim set (P)
<code>su</code>	Submit a setup experiment to acquisition (M)

setcolor Set colors for graphics window and for plotters (C)

Syntax: (1) `setcolor('pcl', item_index, 'color')`
 (2) `setcolor('hpgl', item_index, 'color')`
 (3) `setcolor('pen', pen_number, 'color')`
 (4) `setcolor('graphics', item_index, red, green, blue)`
 (5) `setcolor('ps', item_index, red, green, blue)`
 (6) `setcolor('plotter', black_plane, color_planes)`

Description: Sets colors used on the graphics window and on plotters. This command is a utility program used by the `color` macro and other macros. It is not expected that `setcolor` would be entered directly from the input window.

Arguments: 'pcl' is a keyword to set colors on a plotter device that uses the PCL language. PCL plotters are the laser type of plotter.
 'hpgl' is a keyword to set colors on a plotter device that uses the HPGL language. HPGL plotters are the pen type of plotter.
 'pen' is a keyword that next two arguments set the color for a physical pen on a plotter device that uses the HPGL language.
 'graphics' is a keyword to set colors on the graphics window.
 'ps' is a keyword to set colors on a plotter using the PostScript language.
 red, green, blue are three integers between 0 and 255 that set the amount of red, green, and blue color on the graphics window or PostScript plotter.
 'plotter' is a keyword that the next two arguments set the black mode and number of colors available for a plotter device.
 item_index is an index number from the following list that represents a specific drawing item.

8	background of images
9	real channel of an FID
10	imaginary channel of an FID
11	spectrum
12	integral
13	parameters
14	scale
15	threshold line (graphics device only)
16	second spectrum or FID in <code>addi</code> (graphics device only)
17	result spectrum or FID in <code>addi</code> (graphics device only)
18	cursors (graphics device only)
19	foreground of images
20	background color of graphics window (graphics device only)
20-35	contour 0 to contour 15 of absolute value 2D display
36-42	contours -7 to -1 of phased 2D display
44-50	contours 1 to 7 of phased 2D display

pen_number is an integer from 1 to 8 that specifies the physical pen used.
 color is a string for the color set for the device: 'red', 'green', 'blue', 'cyan', 'magenta', 'yellow', 'white', or 'black'.

`black_plane` is 1 or 0, specifying whether the plotter has a separate black mode. Because all currently supported plotters have this feature, the value is usually 1.

`color_planes` specifies how many colors are available. Use 3 for color plotters and 0 for black and white plotters.

Examples: `setcolor('pcl',11,'green')`
`setcolor('hpgl',11,'red')`
`setcolor('pen',2,'red')`
`setcolor('graphics',11,255,0,0)`
`setcolor('ps',11,255,255,0)`
`setcolor('plotter',1,0)`

See also: *NMR Spectroscopy User Guide*

Related: `addi` Start interactive add/subtract mode (C)
`color` Select plotting colors from a graphical interface (M)

setdecpars Set decoupler parameter values from probe file (M)

Syntax: `setdecpars`

Description: Reads from the probe file `pwxlvl`, `pw`, `pplvl`, `pp`, `dpwr`, `dmf`, `dmm`, `dres`, and `dseq` values, if they exist, and updates the current experiment parameters.

Related: `setdec2pars` Set decoupler 2 parameter values from probe file (M)

setdec2pars Set decoupler 2 parameter values from probe file (M)

Syntax: `setdec2pars`

Description: Reads from the probe file `pw2lvl`, `pw2`, `dpwr2`, `dmf2`, `dmm2`, `dres2`, and `dseq2` values, if they exist, and updates the current experiment parameters.

Related: `setdecpars` Set decoupler parameter values from probe file (M)

setdgroup Set the Dgroup of a parameter in a tree (C)

Syntax: `setdgroup(parameter,dgroup<,tree>)`

Description: Sets the Dgroup of a parameter in a tree. The application determines the usage of `setdgroup`. Only Tcl-dg currently uses this feature.

Arguments: `parameter` is the name of the parameter.
`dgroup` is an integer.
`tree` is 'current', 'global', 'processed', or 'systemglobal'. The default is 'current'. Refer to the description of the `create` command for more information on types of trees.

Examples: `setdgroup('a',1)`
`setdgroup('b',3,'global')`

See also: *User Programming*

Related: `create` Create new parameter in a parameter tree (C)

setenumer1 Set values of a string parameter in a tree (C)

Syntax: `setenumer1(parameter,N,enum1,enum2,...,enumN<,tree>)`

Description: Sets the possible values of a string parameter in a parameter tree. To remove enumerated values from a parameter, set argument `N` to 0 (see example below).

Arguments: `parameter` is the name of the parameter.
`N` is the number of enumeral values to be assigned to `parameter` (or removed from `parameter` if `N` is set to 0).
`enum1` to `enumN` are the possible string values of the parameter.
`tree` is 'current', 'global', 'processed', or 'systemglobal'.
The default is 'current'. Refer to the description of the `create` command for more information on types of trees.

Examples: `setenumeral('size',0)`
`setenumeral('size',2,'large','small')`
`setenumeral('user',3,'user','superuser','master',`
`'global')`

See also: *User Programming*

Related: `create` Create new parameter in a parameter tree (C)

setether Connect or reconnect host computer to Ethernet (U)

Description: Connects or reconnects the host computer to the Ethernet network. Only `root` can execute this shellscript properly. If the system is already connected to the Ethernet network, `setether` does nothing.

On systems running Solaris, `setether` undoes the work of `setnoether`. You cannot use `setether` unless you previously entered the `setnoether` command. `setether` restores the files `hostname.le0`, `defaultdomain`, and `defaultrouter` so that Ethernet is activated on the host computer when UNIX is rebooted.

See also: *VnmrJ Installation and Administration*

Related: `setnoether` Disconnect host computer from Ethernet (U)

setexport Set parameter bits for use with protocols (M)

Description: Set the parameter protection bits for use with the `rtx` command. Usually called by other macros, and not used from the command line.

Related: `rtx`
`cqprotocol` Create study queue parameters for liquids (M)

setfrq Set frequency of rf channels (C)

Syntax: `setfrq<(channel)><('nucleus')>`

Description: Calculates frequencies based on the nucleus (`tn`, `dn`, `dn2`, etc.), referencing (`lockfreq`), solvent, and the offset parameter (`tof`, `dof`, etc.). The result of the calculation is stored in parameters `sfrq`, `dfrq`, `dfrq2`, etc. The parameters are rounded to the resolution of the channel—either 0.1 or 100 Hz.

The `setfrq` command should never need to be entered from the keyboard. It is called automatically when the appropriate parameters are changed or a parameter set is returned. If a parameter is entered that affects a single frequency, `setfrq` is called from an internal underscore macro (e.g., `_tn`, `_tof`, `_dn`, `_dof`) to recalculate the frequency for that channel. Likewise, if a parameter is entered that affects all frequencies, `setfrq` is called from an internal underscore macro (e.g., `_solvent`, `_lockfreq`) to recalculate the frequencies.

Arguments: `channel` is a single integer specifying the rf channel to be set. The default is to calculate the frequencies for all rf channels.

nucleus displays or returns the frequency of the supplied nucleus. Channel 1 is assumed for rounding information and an offset (e.g., `tof` or `dof`) is not added to the result.

Examples: `setfrq`
`setfrq(2)`
`setfrq('P31'):freq`

See also: *NMR Spectroscopy User Guide*

Related: `spcfrq` Display frequencies of rf channels (M)

setgauss Set a Gaussian fraction for lineshape (M)

Syntax: (1) `setgauss(fraction)`
 (2) `setgauss(fraction*)`

Description: Modifies the output of a deconvolution using pure Lorentzian lineshape (`fitspec.outpar`) and makes it the input for a subsequent analysis (`fitspec.inpar`), after first modifying the Gaussian fraction. To allow this fraction to vary, use syntax 1; to fix the fraction, use syntax 2.

Arguments: `fraction` is the Gaussian fraction of the lineshape, a number from 0 to 1. To fix the fraction (syntax 2), suffix the value with an asterisk (*) and enclose the value in single quotes (see the second example below).

Examples: `setgauss(0.4)`
`setgauss('1.0*')`

See also: *NMR Spectroscopy User Guide*

Related: `fitspec` Perform spectrum deconvolution (C)

setgcal Set the gradient calibration constant (M)

Applicability: Systems with pulsed field gradients (PFG) or imaging capabilities.

Description: Determines the gradient calibration constant `gcal` by using a proton phantom of known dimensions. `setgcal` requests the linear dimension of the phantom in the readout direction. It uses the value entered, together with cursor separation of this dimension from the image profile and the strength of the readout gradient `gzlvl1` if pulsed field gradients, to calculate `gcal` in units of gauss/cm-DAC units. You are then prompted whether this value should be entered. If you answer yes, it is stored as a system constant in the your global file.

Note that a particular value of `gcal` is closely related to the current eddy current compensation settings. If these settings are changed (e.g., reading in a new `curecc` file), a different value of `gcal` should be expected.

Before running `setgcal`, use the pulse sequence set up by `profile` to acquire a signal from a known sized object while the gradient is on.

See also: *Pulsed Field Gradient Modules Installation; VnmrJ Imaging NMR*

Related: `gcal` Gradient calibration constant (P)
`profile` Set up pulse sequence for gradient calibration (M)

setgcoil Assign sysgcoil configuration parameter (M)

Syntax: `setgcoil<(file)>`

Description: Allows users to change the configured `gcoil` for the system. `setgcoil` updates the systemglobal parameter `sysgcoil` to the named table and updates the assignment value of the parameter `gcoil` in the named table. The directory

`$vnmrsystem/imaging/gradtables` must have write permission for all users for the macro to be effective. This table now exists in the system local `/var/vnmr/gradtables` directory, with a soft link from `$vnmrsystem/imaging/gradtables` to that directory.

Arguments: `file` is the any legal file name defined for the parameter `gcoil`.

See also: *VnmrJ Imaging NMR*

Related:	<code>config</code>	Display current configuration and possible change it (M)
	<code>gcoil</code>	Read data from gradient calibration tables (P)
	<code>sysgcoil</code>	System value for <code>gcoil</code> parameter (P)

setgrid **Divide graphics window into rows and columns (C)**

Syntax: `setgrid(row<,column>)`

Description: Divides graphics window into an array of rows and columns (or window panes). Only one pane is active at a time. An individual pane can be activated by double-clicking in it with the left mouse button or by entering `setwin` in the input window.

Arguments: `row` is the number of rows (maximum is 3) in the graphics window. If 0 is entered, the number of rows remains the same; e.g., in `setgrid(0,2)`, the number of rows is unchanged and two columns are created in each row.

`column` is the number of columns (maximum is 3) in the graphics window.

Examples: `setgrid(3)`
`setgrid(3,3)`
`setgrid(0,2)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>curwin</code>	Current window (P)
	<code>fontselect</code>	Open FontSelect window (C)
	<code>jwin</code>	Activate current window (M)
	<code>mapwin</code>	List of experiment numbers (P)
	<code>setwin</code>	Activate selected window (C)

setgroup **Set group of a parameter in a tree (C)**

Syntax: `setgroup(parameter,group<,tree>)`

Description: Sets the group of a parameter in a tree.

Arguments: `parameter` is the name of the parameter.

`group` is one of the following keywords: 'all', 'sample', 'acquisition', 'processing', 'display', or 'spin'.

`tree` is one of the keywords 'current', 'global', or 'processed'. The default is 'current'. See the `create` command for information on the types of trees.

Examples: `setgroup('a','sample')`
`setgroup('b','all','global')`

See also: *User Programming*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>destroy</code>	Destroy a parameter (C)
	<code>destroygroup</code>	Destroy parameters of a group in a tree (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>groupcopy</code>	Copy parameters of group from one tree to another (C)
	<code>paramvi</code>	Edit a parameter and its attributes using <code>vi</code> text editor (M)

<code>setlimit</code>	Set limits of a parameter in a tree (C)
<code>setprotect</code>	Set protection mode of a parameter (C)

sethtfrq1 **Set a Hadamard frequency list from a line list ((M)**

Description: A macro to set the Hadamard frequency list `htfrq1` from a line list `curexp+ ' / dll.out '`. It assumes that the line list has already been created. The macro also sets `ni` to the Hadamard matrix size, creates `htofs1`, and sets `fn1` from the minimum frequency difference in `htfrq1`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>htfrq1</code>	Hadamard frequency list in <code>ni</code> (P)
	<code>dll</code>	Display listed line frequencies and intensities (C)
	<code>htofs1</code>	Hadamard offset in <code>ni</code> (P)
	<code>fn1</code>	Fourier number in the 1st indirectly detected dimension (P)
	<code>ni</code>	Number of increments in the 1st indirectly detected dimension (P)

sethw **Set values for hardware in acquisition system (C)**

Applicability: Syntax 1 through 5 apply to all systems. Syntax 6 applies only to systems with a sample changer. Syntax 7 and 8 apply only to systems with a variable temperature (VT) controller.

Syntax: The following syntax is used with the `sethw` command:

- (1) `sethw(<'wait' | 'nowait', >par1, val1<, par2, val2, ...)`
- (2) `sethw('lock', 'on' | 'off')`
- (3) `sethw('spin', speed)`
- (4) `sethw('spinner', 'bump')`
- (5) `sethw('eject', 'on' | 'off')`
- (6) `sethw('loc', location)`
- (7) `sethw('vt', 'reset' | 'off')`
- (8) `sethw('temp', temperature)`
- (9) `sethw('lockfreq', lockfreq_value)`

Description: Sets acquisition system hardware values. `sethw` cannot be used when an acquisition is in progress or when the `acqi` program is active.

Syntax 1 can be used to set the lock system parameters `lockpower`, `lockgain`, `lockphase`, and `z0`. This syntax can also be used to set the values of the shims. The particular shim that can be set depends upon the type of shim hardware present in the system. See the description of `shimset` for a list of the shim names for each type of shim hardware.

Syntax 2 turns the hardware lock on or off.

Syntax 3 controls spinning speed.

Syntax 4 carries the sample to bump by giving it a short burst of eject air. This is sometimes useful to reseal the sample if it is failing to spin.

Syntax 5 ejects and inserts samples into the probe. Entering the command `sethw('eject', 'on')` is equivalent in function to macros `eject` and `e`; and `sethw('eject', 'off')` is equivalent to macros `insert` and `i`.

Syntax 6 sets a location for the sample currently in the magnet on a system with a sample changer. The parameter `loc` is updated.

Syntax 7 resets the VT controller, useful when changing the probe in a system with VT regulation. By entering `sethw('vt', 'reset')` after installing a new probe in the magnet and attaching the VT controller interface to the probe, the VT controller is ready to regulate the temperature. No other parameters can be modified by the command. As an alternate, you can manually turn the VT

controller unit off and then back on. Syntax 7 also turns the VT controller off by entering `sethw('vt','off')`.

Syntax 8 sets the temperature in degrees celsius. The host computer does not wait for the temperature to regulate.

Syntax 9 sets the lock frequency, in MHz.

Arguments: 'wait' or 'nowait' keyword must be either the first or last argument.

- 'wait' sends the new values to the acquisition console, verifies these values, and updates the corresponding parameters. This is the default.
- 'nowait' sends the new values to the console without verifying them or changing parameters.

`parameter1,value1,parameter2,value2,...` are pairs of parameter names and their values (see the first two examples below). At least one parameter name and its value must be specified. A maximum of ten parameters can be set.

'lock','on' is a keyword pair to turn the hardware lock on.

'lock','off' is a keyword pair to turn the hardware lock off.

'liqbear' sets the bearing air on level; see [liqbear](#) parameter.

'pneufault' second argument is 'clear', 'n', 'w', or 'y' to clear or set the pneumatics fault code.

'spin' is a keyword that identifies the next argument, speed, as the sample spinning speed, in Hz.

'spinner','bump' is a keyword pair to bump the sample.

'eject','on' is a keyword pair to eject the sample from the probe.

'eject','off' is a keyword pair to insert the sample into the probe.

'loc' is a keyword to identify that the next argument, location, is a number for the sample currently in the magnet ('loc' is unrelated to the [loc](#) parameter).

'vt','reset' is a keyword pair to reset the VT controller after the controller has been disconnected from the probe. This is equivalent to turning the VT controller power off and on.

'vt','off' is a keyword pair to turn the VT controller off.

'temp' is a keyword that identifies the next argument, temperature, as the requested sample temperature, in degrees celsius.

'lockfreq' is a keyword that the next argument is the lock frequency.

`lockfreq_value` is the [lockfreq](#) value, in MHz, for the lock frequency.

'lockrate' is a number <5000 used internally; usually 20 or 2000.

Examples: `sethw('z1c',30,'z2c',-50)`
`sethw('wait','z1',150,'z2',-400)`
`sethw('lock','on')`
`sethw('spin',20)`
`sethw('spinner','bump')`
`sethw('eject','on')`
`sethw('loc',5)`
`sethw('vt','reset')`
`sethw('lockfreq',46.042)`

See also: *NMR Spectroscopy User Guide*

Related:	loc	Location of sample in tray (P)
	lockpower	Lock power (P)
	lockfreq	Lock frequency (P)
	lockgain	Lock gain (P)

<code>lockphase</code>	Lock phase (P)
<code>readhw</code>	Read current values of acquisition hardware (C)
<code>spin</code>	Sample spin rate (P)
<code>z0</code>	Z0 field position (P)

setint **Set value of an integral (M)**

Syntax: `setint(int_number<,value>)`

Description: Sets the value of an integral.

Arguments: `int_number` is the integral number. It corresponds to the index number displayed by `dli` if all integrals are shown (i.e., `intmod= 'full'`) or the region if alternating integrals are shown (i.e., `intmod= 'partial'`).
`value` sets the actual value of the selected integral. The default is `ins`.

Examples: `setint(2)`
`setint(1,3)`

See also: *NMR Spectroscopy User Guide*

Related: `dli` Display list of integrals (C)
`ins` Integral normalization scale (P)
`intmod` Integral display mode (P)

setlimit **Set limits of a parameter in a tree (C)**

Applicability: All

Syntax: `setlimit(name, max,min,step [,tree])`
`setlimit(name, index[,tree])`

Description: `setlimit` sets the limits of a variable in a tree.

The limits are max value, min. value and step size. A variable, such as an index into the table, can look up maximum, minimum, and step sizes in a table.

Supplying all three (max, min., and step) arguments sets the parameter's protection bits (see `setprotect`) so that the table lookup is turned off. The parameter's protection bits are set so that table lookup is turned on if only a single index argument is supplied.

The step value is only used if the parameter is a real number.

Step Value Parameter setting

<code>< -1</code>	The parameter is set to the nearest larger value that is a power of 2. The <code>fn</code> parameter uses a step of -2 to select this case.
<code>>-1 and < 0</code>	The inverse of the parameter is set to the nearest multiple of the absolute value of the step. The <code>sw</code> parameter uses a step of negative of the minimum dwell time to select this mode.
<code>>0 and <1</code>	The parameter is set to the nearest multiple of the step value. As an equation, $value = n * step$ where n is a positive or negative integer.
<code>≥ 1</code>	The parameter is set to nearest value that is a multiple of step relative to the minimum value. For example, <code>setlimit('var', 3, -3, 2)</code> allows only the following values -3, -1, 1, and 3. As an equation, $value = min + n*step$ where n is an integer ≥ 0 . In this example, the equation is: $value = (-3) + (n * 2)$.

Up to four optional return arguments can be used. The first will return the maximum, the second will return the minimum, and the third will return the step size. The fourth argument will return a 0 if the parameter is not using an indexed table lookup for the maximum, minimum, and step size. If the parameter is

using the table lookup mechanism, the fourth argument will be set to the index for that table.

The variable trees are 'current', 'global', 'processed' and 'systemglobal'. The default tree is 'current'.

Arguments: name — the name of the variable.

tree — the variable tree: current (the default), global, processed, or systemglobal.

Examples: `setlimit('a',10000,0,.3)`

`setlimit('b',1e5,-3e2,1,'global')`

`setlimit('dpwr',9)`

See also: *User Programming*

Related:	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>destroy</code>	Destroy a parameter (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>fread</code>	Read parameters from file and load them into a tree (C)
	<code>fsave</code>	Save parameters from a tree to a file (C)
	<code>getlimit</code>	Get the limits of a variable in a tree (C)
	<code>paramvi</code>	Edit a parameter and its attributes using vi text editor (M)
	<code>parmax</code>	Parameter maximum values (P)
	<code>parmin</code>	Parameter minimum values (P)
	<code>parstep</code>	Parameter step size values (P)
	<code>prune</code>	Prune extra parameters from current tree (C)
	<code>setgroup</code>	Set group of a parameter in a tree (C)
	<code>setprotect</code>	Set protection mode of a parameter (C)
	<code>settype</code>	Change type of a parameter (C)
	<code>setvalue</code>	Set value of any parameter in a tree (C)

setlk Set up lock parameters (M)

Syntax: `setlk(solvent)`

Description: Called from other macros to provide adjustment of locking and shimming as a function of solvent. Removing quotation marks from around different parts of the text file of the macro places that particular section into effect. If the macro is left unchanged, setting `alock='s'` is required in the parameter sets where used.

Arguments: solvent is the solvent to be used.

See also: *NMR Spectroscopy User Guide*

Related: `alock` Automatic lock status (P)

setlockfreq Set lock frequency (M)

Description: Calculates and sets the lock frequency parameter `lockfreq`. Before using `setlockfreq`, you must acquire a signal using ^1H as the transmitter nucleus (`tn='H1'`). To avoid errors in calculating frequencies, set `lockfreq='n'` before starting the acquisition.

See also: *VnmrJ Installation and Administration*

Related: `lockfreq` Lock frequency (P)
`tn` Nucleus for observe transmitter (P)

setLP Set up linear prediction in the direct dimension (M)

Applicability: ALL

Syntax: `setLP (n)`

Description: Sets up linear prediction in the direct dimension using the number of coefficients specified.

Examples: `setLP (3)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>lpext</code>	LP data extension in np dimension (P)
	<code>lpfilt</code>	LP coefficients to calculate in np dimension (P)
	<code>lpnupts</code>	LP number of data points in np dimension (P)
	<code>lpopt</code>	LP algorithm data extension in np dimension (P)
	<code>proc</code>	Type of processing on np FID (P)
	<code>setrc</code>	Set frequency referencing based upon lock signal shift (M)
	<code>strtext</code>	Starting point for LP data extension in np dimension (P)
	<code>strtlp</code>	Starting point for LP calculation in np dimension (P)

setLP1 Set F1 linear prediction parameters (M)

Syntax: `setLP1<(extended_length<, current_length>) >`

Description: Sets F1 linear prediction parameters. If no arguments are specified, the interferograms are quadrupled in length.

Arguments: `extended_length` is the number of complex points now existing (`ni`).
`current_length` is the number of points desired after the (forward) linear prediction.

See also: *NMR Spectroscopy User Guide*

Related: `ni` Number of increments in 1st indirectly detected dimension (P)

setlp0 Set parameters for zero linear phase (M)

Syntax: `setlp0`

Description: A new value of `ddrtc` is calculated by `setlp0` using the current values of `alfa`, `rof2`, and `lp` to achieve a zero linear phase condition (`lp=0`). A trial experiment must first be acquired and phased for pure absorption before running `setlp0`. A value of `lp` near zero is required for flat base line.

See also: *NMR Spectroscopy User Guide*

Related	<code>alfa</code>	Set alfa delay before acquisition (P)
	<code>ddrtc</code>	Set ddr time constant (P)
	<code>lp</code>	First-order phase in directly detected dimension (P)
	<code>rp</code>	Zero-order phase in directly detected dimension (P)
	<code>sw</code>	Spectral width in directly detected dimension (P)
	<code>rof2</code>	Receiver gating time following pulse (P)

setnoether Disconnect host computer from Ethernet (U)

Description: Disconnects the host computer from the Ethernet network. Only `root` can execute this shellscript properly. `setnoether` does nothing if the system is already disconnected from the Ethernet network.

On systems running Solaris, `setnoether` renames the `hostname.le0`, `defaultdomain`, and `defaultrouter` files so that Ethernet is not activated when the system is rebooted.

See also: *VnmrJ Installation and Administration*

Related: [setether](#) Connect or reconnect host computer to Ethernet (U)

setoffset Calculate offset frequency for given nucleus and ppm (M)

Syntax: `setoffset (nucleus, ppm) :offsetfreq`

Description: Using the [setref](#) macro, `setoffset` calculates the offset frequency for a given chemical shift and returns the value.

Arguments: `nucleus` is the given nucleus.

`ppm` is the chemical shift.

`offsetfreq` returns the offset frequency for the given chemical shift.

Examples: `setoffset (tn, 5) :tof`
`setoffset ('C13', 85) :dof`

See also: *NMR Spectroscopy User Guide*

Related: [setref](#) Set frequency referencing for proton spectra (M)

setparams Write parameter to current probe file (M)

Syntax: `setparams (param, value<, nucleus>)`

Description: Writes the value of a parameter to the current probe file. The name of the probe file is referenced from the parameter [probe](#).

Arguments: `param` is the name of the parameter to write.

`value` is a string with the value to be written for the parameter.

`nucleus` is the nucleus to write in the probe file. The default is the current value of the parameter `tn`.

Examples: `setparams ('pw90', '10')`
`setparams ('pplvl', '60')`
`setparams ('dpwr', $strdpwr, 'H1')`

See also: *NMR Spectroscopy User Guide*

Related: [addnucleus](#) Add new nucleus to existing probe file (M)
[addparams](#) Add parameter to current probe file (M)
[addprobe](#) Create new probe directory and probe file (M)
[getparam](#) Retrieve parameter from probe file (M)
[probe](#) Probe type (P)
[tn](#) Nucleus for the observe transmitter (P)
[updateprobe](#) Update probe file (M)

setpen Set maximum number of HP plotter pens (M)

Syntax: `setpen< (maxpen, max_number_pens) >`

Description: Allows the user to interactively define the maximum number of pens when changing to a Hewlett-Packard plotter.

Arguments: `maxpen` is the current value of the parameter [maxpen](#).

`maximum_number_pens` is the maximum number of pens to be used. If the value of `max_number_pens` is less than or equal to the current value of the parameter [maxpen](#), this value becomes the new value of [maxpen](#).

See also: *NMR Spectroscopy User Guide*

Related: [color](#) Select plotting colors from a graphical interface (M)
[maxpen](#) Maximum number of pens to use (P)

setplotdev **Return characteristics of a named plotter (C)**

Syntax: `setplotdev<:plotter_type,plotter_host,ppmm,raster>`

Description: Returns information from the `devicenames` and `devicetable` files to identify the characteristics of a plotter. This command need never be entered directly by a user because it is automatically called whenever the `plotter` parameter is set. Note that different “types” of plotters (and printers) are characterized in `devicetable`. The `devicenames` file associates different “names” to a given “type.”

Arguments: `plotter_type` returns the type of the named plotter.
`plotter_host` returns the host associated with the plotter.
`ppmm` returns the plotter resolution in points per millimeter.
`raster` returns the value from the `devicetable` file.

See also: *VnmrJ Installation and Administration*

Related: `plotter` Plotter device (P)

setpower **Set power and pulsewidth for a given γ B1 value (M)**

Syntax: `setpower( $\gamma$ B1,nucleus)`

Description: Sets power level and `pw90` values. For `tn`, `setpower` uses `ref_pwr` and `ref_pw90` from the parameter set or from the probe table. For `dn`, it uses `ref_pwx1v1` and `ref_pwx90` from the parameter set or from the probe table. For `dn2`, it uses `ref_pwx21v1` and `ref_pwx290` from the parameter set or from the probe table. If the reference power levels and pulse width do not exist, `setpower` uses `tpwr` (`pw90`), `dpwr` (`1/dmf`) or `dpwr2` (`1/dmf2`) (if the nucleus is `tn`, `setpower` uses `tpwr`; if the nucleus is `dn`, it uses `dpwr`; if the nucleus is `dn2`, it uses `dpwr2`).

Arguments: `$\gamma$ B1` is a given γ B1 value.
`nucleus` is a given nucleus.

Examples: `setpower(sw,tn)`
`setpower(5000,H1)`

Related: `dn` Nucleus for first decoupler (P)
`dn2` Nucleus for second decoupler (P)
`dpwr` Power level for first decoupler with linear amplifiers (P)
`dpwr2` Power level for second decoupler (P)
`pw90` 90° pulse width (P)
`sw` Spectral width in directly detected dimension (P)
`tpwr` Observe transmitter power level with linear amplifiers (P)

setprotect **Set protection mode of a parameter (C)**

Syntax: `setprotect(parameter,'set'|'on'|"off',bit_vals<,tree>)`

Description: Enables changing the protection bits associated with a parameter.

Arguments: `parameter` is the name of the parameter.
`'set'` causes the current protection bits for the parameter to be completely replaced with the bits specified by `bit_vals`.
`'on'` causes the bits specified in `bit_vals` to be turned on without affecting any other protection bits.
`'off'` causes the bits specified in `bit_vals` to be turned off without affecting any other protection bits.

'list' causes all parameter with the specified bit_vals to be listed. This list may be returned to the calling macro.

'clear' option clears the specified bit_vals from all parameters. For both the list and clear options, the names argument can be ''. The return value when setprotect is called with the list option can be used as the 'names' argument for other forms of setprotect. It can also be names for other commands which use lists of parameter names, such as writeparam and readparam.

bit_vals is the *sum* of the *values* of bits selected from the following list:

Bit	Value	Description
0	1	Cannot array the parameter
1	2	Cannot change active/not active status
2	4	Cannot change the parameter value
3	8	Causes <code>_parameter</code> macro to be executed (e.g., if parameter is named <code>sw</code> , macro <code>_sw</code> is executed when <code>sw</code> is changed)
4	16	Avoids automatic redisplay
5	32	Cannot delete parameter
6	64	System ID for spectrometer or data station
7	128	Cannot copy parameter from tree to tree
8	256	Will not set <code>array</code> parameter
9	512	Cannot set parameter enumerals values
10	1024	Cannot change the parameter's group
11	2048	Cannot change protection bits
12	4096	Cannot change the display group
13	8192	Look up minimum, maximum, step values in table
14	16384	Parameter marked for locking (P_LOCK; see <code>rtx</code>)
15	32768	Global parameter not shared in multiple VJ viewports
16	65536	Force automatic redisplay in VJ templates

For example, to change the first two protection bits, with values 1 and 2, either enter `setprotect` twice (once for each value) with the keyword 'on', or enter `setprotect` once with `bit_vals` set to 3 (sum of 1 and 2) with the keyword 'set'.

`tree` is one of the keywords 'global', 'current', 'processed', or 'systemglobal'. The default is 'current'. Refer to the `create` command for more information on the types of parameter trees.

Examples: `setprotect('syn','on',2)`
`setprotect('pslabel','on',8)`

See also: *User Programming*

Related:	<code>array</code>	Parameter order and precedence (P)
	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>destroy</code>	Destroy a parameter (C)
	<code>display</code>	Display parameters and their attributes (C)
	<code>fread</code>	Read parameters from file and load them into a tree (C)
	<code>fsave</code>	Save parameters from a tree to a file (C)
	<code>getlimit</code>	Get the limits of a variable in a tree (C)
	<code>paramvi</code>	Edit a parameter and its attributes using <code>vi</code> text editor (M)
	<code>prune</code>	Prune extra parameters from current tree (C)
	<code>setlimit</code>	Set limits of a parameter in a tree (C)

setrc Set receiver constants (M)

Applicability: VNMR5 and 400 - MR systems

Syntax: `setrc`

Description: Sets receiver time constants to optimal values. `alfa` is set to a minimum value from the probe file (default is 10 μ s). `rof2` is set to a minimum value from the probe file (default is 25 μ s). `lp` is set to zero. `ddrtc` is set to a value based upon the `ddrpm` parameter, which is set based upon pulse sequence type (default value `ddrpm` = 'p'). Linear prediction is turned on in the direct dimension if the `ddrtc` value is more than a dwell time. `setrc` is used in the `apptype` macros for setting up pulse sequences or from the command line to optimize receiver constants.

Description: sets receiver time constants to optimal values.

See also: *NMR Spectroscopy User Guide*

Related	<code>alfa</code>	Set alfa delay before acquisition (P)
	<code>rof2</code>	Receiver gating time following pulse (P)
	<code>pw</code>	Pulse width (P)
	<code>probe</code>	Probe type (P)
	<code>ddrtc</code>	Set ddr precession mode (P)
	<code>ddrpm</code>	Set ddr precession mode (P)
	<code>sw</code>	Spectral width in directly detected dimension (P)
	<code>setLP</code>	Set F1 linear prediction parameters (M)

setref Set frequency referencing (M)

Syntax: `setref<(nucleus)>:$rfl,$rfp,$reffrq,$refpos`

Description: Calculates the referencing for a given parameter or FID data set, for samples locked on deuterium, and based on the chemical shift of the lock solvent line. `setref` uses information in `/vnmr/solvents` (^2H chemical shift for current solvent) and `/vnmr/nuctables/nuctabref` (absolute reference frequencies for NMR nuclei) to predict the position of the reference frequency with the current solvent, spectral window, and spectrometer frequency. `setref` assumes a locked sample.

The macro calculates the (auxiliary) ^2H reference frequency (TMS-d1) from the lock frequency (`lockf` = `lockfreq` + `lkof`/1e6) as follows:

$$\text{H2\_TMSfreq} = \text{lockf} / (1 + \text{solppm}/1e6)$$

then takes the Ξ values for ^2H and `tn` and calculates the auxiliary reference frequency (`reffrq`) for the observe nucleus at the given field strength:

$$\text{reffrq} = (\text{H2\_TMSfreq} / \Xi(\text{H2})) * \Xi(\text{tn})$$

from this, `rfl` and `rfp` are set:

$$\text{rfp}=0 \quad \text{rfl} = \text{sw}/2 - (\text{sfrq} - \text{reffrq}) * 1e6.$$

Setting the global (or local) flag `bioref='y'` uses Bio-NMR referencing (based on `nuctables/nuctabrefBio`) rather than standard IUPAC / organic chemistry referencing (based on `nuctables/nuctabref`)

Ξ is the normalized frequency such that the ^1H signal from TMS is 100.00 MHz.

This estimate of the frequency based upon the chemical shift value of the lock signal and does not account for temperature, pH, or other factors affecting the chemical shift of the lock solvent.

The default tree is 'current'.

Arguments: An argument and return values are beneficial for the use of `setref` within other macros such as `setref1` and `setref2`. By default (i.e., without an

argument), `setref` calculates the referencing for 1D spectra or for the directly detected dimension in nD spectra (f2 in 2D, f3 in 3D).

When only `nucleus` is used as an argument, `setref` returns values without setting parameters.

`$rfl`, `$rfp`, `$reffrq`, `$refpos` are return values for reference peak position, reference peak frequency, reference line frequency, and reference line position, respectively.

Examples: `setref`
`setref('C13'):$rfl,$rfp`

See also: *NMR Spectroscopy User Guide*

Related:	<code>reffrq</code>	Reference frequency of reference line (P)
	<code>refpos</code>	Position of reference frequency (P)
	<code>rfl</code>	Reference peak position (P)
	<code>rfp</code>	Reference peak frequency (P)
	<code>rl</code>	Set reference line in directly detected dimension (M)
	<code>setref1</code>	Set frequency referencing for 1st indirectly detected dimension (M)
	<code>setref2</code>	Set frequency referencing for 2nd indirectly detected dimension (M)
	<code>setup</code>	Set up parameters for basic experiments (M)
	<code>tmsref</code>	Reference 1D proton or carbon spectrum to TMS (M)
	<code>bioref</code>	Use <code>nuctables/nuctabrefBio</code> rather than standard IUPAC / organic chemistry

setref1 **Set freq. referencing for 1st indirectly detected dimension (M)**

Syntax: `setref1(nucleus)`

Description: Calculates the referencing for the first indirect dimension (f1) in nD parameters and FID data sets, for samples locked on deuterium, and for the solvent specified by the `solvent` parameter. `setref1` uses the `setref` macro to calculate the reference frequency and based on the chemical shift of the lock solvent line and `/vnmr/nuctables/nuctabref` (absolute reference frequencies for NMR nuclei) to predict the referencing in f1 (`reffrq1`, `rfl1`, `rfp1`) with the current solvent, `sw1`, and for the frequency of the specified nucleus.

This estimate of the frequency based upon the chemical shift value of the lock signal, as in `setref`, and does not account for temperature, pH, or other factors affecting the chemical shift of the lock solvent. Using `setref`, `setref1`, and `setref2`, maintains a consistent reference for all dimensions.

Ξ is the normalized frequency such that the ^1H signal from TMS is 100.00 MHz.

Setting the global (or local) flag `bioref='y'` uses bio-NMR referencing (based on `nuctables/nuctabrefBio`) rather than standard IUPAC / organic chemistry referencing (based on `nuctables/nuctabref`)

See `/vnmr/nuctables/nuctabref`.

Arguments: `nucleus` is the frequency-relevant nucleus in f1.

Examples: `setref1(tn)`
`setref1('C13')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>reffrq1</code>	Reference frequency of reference line in 1st indirect dimension (P)
	<code>refpos1</code>	Position of reference frequency in 1st indirect dimension (P)
	<code>rfl</code>	Reference peak position (P)
	<code>rfl1</code>	Reference peak position in 1st indirectly detected dimension (P)
	<code>rfp1</code>	Reference peak frequency in 1st indirectly detected dimension (P)

`setref` Set frequency referencing (M)
`bioref` Use nuctables/nuctabrefBio

setref2 Set freq. referencing for 2nd indirect detected dimension (M)

Syntax: `setref2 (nucleus)`

Description: Calculates the referencing for the second indirect dimension (f2) in nD parameters and FID data sets, for samples locked on deuterium, and for the solvent specified by the `solvent` parameter. `setref2` uses `setref` to calculate the reference frequency and based on the chemical shift of the lock solvent line and `/vnmr/nuctables/nuctabref` (absolute reference frequencies for NMR nuclei) to predict the referencing in f2 (`reffrq2`, `rfl2`, `rfp2`) with the current solvent, `sw2`, and for the frequency of the specified nucleus.

This estimate of the frequency based upon the chemical shift value of the lock signal, as in `setref`, and does not account for temperature, pH, or other factors affecting the chemical shift of the lock solvent. Using `setref`, `setref1`, and `setref2`, maintains a consistent reference for all dimensions.

Setting the global (or local) flag `bioref='y'` uses bio-NMR referencing (based on `nuctables/nuctabrefBio`) rather than standard IUPAC / organic chemistry referencing (based on `nuctables/nuctabref`)

See `/vnmr/nuctables/nuctabref`.

Arguments: `nucleus` is the frequency-relevant nucleus in f2.

Examples: `setref2 (tn)`
`setref2 ('C13')`

See also: *NMR Spectroscopy User Guide*

Related: `reffrq2` Reference frequency of reference line in 2nd indirect dimension (P)
`refpos2` Position of reference frequency in 2nd indirect dimension (P)
`rfl2` Reference peak position in 2nd indirectly detected dimension (P)
`rfp2` Reference peak frequency in 2nd indirectly detected dimension (P)
`rl2` Set reference line in 2nd indirectly detected dimension (M)
`setref` Set frequency referencing (M)
`bioref` Use nuctables/nuctabrefBio

setscout Set up a scout run (M)

Applicability: Systems with LC-NMR accessory.

Description: Designed to help run simple experiments during the setup phase of LC-NMR or to be the first of two experiments run on peaks in a stopped-flow or loop-flushing mode. In the latter application, you can set `wexp='setwet au'` so that the scout run is analyzed, parameters adjusted, and an appropriate solvent-suppressed experiment run.

If parameters already exist in the current experiment for performing the `lc1d` pulse sequence, `setscout` turns off the solvent suppression portion of the sequence; if they do not exist, they are created and set to default values using `lc1d`.

See also: *NMR Spectroscopy User Guide*

Related: `lc1d` Pulse sequence for LC-NMR (M)
`setwet` Set up a solvent-suppressed experiment (M)

S

setssfilter Set ssfsfrq to the frequencies of each suppressed solvents (M)

Applicability: Systems with LC-NMR accessory.

Description: Sets `ssfsfrq` to the frequencies of each of the suppressed solvents.

See also: *NMR Spectroscopy User Guide*

setsw Set spectral width (M)

Syntax: `setsw(downfieldppm,upfieldppm)`

Description: Sets `sw` and `tof` for the given spectral window and also does referencing.

Arguments: `downfieldppm` is the downfield frequency, in ppm.

`upfieldppm` is the upfield frequency, in ppm.

Examples: `setsw(12,0)`
`setsw(235,-15)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>setsw1</code>	Set spectral width in evolution dimension (M)
	<code>setsw2</code>	Set spectral width in 2nd evolution dimension (M)
	<code>sw</code>	Spectral width in directly detected dimension (P)
	<code>tof</code>	Frequency offset for observe transmitter (P)

setsw1 Set spectral width in evolution dimension (M)

Syntax: `setsw1(nucleus,downfieldppm,upfieldppm):offset`

Description: Sets `sw1` for the given spectral window and also does referencing.

Arguments: `nucleus` returns the nucleus.

`downfieldppm` is the downfield frequency, in ppm.

`upfieldppm` is the upfield frequency, in ppm.

`offset` returns the appropriate offset.

Examples: `setsw1(tn,12,0)`
`setsw1(dn,235,-15):dof`

See also: *NMR Spectroscopy User Guide*

Related:	<code>setsw</code>	Set spectral width (M)
	<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)

setsw2 Set spectral width in 2nd evolution dimension (M)

Syntax: `setsw2(nucleus,downfieldppm,upfieldppm):offset`

Description: Sets `sw2` for the given spectral window and also does referencing.

Arguments: `nucleus` returns the nucleus.

`downfieldppm` is the downfield frequency, in ppm.

`upfieldppm` is the upfield frequency, in ppm.

`offset` returns the appropriate offset.

Examples: `setsw2(tn,12,0)`
`setsw2(dn,235,-15):dof`

See also: *NMR Spectroscopy User Guide*

Related:	<code>setsw</code>	Set spectral width (M)
	<code>sw2</code>	Spectral width in 2nd indirectly detected dimension (P)

setselfrqc Set selective frequency and width (M)

Description: Sets selective frequency and width of the excitation bandwidth for selective excitation. Used after **TOCSY1D** and **Noesy1d** selection. Selected frequencies and widths of the excitation bandwidth are used by **suselfrq**.

Related: **Noesy1d** Change parameters for NOESY1D experiment (M)
suselfrq Select peak, continue selective excitation experiment (M)
TOCSY1D Change parameters for TOCSY1D experiment (M)

setselinv Set up selective inversion (M)

Description: Sets power, pulsewidth, and shape for selective inversion; used by **suselfrq**. By default, **setselinv** selects a q3 gaussian cascade pulse if a waveform generator or linear modulator is present. Otherwise, **setselinv** selects a “rectangular” pulse.

Related: **setselfrqc** Select selective frequency and width (M)
suselfrq Select peak, continue selective excitation experiment (M)

settclddefault Select default display templates for pulse sequence (M)

Syntax: `settclddefault(<default><, sequence>)`

Description: Selects the display templates to use as the default for a pulse sequence.

Arguments: **default** is the name of the set of display templates to use for the default display of the current pulse sequence (defined by the parameter **seqfil**). If no arguments are given, the user is prompted for the name of the display templates.
sequence defines which pulse sequence will use the default displays of the pulse sequence given as the first argument. The default is the pulse sequence defined by the parameter **seqfil**.

Examples: `settclddefault`
`settclddefault('cosy')`
`settclddefault('default2d', 'HMQC8')`

See also: *User Programming*

Related: **seqfil** Pulse sequence name (P)

settone Opens the Auto Tune Setup dialog (M)

Applicability: *VnmrJ Walkup*, Automation

Syntax: `settone`

Description: Opens a dialog for setting when to tune in automation using ProTune.

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: **protune** **Macro to start ProTune (M)**
wtune Specify when to tune (P)

settype Change type of a parameter (C)

Syntax: `settype(parameter, type<, tree>)`

Description: Changes the type of an existing parameter. A string parameter can be changed into a string or flag type, or a real parameter can be changed into a real, delay, frequency, pulse, or integer type. Note that **settype** cannot change a string parameter into a real, or change a real into a string.

Arguments: `parameter` is the name of an existing parameter.
`type` is one of the keywords 'string', 'flag', 'real', 'delay', 'frequency', 'pulse', or 'integer'.
`tree` is one of the keywords 'global', 'current', 'processed', or 'systemglobal'. The default is 'current'. Refer to the [create](#) command for more information on the types of parameter trees.

Examples: `settype('in','flag','global')`
`settype('p12','pulse')`

See also: *User Programming*

Related:	create	Create new parameter in a parameter tree (C)
	display	Display parameters and their attributes (C)
	setgroup	Set group of a parameter in a tree (C)
	setlimit	Set limits of a parameter in a tree (C)
	setprotect	Set protection mode of a parameter (C)
	setvalue	Set value of any parameter in a tree (C)

setup **Set up parameters for basic experiments (M)**

Syntax: `setup<(nucleus<,solvent>)>`

Description: Returns a parameter set to do the experiment requested, complete with positioning of the transmitter and decoupler. Parameters set by `setup` are recalled from the `/vnmr/stdpar` directory or from the user's `stdpar` directory if the appropriate file exists there. Any changes made to the files in these directories are reflected in `setup`. The default parameters for carbon and proton survey spectra are in files `/vnmr/stdpar/C13.par` and `/vnmr/stdpar/H1.par`, respectively. These files should be modified as desired to produce spectra under desirable conditions.

Arguments: `nucleus` is a nucleus chosen from the files in `/vnmr/stdpar` or in the user's `stdpar` directory (e.g., 'H1', 'C13', 'P31').
`solvent` is a solvent chosen from the file `/vnmr/solvents` (e.g., 'CDC13', 'C6D6', 'D2O'). The default is 'CDC13'.

Examples: `setup`
`setup('H1')`
`setup('C13','DMSO')`

See also: *NMR Spectroscopy User Guide*

setup_dosy **Set up gradient levels for DOSY experiments (M)**

Description: Initiates a dialogue to set up an array of `gzlv11` values for DOSY experiments. `setup_dosy` requests the number of array increments and an initial and a final `gzlv11` value and sets up an array that gives increments in `gzlv11` squared between these limits. `setup_dosy` retrieves the gradient strength from the probe calibration file if `probe<>' '` and stores it in the local experimental parameter `DAC_to_G`. If `probe=' '` (i.e., the probe is not defined), then `DAC_to_G` is set to the current value of the global parameter `gcal`.

See also: *NMR Spectroscopy User Guide*

Related:	dosy	Process DOSY experiments (M)
	DAC_to_G	Parameter to store gradient calibration value in DOSY sequences (P)
	setgcal	Set the gradient calibration constant (M)

setvalue Set value of any parameter in a tree (C)

Syntax: `setvalue (parameter, value<, index><, tree>)`

Description: Sets the value of any parameter in a tree. This command bypasses the normal range checking for parameter entry, as well as bypassing any action that would be invoked by the parameter's protection mode (see the [setprotect](#) command). If the parameter entry normally causes a `_parameter` macro to be executed, this action also is bypassed.

Arguments: `parameter` — name of the parameter.

`value` — set value for the parameter.

`index` — number of a single element in an arrayed parameter.

The default is 1. A value of 0 for the index resets an arrayed (or non-arrayed) parameter to the one element supplied as the second argument to `setvalue`.

`tree` — keyword 'global', 'current', 'processed', or 'systemglobal'. The default is 'current'. Refer to the [create](#) command for more information on the types of parameter trees.

Examples: `setvalue ('arraydim', 128, 'processed')`

See also: *User Programming*

Related: [create](#) Create new parameter in a parameter tree (C)
[setprotect](#) Set protection mode of a parameter (C)

setwave Write a wave definition string into Pbox.inp file (M)

Syntax: `setwave ('sh bw/pw ofs st ph fla trev d1 d2 d0')`

Description: Sets up a single excitation band in the `Pbox.inp` file. An unlimited number of waves can be combined by reapplying `setwave`.

Arguments: A single string of 1 to 10 wave parameters in predefined order. Note that a single quote is required at the start and the end of the entire string, but no single quotes are required surrounding characters and strings inside the entire string.

<code>sh</code>	name of a shape file.
<code>bw/pw</code>	either the bandwidth, in Hz, or the pulsewidth, in sec.
<code>ofs</code>	offset, in Hz.
<code>st</code>	number specifying the spin status: 0 for excitation 1 for de-excitation 0.5 for refocusing.
<code>ph</code>	phase (or phase cycle, see <code>wavelib/supercycles</code>).
<code>fla</code>	flip angle. <code>fla</code> can override the default flip angle.
<code>trev</code>	time reversal. This can be used to cancel time reversal if spin status (<code>st</code>) is set to 1 for Mxy.
<code>d1</code>	delay, in sec, prior the pulse.
<code>d2</code>	delay, in sec, after the pulse.
<code>d0</code>	delay or command prior to <code>d1</code> . If <code>d0=a</code> , the wave is appended to the previous wave.

Examples: `setwave ('eburp1')`
`setwave ('GARP 12000.0')`
`setwave ('esnob 600 -1248.2 1 90.0 n n 0.001')`

See also: *NMR Spectroscopy User Guide*

Related: [Pbox](#) Pulse shaping software (U)

S

setwin Activate selected window (C)

Syntax: `setwin (row<, column>)`

Description: Activates a specific pane in the graphics window. Panes are numbered sequentially from left to right and top to bottom.

Arguments: `row` is the number of the row containing the pane to be activated.
`column` is the number of the column containing the pane to be activated.

Examples: `setwin (3)`
`setwin (1, 2)`

See also: *NMR Spectroscopy User Guide*

Related: `curwin` Current window (P)
`fontselect` Open FontSelect window (C)
`jwin` Activate current window (M)
`mapwin` List of experiment numbers (P)
`setgrid` Activate selected window (M)

sf Start of FID (P)

Description: Sets the start of the FID display. This parameter can be entered in the usual way or interactively controlled by the `sf wf` button during a FID display.

Values: 0 to the value of `at`, in seconds.

See also: *NMR Spectroscopy User Guide*

Related: `at` Acquisition time (P)
`dcon` Display noninteractive color intensities map (C)
`dconi` Interactive 2D data display (C)
`df` Display a single FID (C)
`sf1` Start of interferogram in 1st indirectly detected dimension (P)
`sf2` Start of interferogram in 2nd indirectly detected dimension (P)
`vf` Vertical scale of FID (P)
`wf` Width of FID (P)

sf1 Start of interferogram in 1st indirectly detected dimension (P)

Description: Sets the start of the interferogram display in the first indirectly detected dimension.

Values: 0 to $(2 \times \text{ni})/\text{sw1}$, in seconds.

See also: *NMR Spectroscopy User Guide*

Related: `ni` Number of increments in 1st indirectly detected dimension (P)
`sf` Start of FID (P)
`sw1` Spectral width in 1st indirectly detected dimension (P)
`wf1` Width of interferogram in 1st indirectly detected dimension (P)

sf2 Start of interferogram in 2nd indirectly detected dimension (P)

Description: Sets the start of the interferogram display in the second indirectly detected dimension.

Values: 0 to $(2 \times \text{ni2})/\text{sw2}$, in seconds.

See also: *NMR Spectroscopy User Guide*

Related: `ni2` Number of increments in 2nd indirectly detected dimension (P)
`sf` Start of FID (P)

sw2 Spectral width in 2nd indirectly detected dimension (P)
wf2 Width of interferogram in 2nd indirectly detected dimension (P)

sfrq Transmitter frequency of observe nucleus (P)

Description: Contains the frequency for the observe transmitter. **sfrq** is automatically set when **tn** is changed, and it should not be necessary for the user to manually set this parameter.

Values: Number, in MHz.

See also: *NMR Spectroscopy User Guide*

Related: **dfrq** Transmitter frequency of first decoupler (P)
dfrq2 Transmitter frequency of second decoupler (P)
dfrq3 Transmitter frequency of third decoupler (P)
tn Nucleus for observe transmitter (P)
tof Frequency offset for observe transmitter (P)
spcfrq Display frequencies of rf channels (M)

sh2pul Set up for a shaped observe excitation sequence (M)

Applicability: Systems with waveform generators.

Syntax: **sh2pul**

Description: Behaves like standard two-pulse sequence S2PUL but with the normal hard pulses changed into shaped pulses from the waveform generator. The name of the shaped pulse associated with **pw** is **pwpat** and **p1** is **p1pat**. Information about the specifics of power settings and bandwidths is available from the macros **bandinfo** and **pulseinfo**.

See also: *User Programming*

Related: **bandinfo** Shaped pulse information for calibration (M)
p1pat Shape of an excitation pulse (P)
pwpat Shape of refocusing pulse (P)
pulseinfo Shaped pulse information for calibration (M)

shdec Set up for shaped observe excitation sequence (M)

Applicability: Systems with waveform generators.

Description: Sets up the SHDEC pulse sequence that generates a shaped pulse on the observe channel using the waveform generator. It also allows for programmed (e.g.: multiselective) homodecoupling or solvent presaturation using the observe transmitter, and an optional gradient pulse following the excitation pulse.

See also: *NMR Spectroscopy User Guide*

Related: **Pbox** Pulse shaping software (U)

shell Start a UNIX shell (C)

Syntax: **shell**<(command)>:\$var1,\$var2,...

Description: Brings up a normal UNIX shell for the user. On the Sun, a pop-up window is created. On the GraphOn terminal, the entire terminal is used.

Arguments: **command** is a UNIX command line to be executed by **shell**. The default is to bring up a UNIX shell. If the last character in the command line is the symbol **&**, the command is executed in background, which allows commands to be

entered and executed while the `shell` command is still running. Note that if this background feature is used, any printed output should be redirected to a file. Otherwise, the output may pop up in the text window at random times.

`shell` calls involving pipes or input redirection (<) require either an extra pair of parentheses or the addition of `; cat` to the `shell` command string.

`$var1`, `$var2`, ... are names of variables to hold text lines that are generated as a result of the UNIX command. The default is to display the text lines. Each variable receives a single display line. `shell` always returns a text line; in many cases, it is a simple carriage return. To prevent this carriage return from being shown, capture it in a dummy variable, such as

```
shell('command'):$dum
```

Examples: `shell`
`shell('ps')`
`shell('ls -lt'):$filelist`
`shell(systemdir+'/acqbin/Acqstat '+hostname+' &')`
`shell('ls -t|grep May; cat')`
or
`shell('(ls -t|grep May)')`

See also: *NMR Spectroscopy User Guide, User Programming*

Related: [shell](#) Start an interactive UNIX shell (C)

shell Start an interactive UNIX shell (C)

Syntax: `shell(command)`

Description: On a terminal, runs interactively the UNIX command line given as the argument. No return or output variables are allowed.

Arguments: `command` is a UNIX command line to be executed.

Examples: `shell('vi myfile')`

See also: *NMR Spectroscopy User Guide, User Programming*

Related: [shell](#) Start a UNIX shell (C)

shim Submit an Autoshim experiment to acquisition (C)

Description: Performs validity checks on the acquisition parameters and then submits an Autoshim experiment to acquisition.

See also: *NMR Spectroscopy User Guide*

Related: [au](#) Submit experiment to acquisition and process data (C)
[change](#) Submit a change sample experiment to acquisition (M)
[ga](#) Submit experiment to acquisition and FT the result (C)
[go](#) Submit experiment to acquisition (C)
[lock](#) Submit an Autolock experiment to acquisition (C)
[sample](#) Submit change sample, autoshim experiment to acquisition (M)
[spin](#) Submit a spin setup experiment to acquisition (C)
[su](#) Submit a setup experiment to acquisition (M)

shimset Type of shim set (P)

Description: Configuration parameter for the type of shims on the system. The value of `shimset` is set using the Shimset label in the Spectrometer Configuration window.

Values: 1 to 14, where the value identifies one of the following shim sets:

1 is a shim set in a Varian 13-shim supply with computer-controlled axial shims z1, z1c, z2, z2c, z3, z4, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3. Shims can be adjusted from -2047 to +2047. This value is used with the Ultra•nmr shim system when operated from the HIM box (Varian 13 Shims choice in Spectrometer Configuration window).

2 is a shim set in a Oxford 18-shim supply with computer-controlled axial shims z1, z1c, z2, z2c, z3, z4, z5, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, xz2, yz2, zxy, zx2y2. Shims can be adjusted from -2047 to +2047 (Oxford 18 Shims choice in Spectrometer Configuration window).

3 is a shim set in a Varian 23-shim supply with computer-controlled axial shims z1, z2, z3, z4, z5, z6, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, xz2, yz2, zxy, zx2y2, z3x, z3y, z2x2y2, z2xy. Shims can be adjusted from -32767 to +32767 (Varian 23 Shims choice in Spectrometer Configuration window).

4 is a shim set in a Varian 28-shim supply with computer-controlled axial shims z1, z2, z3, z4, z5, z6, z7, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, xz2, yz2, zxy, zx2y2, z3x, z3y, z2x2y2, z2xy, zx3, zy3, z4x, z4y. Shims can be adjusted from -32767 to +32767 (Varian 28 Shims choice in Spectrometer Configuration window).

5 is a shim set in an Ultra•nmr shim system (39 shim channels) with computer-controlled axial shims z1, z1c, z2, z2c, z3, z3c, z4, z4c, z5, z6, z7, z8, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, xz2, yz2, zxy, zx2y2, z3x, z3y, z2x2y2, z2xy, zx3, zy3, z4x, z4y, z3x2y2, z3xy, z2x3, z2y3, z3x3, z3y3, z4x2y2, z4xy, z5x, z5y. Shims can be adjusted from -32767 to +32767 (Ultra Shims choice in Spectrometer Configuration window).

6 is a shim set in a Varian 18-shim supply with computer-controlled axial shims z1, z2, z3, z4, z5, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, xz2, yz2, zxy, zx2y2. Shims can be adjusted from -32767 to +32767 (Varian 18 Shims choice in Spectrometer Configuration window).

7 is a shim set in a Varian 20-shim supply with computer-controlled axial shims z1, z2, z3, z4, z5, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, xz2, yz2, zxy, zx2y2, z3x, z3y. Shims can be adjusted from -32767 to +32767 (Varian 20 Shims choice in Spectrometer Configuration window).

8 is a shim set in a Oxford 15-shim supply with computer-controlled axial shims z1, z2, z3, z4, and radial shims x1, y1, xz, yz, xy, x2y2, zx2y2, xz2, yz2, zxy. Shims can be adjusted from -2047 to +2047 (Oxford 15 Shims choice in Spectrometer Configuration window).

9 is a shim set in a Varian Ultra•nmr shim system II (40 shim channels) with computer-controlled axial shims z1, z1c, z2, z2c, z3, z3c, z4, z4c, z5, z6, z7, z8, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, x4, y4, xz2, yz2, zxy, zx2y2, z3x, z3y, z2x2y2, z2xy, zx3, zy3, z4x, z4y, z3x2y2, z3xy, z2x3, z2y3, z3x3, z3y3, z4x2y2, z4xy, z5x, z5y. Shims can be adjusted from -32767 to +32767 (Varian 40 Shims choice in Spectrometer Configuration window).

10 is a shim set in a Varian 14-shim supply with computer-controlled axial shims z1, z1c, z2, z2c, z3, z4, z5, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3. Shims can be adjusted from -2047 to +2047 (Varian 14 Shims choice in Spectrometer Configuration window).

11 is a shim set in a Varian 8-shim supply with computer-controlled axial shims z1, z2, and radial shims x1, y1, xz, yz, xy, x2y2. Shims can be adjusted from -32767 to +32767 (Whole Body Shims choice in Spectrometer Configuration window).

12 is a shim set in a Varian 26-shim supply with computer-controlled axial shims z1, z2, z3, z4, z5, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, xz2, yz2, zxy, zx2y2, z3x, z3y, z2x2y2, z2xy, zx3, zy3, x4, y4. Shims can be adjusted

from -32767 to +32767 (Varian 26 Shims choice in Spectrometer Configuration window).

13 is a shim set in an Varian 29-shim supply with computer-controlled axial shims z1, z2, z3, z4, z5, z6, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, xz2, yz2, zxy, zx2y2, z3x, z3y, z2x2y2, z2xy, zx3, zy3, z4x, z4y, z5x, z5y. Shims can be adjusted from -32767 to +32767 (Varian 29 Shims choice in Spectrometer Configuration window).

14 is a shim set in a Varian 35-shim supply with computer-controlled axial shims z1, z2, z3, z4, z5, z6, and radial shims x1, y1, xz, yz, xy, x2y2, x3, y3, x4, y4, xz2, yz2, zxy, zx2y2, z3x, z3y, z2x2y2, z2xy, zx3, zy3, z4x, z4y, z3x2y2, z3xy, z4x2y2, z4xy, z5x, z5y. Shims can be adjusted from -32767 to +32767 (Varian 35 Shims choice in Spectrometer Configuration window).

15 is the Varian 15 Shim.

16 is the Ultra 18 Shims.

See also: *VnmrJ Installation and Administration*

Related: `config` Display current configuration and possibly change it (M)
`readhw` Read current values of acquisition hardware (C)

showconfig Show system configuration settings (M)

See also: Displays the system configuration settings in the text window. To print the settings, enter the following in the VnmrJ command line:

printon showconfig printoff.

See also: *VnmrJ Installation and Administration*

Related: `config` Display current configuration and possibly change it (M)

showconsole Show system configuration settings (U)

Description: Displays console hardware configuration parameters and system versions. This information is recorded during console bootup and represents the system hardware options recognized by the acquisition computer. The command is used mainly when troubleshooting or performing diagnostics.

See also: *NMR Spectroscopy User Guide*

Related: `ihwinfo` Hardware status of console (C)

showfit Display numerical results of deconvolution (M)

Description: After a deconvolution, the results are written into file `fitspec.outpar` in an abbreviated format. `showfit` converts these data to an output format more suitable for examination and printing.

See also: *NMR Spectroscopy User Guide*

Related: `fitspec` Perform spectrum deconvolution (C)
`plfit` Plot deconvolution analysis (M)
`usemark` Use "mark" output as deconvolution starting point (M)

showloginbox Shows operator login dialog (M)

Description: Shows the login dialog for operators.

shownumx Show x position of number (P)

Description: Show the X position of the number. The bottom left of every spectrum is defined as 0.

See also: *User Programming*

Related: `shownumy` y position counting from bottom left of every spectrum (P)

shownumy Show y position of number (P)

Description: Show the Y position of the number. The bottom left of every spectrum is defined as 0.

See also: *User Programming*

Related: `shownumx` x position counting from bottom left of every spectrum (P)

showoriginal Restore first 2D spectrum in 3D DOSY experiment (M)

Description: Restores the first 2D spectrum in a 3D DOSY experiment (if it has been saved by the `dosy` macro).

See also: *NMR Spectroscopy User Guide*

Related: `dosy` Process DOSY experiments (M)

showplotter Show list of currently defined plotters and printers (M)

Description: Shows a list of currently defined plotters and printers.

See also: *NMR Spectroscopy User Guide*

Related: `plotter` Plotter device (P)
`printer` Printer device (P)

showplotq Display plot jobs in plot queue (M)

Description: Displays current plot jobs in the plot queue for the active plotter.

See also: *NMR Spectroscopy User Guide*

Related: `killplot` Stop plot jobs and remove from plot queue (C)
`showprintq` Display print jobs in print queue (C)

showprintq Display print jobs in print queue (M)

Description: Displays current print jobs in the print queue for the active printer.

See also: *NMR Spectroscopy User Guide*

Related: `killprint` Stop print jobs and remove from print queue (C)
`showplotq` Display plot jobs in plot queue (M)

showprotunegui show the graphical interface while tuning (P)

Syntax: `showprotunegui='argument'`

Description: This is a global string parameter that does not exist by default. The user can create it to force the ProTune GUI to be shown during normal tuning operation.

Arguments: 'n' — Do not force the GUI to be shown.

'y' — Show the GUI, except in automation.

'a' — Always show the GUI, even in automation.

Set `showprotunegui='a'` will cause ProTune to fail in automation unless the proper display permission has been set. Set the display permissions on Linux systems by executing "`xhost local:`" on the Linux command line.

See also: *NMR Spectroscopy User Guide*

Related: [protune](#) Macro to start ProTune (M)

showrfmon Show RF Monitor Button in Hardware Bar (P)

Applicability: Imaging

Syntax: `showrfmon=<value>`

Description: Show RF Monitor Button in Hardware Bar.

Values: 1 show RF Monitor button.

-1 hide RF Monitor button.

See also: *VnmrJ Imaging User Guide*

showstat Display information about status of acquisition (M,U)

Syntax: (From VnmrJ) `showstat<(remote_system)>`
(From UNIX) `showstat <remote_system>`

Description: Displays information in the text screen about the status of acquisition on a spectrometer. The command is similar to [Acqstat](#), but displays the information in a non-graphical manner and only once.

Arguments: `remote_system` is the host name of a remote spectrometer. The default is to display information about acquisition on the local system.

See also: *NMR Spectroscopy User Guide*

Related: [Acqstat](#) Bring up the acquisition status display (U)

sin Find sine value of an angle (C)

Syntax: `sin(angle)<:n>`

Description: Finds the sine value of an angle.

Arguments: `angle` is the angle given in radians.

`n` is a return value giving the sine of `angle`. The default is to display the sine value in the status window.

Examples: `sin(.5)`
`sin(val):sin_val`

See also: *User Programming*

Related	asin	Find arc sine of number (C)
	atan	Find arc tangent of a number (C)
	cos	Find cosine value of an angle (C)
	exp	Find exponential value (C)
	ln	Find natural logarithm of a number (C)
	tan	Find tangent value of an angle (C)

sine Find values for a sine window function (M)

Syntax: `sine<(shift<,number_points<,domain)>>`

Description: Calculates appropriate values for parameters [sb](#) and [sbs](#) (if the domain argument is 'f2') or for parameters [sb1](#) and [sbs1](#) (if the domain argument is 'f1') in order to achieve a sine window function. The value of the parameter [trace](#) is used if the domain argument is not entered.

Arguments: If `shift` is greater than 1, the `sbs` parameter is calculated as $2*sb/shift$ (`sbs1` is calculated as $2*sb1/shift$). `sine(2)` gives a “PI/2-shifted” sine

window, i.e., cosine weighting. `sine(3)` gives a “PI/3” shifted sine window, etc. If `shift` is less than or equal to 1, an unshifted sine window is used (`sbs='n'` or `sbs1='n'`).

`number_points` specifies the number of real points that the window function spans. The value of the window function for subsequent points is 0.

`number_points` must be greater than 0 and a multiple of 2. The default is `ni*2` if `trace='f1'`, or `np` if `trace='f2'`.

`domain` is `'f1'` or `'f2'`. The default is the current setting of `trace`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>np</code>	Number of data points (P)
	<code>sb</code>	Sinebell const. in directly detected dimension (P)
	<code>sb1</code>	Sinebell const. in 1st indirectly detected dimension (P)
	<code>sbs</code>	Sinebell shift const. in directly detected dimension (P)
	<code>sbs1</code>	Sinebell shift const. in 1st indirectly detected dimension (P)
	<code>sinesq</code>	Find values for a sine squared window function (M)
	<code>trace</code>	Mode for <i>n</i> -dimensional data display (P)

sinebell **Select default parameters for sinebell weighting (M)**

Description: Generates initial guess at good sinebell weighting parameters by setting the `sb` and `sb1` parameters to one-half the acquisition time and turning off all other weighting. Use `sinebell` in absolute-value 2D experiments only.

See also: *NMR Spectroscopy User Guide*

Related:	<code>pseudo</code>	Set default parameters for pseudo-echo weighting (M)
	<code>sb</code>	Sinebell const. in directly detected dimension (P)
	<code>sb1</code>	Sinebell const. in 1st indirectly detected dimension (P)

sinesq **Find values for a sine-squared window function (M)**

Syntax: `sinesq<(shift<, number_points<, domain>)>`

Description: Calculates appropriate values for parameters `sb` and `sbs` (if the `domain` argument is `'f2'`) or for parameters `sb1` and `sbs1` (if the `domain` argument is `'f1'`) in order to achieve a sine-squared window function. The value of parameter `trace` is used if the `domain` argument is not entered.

Arguments: `shift` sets the starting value for the window function. If `shift` is greater than 0, the starting value is given by $\sin p/\text{shift}$; otherwise, if `shift` is less than or equal to 0, the starting value is 0. The default value is 0.

`number_points` specifies the number of real points that the window function spans. The value of the window function for subsequent points is 0. The `number_points` argument must be greater than 0 and a multiple of 2. The default is `ni*2` if `trace='f1'`, or `np` if `trace='f2'`.

`domain` is `'f1'` or `'f2'`. The default is the current setting of `trace`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
	<code>np</code>	Number of data points (P)
	<code>sb</code>	Sinebell const. in directly detected dimension (P)
	<code>sb1</code>	Sinebell const. in 1st indirectly detected dimension (P)
	<code>sbs</code>	Sinebell shift const. in directly detected dimension (P)
	<code>sine</code>	Find values for a sine window function (M)
	<code>trace</code>	Mode for <i>n</i> -dimensional data display (P)

S

size Returns the number of elements in an arrayed parameter (O)

Description: In MAGICAL programming, an operator that returns the number of elements in an arrayed parameter.

Examples: `r1 = size('d2')`

See also: *User Programming*

Related: `arraydim` Dimension of experiment (P)
`typeof` Return identifier for argument type (O)
`length` Determine length of a string (C)

slfreq Measured line frequencies (P)

Description: Contains a list of measured line frequencies. In iterative spin simulation, a calculated spectrum is matched to the lines in the list. The `spinll` macro fills in `slfreq` from the last line listing or a `mark` operation. Use `assign` to make assignments between the measured lines and the calculated transitions. `slfreq` is a global parameter and is displayed by `dla`.

See also: *NMR Spectroscopy User Guide* .

Related: `assign` Assign transitions to experimental lines (M)
`cla` Clear all line assignments (M)
`dla` Display spin simulation parameter arrays (M)
`fitspec` Perform spectrum deconvolution (C)
`mark` Determine intensity of a spectrum at a point (C)
`spinll` Set up an `slfreq` array (M)

slw Spin simulation linewidth (P)

Description: Sets linewidth for individual transitions in the displayed spectrum. Only one linewidth is provided, so all transitions must be given the same linewidth. If the Set Params button is used in setting up spin simulation parameters, `slw` is automatically set to the measured linewidth of the tallest line displayed.

`slw` is also the starting default linewidth for deconvolution calculations. This linewidth will be set automatically when deconvolution is operated using the menu mode and is bypassed if the `usemark` command has been used in conjunction with two cursor input.

Values: 0.01 to 1e6. The typical value is 1.

See also: *NMR Spectroscopy User Guide*

Related: `usemark` Use “mark” output as deconvolution starting point (M)

smaxf Maximum frequency of any transition (P)

Description: Sets the maximum frequency limit for the calculation of the final simulated spectrum. It should be set before the calculation is performed. If the Set Params button is used in setting up spin simulation parameters, `smaxf` is initialized to `sp+wp`; which assumes that you have already expanded the region of the spectrum that you wish to simulate before beginning the spin simulation process.

Values: -1e10 to 1e10, in Hz. The typical value is the maximum chemical shift + 50.

See also: *NMR Spectroscopy User Guide*

Related: `sminf` Minimum frequency of any transition (P)
`sp` Start of plot (P)
`wp` Width of plot (P)

sminf **Minimum frequency of any transition (P)**

Description: Sets the minimum frequency limit for the calculation of the final simulated spectrum. It should be set before the calculation is performed. If the Set Params button is used in setting up spin simulation parameters, `sminf` is initialized to `sp`, which assumes that you have already expanded the region of the spectrum that you wish to simulate before beginning the spin simulation process.

Values: $-1\text{e}10$ to $1\text{e}10$, in Hz. The typical value is 0.

See also: *NMR Spectroscopy User Guide*

Related: `smaxf` Maximum frequency of any transition (P)
`sp` Start of plot (P)
`wp` Width of plot (P)

smsport **Sample Management System serial port connection (P)**

Description: Sets which serial port on the host computer is connected to a Sample Management System (i.e., a sample changer). The value of `smsport` is set using the Sample Changer Serial Port label in the Spectrometer Configuration window.

Values: 'a' sets the connection for serial port A. This value is the default.
'b' sets the connection for serial port B.

See also: *VnmrJ Installation and Administration*; *NMR Spectroscopy User Guide*

Related: `config` Display current configuration and possibly change it (M)

sn **Signal-to-noise ratio (P)**

Description: Sets a ratio for testing signal-to-noise. The `testsn` macro checks whether a signal-to-noise ratio equal to `sn` has been achieved.

Values: Typical value is 35.

See also: *NMR Spectroscopy User Guide*

Related: `dsn` Measure signal-to-noise (C)
`getsn` Get signal-to-noise estimate of a spectrum (M)
`testsn` Test signal-to-noise of a spectrum (M)
`testct` Check `ct` for resuming signal-to-noise testing (M)

solppm **Return ppm and peak width of solvent resonances (M)**

Syntax: `solppm:chemical_shift,peak_width`

Description: Returns to the calling macro information about the chemical shift and peak spread of solvent resonances in various solvents for either ^1H or ^{13}C , depending on the observe nucleus `tn` and the parameter `solvent`. This macro is used “internally” by other macros only.

Arguments: `chemical_shift` returns the chemical shift of the solvent in ppm.

`peak_width` returns the approximate peak spread of solvent resonances.

See also: *User Programming*

Related: `solvent` Lock solvent (P)
`tn` Nucleus for observe transmitter (P)

solvent Lock solvent (P)

Description: Contains one of a series of lock solvents from the `/vnmr/solvents` file, which contains the ^2H chemical shift of each lock solvent. By editing the file, additional solvents can be added. Values for `solvent` are not case-sensitive (e.g., `solvent='C6D6'` and `solvent='c6d6'` are identical)

The `auto_dir` macro now controls most of the automation features, including setting the value of `solvent`.

Values: Standard values in `/vnmr/solvents` include:

Deuterium Oxide	CDCl3	MethyleneChloride
D2O	Cyclohexane	MethylAlcohol-d4
Acetone	C6Dl2	CD2Cl2
CD3COCD3	Toluene	CD3OD
Benzene	C6D5CH3	Chloroform
C6D6	Acetic_Acid	
DMSO	CD3COOD	

See also: *NMR Spectroscopy User Guide*

Related: `lastlk` Last lock solvent used (P)
`solvinf` Retrieve information from solvent table (C)
`tof` Frequency offset for observe transmitter (P)

solvinf Retrieve information from solvent table (C)

Syntax: `solvinf(solvent):$chemical_shift,$name`

Description: Retrieves solvent shift and solvent name from the solvent table.

Arguments: `solvent` is the name of a solvent from the `/vnmr/solvents` file. This argument is not case-sensitive (e.g., `'c6d6'` is the same as `'C6D6'`).

`chemical_shift` returns the chemical shift of the solvent, in ppm.

`name` returns the name of the solvent. The name returned will match the case of the letters (upper or lower) in `/vnmr/solvents`.

Examples: `solvinf('acetone'):$shift`
`solvinf('d2o'):$shift,solvent`

See also: *NMR Spectroscopy User Guide*

Related: `lookup` Look up words and lines from a text file (C)
`solvent` Lock solvent (P)

sort Sort real values of a parameter (M)

Syntax: `sort(parametername<,sortType>:order,val`

Description: Sorts the real values of a parameter. The `sort` macro is not used for parameters holding string values. The default behavior is to sort the array into values of increasing value. A `sortType` can be given to sort into descending order ('r').

If only unique values are wanted, the 'u' `sortType` can be used. The 'ru' `sortType` given unique values in descending order.

The name of a parameter is the first argument to `sort`. Two return values hold the results of the sort. The first return value is an array containing the original indexes of the sorted array. The second return value gives the sorted array.

Examples: With `par=10,8,6,4,2` the `display('par')` command will show:

```
[1] = 10
[2] = 8
[3] = 6
[4] = 4
[5] = 2
```

The command `sort('par'):$order,$val` will set:

```
$order=5,4,3,2,1
$val =2,4,6,8,10
```

sp **Start of plot in directly detected dimension (P)**

Description: Low-frequency limit of the display or plotted region of the spectrum. `sp` is always stored in Hz, but can be entered in ppm by using the `p` suffix (e.g., `sp=2p` sets the start of plot to 2 ppm).

See also: *NMR Spectroscopy User Guide*

Related: `sp1` Start of plot in 1st indirectly detected dimension (P)
 `sp2` Start of plot in 2nd indirectly detected dimension (P)

sp1 **Start of plot in 1st indirectly detected dimension (P)**

Description: Analogous to the `sp` parameter except that `sp1` applies to the first indirectly detected dimension of a multidimensional data set.

See also: *NMR Spectroscopy User Guide*

Related: `sp` Start of plot in directly detected dimension (P)
 `sp2` Start of plot in 2nd indirectly detected dimension (P)

sp2 **Start of plot in 2nd indirectly detected dimension (P)**

Description: Analogous to the `sp` parameter except that `sp2` applies to the second indirectly detected dimension of a multidimensional data set.

See also: *NMR Spectroscopy User Guide*

Related: `sp` Start of plot in directly detected dimension (P)

spadd **Add current spectrum to add/subtract experiment (C)**

Syntax: (1) `spadd<(multiplier<,>,shift>)>`
 (2) `spadd('new')`
 (3) `spadd('trace',index)`

Description: Performs noninteractive spectral addition. The last displayed or selected spectrum is added to the current contents of the add/subtract experiment (`exp5`). A multi-element add/subtract experiment can be created using the `'new'` keyword. Individual spectra in a multi-element add/subtract experiment can be subsequently added to using the `'trace'` keyword followed by an index number of the spectrum.

Arguments: `multiplier` is a value to multiply each spectrum being added to the add/subtract experiment (`exp5`). The normal range of `multiplier` would be +1 to -1 but the range is actually unlimited. The default is 1.0.

`shift` is the number of data points to shift each spectrum. A positive value shifts the spectrum being added to a higher frequency, or to the left. A negative value shifts the spectrum to a lower frequency, or to the right. The default is 0.

`'new'` is a keyword to create a new spectrum in the add/subtract experiment.

'trace' is a keyword to select the spectrum given by the index number argument (*index*) and add it to the add/subtract experiment. The default is to add to the first spectrum in the add/subtract experiment.

index is the index number of the spectrum to be used as a target in a multi-element add/subtract experiment.

Examples: `spadd`
`spadd(.5,25)`
`spadd('new')`
`spadd('trace',2)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>add</code>	Add current FID to add/subtract experiment (C)
	<code>addi</code>	Start interactive add/subtract mode (C)
	<code>clradd</code>	Clear add/subtract experiment (C)
	<code>ds</code>	Display a spectrum (C)
	<code>jexp</code>	Join existing experiment (C)
	<code>select</code>	Select a spectrum without displaying it (C)
	<code>spmin</code>	Take minimum of two spectra in add/subtract experiment (C)
	<code>spsub</code>	Subtract current spectrum from add/subtract experiment (C)

spcfrq Display frequencies of rf channels (M)

Description: Displays the parameters `sfrq`, `dfrq`, `dfrq2`, and `dfrq3` with seven decimal points (to nearest 0.1) to provide the exact frequencies of each rf channel. The number of values displayed depends on `numrfch`.

Prior to VNMR version 4.3, `spcfrq` set the frequency of the observe channel. The parameter `sfrq` now sets the frequency instead of `spcfrq`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dfrq</code>	Transmitter frequency of first decoupler (P)
	<code>dfrq2</code>	Transmitter frequency of second decoupler (P)
	<code>dfrq3</code>	Transmitter frequency of third decoupler (P)
	<code>numrfch</code>	Number of rf channels (P)
	<code>setfrq</code>	Set frequency of rf channels
	<code>sfrq</code>	Transmitter frequency of observe nucleus (P)

specdc3d 3D spectral drift correction (P)

Description: Sets whether a 3D spectral dc correction occurs. The spectral dc correction is the last operation to be performed upon the data prior to forming linear combinations of the data, using the coefficients in the 3D coefficient file (`coef`), and then writing the data to disk. If `specdc3d` does not exist, it is created by the macro `par3d`.

Values: A three-character string selected from 'nnn', 'nny', 'nyn', etc. Each character may take one of two values: n for no spectral dc correction along the relevant dimension, and y for spectral dc correction along the relevant dimension. The first character refers to the f_3 dimension (`sw`, `np`, `fn`), the second character refers to the f_1 dimension (`sw1`, `ni`, `fn1`), and the third character refers to the f_2 dimension (`sw2`, `ni2`, `fn2`). The default is 'nnn'.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dc</code>	Calculate spectral drift correction (C)
	<code>fiddc3d</code>	3D time-domain drift correction (P)
	<code>fn</code>	Fourier number in directly detected dimension (P)
	<code>fn1</code>	Fourier number in 1st indirectly detected dimension (P)
	<code>fn2</code>	Fourier number in 2nd indirectly detected dimension (P)

<code>ft3d</code>	Perform a 3D Fourier transform (M)
<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)
<code>np</code>	Number of data points (P)
<code>par3d</code>	Create 3D acquisition, processing, display parameters (C)
<code>ptspec3d</code>	Region-selective 3D processing (P)
<code>sw</code>	Spectral width in directly detected dimension (P)
<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)
<code>sw2</code>	Spectral width in 2nd indirectly detected dimension (P)

spin **Submit a spin setup experiment to acquisition (C)**

Description: Regulates sample spinning according to the *parameter* `spin`, using the acquisition computer. It also sets rf frequency, decoupler status, and temperature.

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (C)
	<code>change</code>	Submit a change sample experiment to acquisition (M)
	<code>ga</code>	Submit experiment to acquisition and FT the result (C)
	<code>go</code>	Submit experiment to acquisition (C)
	<code>lock</code>	Submit an Autolock experiment to acquisition (C)
	<code>sample</code>	Submit change sample, autoshim experiment to acquisition (M)
	<code>shim</code>	Submit an Autoshim experiment to acquisition (C)
	<code>spin</code>	Sample spin rate (P)
	<code>su</code>	Submit a setup experiment to acquisition (M)

spin **Sample spin rate (P)**

Description: Selects a regulated spin rate. The rate is changed when a sample is inserted or `spin`, `go`, `ga`, `au`, or `sample` are entered.

Values: 0 indicates non-spinning operation.

5 to 39 are spinning rates.

'n' leaves the spin rate at the currently used value and does not wait for regulated spinning before performing acquisition.

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (C)
	<code>ga</code>	Submit experiment to acquisition and FT the result (C)
	<code>go</code>	Submit experiment to acquisition (C)
	<code>sample</code>	Submit change sample, Autoshim experiment to acquisition (M)
	<code>sethw</code>	Set values for hardware in acquisition system (C)
	<code>spin</code>	Submit a spin setup experiment to acquisition (C)

spincad **Run SpinCAD program (C)**

Applicability: SpinCAD Software.

Description: Opens the graphical pulse sequence generation utility.

See also: *SpinCAD*

Related:	<code>vnmr2sc</code>	VNMR to SpinCAD pulse sequence translator (M)

spingen **Compile SpinCAD pulse sequence (M,U)**

Applicability: SpinCAD Software.

Syntax: (From VnmrJ)

```
spingen
spingen(pulsesequence)
spingen(<option>,pulsesequence<,pulsesequence2>)>
spingen(' -psg',pulsesequence)
spingen(' -all',pulsesequence)
spingen(' -dps',pulsesequence)
```

(From UNIX)

```
spingen pulsesequence < pulsesequence2,,>
spingen <option> pulsesequence < pulsesequence2,, >
spingen -psg pulsesequence
spingen -dps pulsesequence
spingen -all pulsesequence
```

Description: Compiles the SpinCAD pulse sequence. The most common usage is the first one (spingen, with no arguments), which compiles the current pulse sequence. Two or more options to SpinCAD compilation are: (1) ' -psg ' option: compilation for the acquisition go command (2) ' -dps ' option: compilation for dps usage and (3) ' -all ' option: include both of the above options and compilation of any Java programs that the pulse sequence may use.

The spingen macro with no arguments does both the go and dps compilations. Individual compilations for go (' -psg ' option) and dps (' -dps ' option) can also be done (these are rarely used)

In case of SpinCAD sequences and C sequences having the same name, the last compiled sequence will be used for the go command. The isspincad macro can be used to check if the current sequence is SpinCAD or of C type.

Compilation of a SpinCAD sequence generates two files in the user's seqlib directory, pulsesequence.psg and pulsesequence_dps.psg, for every source file pulsesequence. Compiled SpinCAD files are distinct from the C files, in that they have .psg extension in the filenames. Java program files (if used) must reside in ~/vnmrsys/spincad/classes directory. Java programs are compiled and the class files placed in the same ~/vnmrsys/spincad/classes directory. The spingen macro checks for any Java files in /vnmr/spincad/classes directory, if it does not exit in the users's classes directory.

Compilation of a SpinCAD sequence differs from the conventional compilation of C sequences; it involves the expansion of any composites used; transformation of parallel events to a format that Jpsg program can resolve.

Arguments: <no option> – compilations for go and dps
 -psg – compilation for go only
 -dps – compilation for dps only
 -all – compilations for go, dps, and also compile any Java programs called from the SpinCAD sequence.

See also: *SpinCAD*

Related: [spincad](#) Display SpinCAD interface (M)

spinll Set up a slfreq array (M)

Syntax: spinll<('mark')>

Description: Copies a list of frequencies to the [slfreq](#) parameter in iterative spin simulation and runs [dla](#). This macro also clears previous line assignments.

Arguments: 'mark' is a keyword to copy the list of frequencies from the markld.out file to [slfreq](#). The default is to copy the frequencies from the last line listing by [nll](#) or [dll](#) to the [slfreq](#). Use the cursor and the mark button to place the

lines to be assigned in `markld.out`. Enter `mark('reset')` to clear the file, and use `nl` to move the cursor to the center of a selected line.

See also: *NMR Spectroscopy User Guide*

Related:	<code>dla</code>	Display line assignments (M)
	<code>dll</code>	Display listed line frequencies and intensities (C)
	<code>mark</code>	Determine intensity of the spectrum at a point (C)
	<code>nl</code>	Position the cursor at the nearest line (C)
	<code>nll</code>	Find line frequencies and intensities (C)
	<code>slfreq</code>	Measured line frequencies (P)

spinner

Open the Spinner Control window (C)

Description: Opens the Spinner Control window. This window has the following capabilities:

- Turn the sample spinner off.
- Turn the sample spinner on at a specified speed, in Hz.
- Enable spinner control from within an experiment using the `spin` parameter and the `spin`, `go`, `ga`, or `au` commands. This mode is the default.
- Alternatively, turn off experiment control of the sample spinner and allow only the Spinner Control window (and `acqi` and `sethw`) to set the spinning speed. This mode has the advantage that, often times, the `spin` parameter is different between experiments. Joining a different experiment and entering `go` can unexpectedly change the spinning speed. This alternate mode prevents this problem. In this mode, when a `go`, `su`, `ga`, or `au` is entered, the `spin` parameter is first set to the speed selected in the Spinner Control window and then the `spin` parameter is set to “Not Used.”
- Select the style of spinner: low-speed style or a high-speed style. If the high-speed style of spinner (used for solids) is selected, the choice of setting the spinning speed or the air flow rate is provided. Setting the air flow rate is useful when setting up the solids spinning apparatus.

If the spinning speed is controlled only through the Spinner Control window, the action to be taken after a spinner error can be selected:

- Display a warning but continue acquisition.
- Stop acquisition and display a warning.

If experiment control of spinning speed is selected, these selections are faded because they are inoperative, and the selection of the action to be taken after a spinning speed error is provided by the parameter `in`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>acqi</code>	Interactive acquisition display process (C)
	<code>au</code>	Submit experiment to acquisition and process data (C)
	<code>change</code>	Submit a change sample experiment to acquisition (M)
	<code>ga</code>	Submit experiment to acquisition and FT the result (C)
	<code>go</code>	Submit experiment to acquisition (C)
	<code>in</code>	Lock and spin interlock (P)
	<code>lock</code>	Submit an Autolock experiment to acquisition (C)
	<code>sample</code>	Submit change sample, autoshim experiment to acquisition (M)
	<code>sethw</code>	Set values for hardware in acquisition system (C)
	<code>shim</code>	Submit an Autoshim experiment to acquisition (C)
	<code>spin</code>	Sample spin rate (P)
	<code>su</code>	Submit a setup experiment to acquisition (M)

spins**Perform spin simulation calculation (C)**

Syntax: `spins<(options)>`

Description: Performs a spin simulation, using the current spin system parameters. Refer to the description of `spsm` for setting up the parameters. Use `dsp` to display the spectrum resulting from the simulation. The output file is `spins.list` in the current experiment. This file includes the calculated transitions ordered by frequency.

Line assignments are required for the iteration. These consist of a list of observed frequencies, which is stored in the arrayed parameter `slfreq`, and the line assignments stored in the array `clindex`. `spinll` copies the frequencies from the last line listing by `nll` or `dll` into the parameter `slfreq`. The line listing can be from an observed spectrum or from the results of deconvolution. After `spinll`, line assignments are most easily made by entering `assign`. `dla` displays the assignments. Single assignments can also be made by `assign(transition_number,line_number)`, where `transition_number` is the index of a transition and `line_number` is the index of the measured line. Setting the `line_number` argument to 0 deletes assignments. `dla('long')` produces an expanded display of assignments.

Be aware that spin simulation line numbers and line list line numbers are *not* the same. Conventional line lists produced by `dll` number the lines from left to right (low- to high-field). The spin simulation software numbers lines according to a more complicated scheme, and these numbers are rarely if ever in frequency order.

The parameters to be iterated are chosen by setting the string parameter `iterate` (e.g., `iterate='A,B,JAB'`). If several parameters have the same value due to symmetry, use `iterate='A,B,C,JAB,JAC=JAB'`. This string sets the iterated parameter JAC to JAB during the iteration. JAB must be defined as an iterated parameter in the string before it can be used at the right side of the equal sign. Sets of parameters with up to six members may be set up in this way. The member in the set that is used on the right side of the equal sign must always come first in the parameter display (e.g., `JAB=JAC` would be wrong). A parameter is held constant during iteration if it is not included in the `iterate` string.

The command `initialize_iterate` sets `iterate` to iterate all spins not named X, Y, or Z and the associated coupling constants.

Following an iterative spin simulation, `dga` displays the new values of the coupling constants and chemical shifts. `undospins` restores a spin system as it was before the last iterative run. It returns the chemical shifts, coupling constants, and line assignments, making it possible to continue from this state with modified line assignments.

Note that major changes in the starting values of parameters may change the numbering of the energy levels and hence the line numbers. The line assignments would then be incorrect and would have to be reentered.

For a successful iteration, it is often necessary to keep some parameters fixed. For example, it is sometimes useful to alternately iterate couplings and shifts, keeping one group fixed while the other is iterated independently.

Arguments: The following variations of `spins` are available:

- `spins('calculate','energy')` puts an energy-level table in the output file.
- `spins('calculate','transitions')` puts a second table of transitions ordered by transition number in the output file.
- `spins('display')` and `dsp` are equivalent.
- `spins('system','spinsystemname')` and `spsm('spinsystemname')` are equivalent.

- `spins('iterate')` runs interactively to match experimental and calculated lines.
- `spins('iterate','iteration')` lists parameters after each iteration in the output file.
- `spins('iterate'<,options>)` provides for determining the chemical shifts and coupling constants to produce a spectrum that matches a table of observed lines. `spins` iterates until the rms (root-mean-square) error of the line matching meets a built-in test, unless it first reaches the value given by `number_iterations`. Iteration also stops if the rms error increases.
- Put multiple list options into the second argument, separated by a blank (e.g., `spins('calculate','transitions energy')`).

Examples: `spins`
`spins('calculate','energy')`
`spins('iterate')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>assign</code>	Assign transitions to experimental lines (M)
	<code>clindex</code>	Index of experimental frequency of a transition (P)
	<code>dga</code>	Display parameter groups (spin simulation) (C)
	<code>dla</code>	Display line assignments (M)
	<code>dll</code>	Display listed line frequencies and intensities (C)
	<code>dsp</code>	Display calculated spectrum (C)
	<code>initialize_iterate</code>	Set <code>iterate</code> to contain relevant parameters (M)
	<code>iterate</code>	Parameters to be iterated (P)
	<code>niter</code>	Number of iterations (P)
	<code>nll</code>	Find line frequencies and intensities (C)
	<code>slfreq</code>	Measured line frequencies (P)
	<code>spinll</code>	Set up <code>slfreq</code> array (M)
	<code>spsm</code>	Enter spin system (M)
	<code>undospins</code>	Restore spin system as before last iterative run (M)

split Split difference between two cursors (M)

Description: Repositions the left-hand cursor halfway between its original position and the position of the other cursor. This macro is very useful for finding the center of a powder pattern: place the two cursors on the horns of the pattern and then enter `split` to give the center.

See also: *NMR Spectroscopy User Guide*

Related: `delta` Difference of two frequency cursors (P)

spintype Spinner Type ((P)

Description: This global parameter determines which spinner hardware is used.

Values: `'liquids'` for low speed spinning of 5 and 10 mm liquids samples
`'tach'` for high speed spinning of 5 and 7 mm Jacobsen probes
`'mas'` for high speed spinning using standalone spinner
`'nano'` for spinning of nano probes
`'none'` for no spinner controller is present, e.g. imaging

S

spmax Take the maximum of two spectra (C)

Description: Takes the maximum of two spectra, considered point-by-point in an absolute-value sense. For example, if the two corresponding values are -2 and $+3$, the **spmax** spectrum will have $+3$; if the two values are $+2$ and -3 , the **spmax** spectrum will have -3 at that point.

spmin Take minimum of two spectra in add/subtract experiment (C)

Description: Takes the minimum of two spectra, considered point-by-point in an absolute-value sense. For example, if the two corresponding values are -2 and $+3$, the **spmin** spectrum will have -2 ; if the two values are $+2$ and -3 , the **spmin** spectrum will have $+2$ at that point.

The function of **spmin** is to essentially select for common features within two spectra while eliminating features that are not common between them. In particular, if two CP/MAS spectra are obtained at different spin rates, the peaks stay in the same place (and hence the **spmin** spectrum also contains the same peaks), but the sidebands move. If spectrum 1 has baseline where spectrum 2 has sideband, and spectrum 2 has baseline where spectrum 1 has sideband, then the **spmin** spectrum will contain only baseline in these regions, eliminating the spinning sidebands.

See also: *NMR Spectroscopy User Guide*

Related:	addi	Start interactive add/subtract mode (C)
	spadd	Add current spectrum to add/subtract experiment (C)
	spsub	Subtract current spectrum from add/subtract experiment (C)

spsm Enter spin system (M)

Syntax: `spsm(spin_system)`

Description: Enables entry of the spin system for spin simulation and creates and initializes the appropriate parameters to describe the various chemical shifts and coupling constants. Chemical shifts can be entered for the X-nucleus, and the spectrum is calculated if that shift is in the window. Generally, however, it is not necessary to enter the X-nucleus chemical shift, and its value has no effect on the spectrum of the remainder of the spin system.

Arguments: `spin_system` is an alphanumeric string of upper-case letters for chemical shift and coupling constant parameters. Chemical shifts are stored in parameters A through Z, and the coupling constants are stored in the parameters starting with JAB and ending with JYZ. Different nucleus types are handled by using letters starting with A for the first type, X for the second, and M for the third. Once created, these parameters are entered and modified in the usual way (e.g., `A=78.5 JAC=5.6`). Entry of chemical shifts in ppm is entered by using **sfrq** (e.g., `B=7.5*sfrq`).

Examples: `spsm('AB')`
`spsm('A3B2')`
`spsm('AB2CMXY')`

See also: *NMR Spectroscopy User Guide*

Related:	sfrq	Transmitter frequency of observe nucleus (P)
	spins	Perform spin simulation calculation (C)

spsub Subtract current spectrum from add/subtract experiment (C)

Syntax: (1) `spsub<(multiplier<,shift>)>`
 (2) `spsub('new')`
 (3) `spsub('trace',index)`

Description: Performs non-interactive spectral subtraction. The last displayed or selected spectrum is subtracted from the current contents of the add/subtract experiment (`exp5`). A multi-element add/subtract experiment can be created using the 'new' keyword. Individual spectra in a multi-element add/subtract experiment can be subsequently subtracted from using the 'trace' keyword followed by an index number of the spectrum.

Arguments: `multiplier` is a value to multiply each spectrum being subtracted from the add/subtract experiment (`exp5`). The normal range of `multiplier` would be +1 to -1 but is actually unlimited. The default is 1.0.

`shift` is the number of data points to shift each spectrum. A positive value shifts the spectrum being added to a higher frequency, or to the left. A negative value shifts the spectrum to a lower frequency, or to the right. The default is 0.

'new' is a keyword to create a new spectrum in the add/subtract experiment.

'trace' is a keyword to select the spectrum given by the index number argument (`index`) and subtract it from the add/subtract experiment. The default is to subtract from the first spectrum in the add/subtract experiment.

`index` is the index number of the spectrum to be used as a target in a multi-element add/subtract experiment.

Examples: `spsub`
`spsub(.5,25)`
`spsub('new')`
`spsub('trace',2)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>clradd</code>	Clear add/subtract experiment (C)
	<code>ds</code>	Display a spectrum (C)
	<code>jexp</code>	Join existing experiment (C)
	<code>spadd</code>	Add current spectrum to add/subtract experiment (C)
	<code>select</code>	Select a spectrum without displaying it (C)
	<code>spmin</code>	Take minimum of two spectra in add/subtract experiment (C)
	<code>sub</code>	Subtract current FID from add/subtract experiment (C)

sqcosine Set up unshifted cosine-squared window function (M)

Syntax: `sqcosine<(<t1_inc><,t2_inc>)>`

Description: Sets up an unshifted cosine-squared window function in 1, 2, or 3 dimensions. The macro checks whether the data is 1D, 2D, and 3D.

Arguments: `t1_inc` is the number of t1 increments. The default is `ni`.
`t2_inc` is the number of t2 increments. The default is `ni2`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>gaussian</code>	Set up unshifted Gaussian window function (M)
	<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
	<code>ni2</code>	Number of increments in 2nd indirectly detected dimension (P)
	<code>pi3ssbsq</code>	Set up pi/3 shifted sinebell-squared window function (M)
	<code>pi4ssbsq</code>	Set up pi/4 shifted sinebell-squared window function (M)
	<code>sq sinebell</code>	Set up unshifted sinebell-squared window function (M)

S

sqdir Study queue directory (P)

Description: Specifies the full path directory where a study is stored. It is set when a new study is created.

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup, VnmrJ Imaging User Guide*

Related: `autodir` Automation directory absolute path (P)
`globalauto` Automation directory name (P)
`save` Save data (M)
`sqname` Study queue parameter template (P)
`startq` Start a chained study queue (M)
`studyid` Study identification (P)
`sqname` Study queue parameter template (P)
`xmunit` Initialize an imaging study queue (M)

sgend End a study queue (M)

Description: End a study queue. Usually called by other macros, and not used from the command line.

Related: `sqfilemenu` Study queue file menu commands (M)

sqexp Load experiment from protocol (M)

Applicability: Imaging

Description: Macro to load an experiment from a protocol.

Syntax: `sqexp(experiment <, 'save'>)`

The first argument is the name of the experiment, and is required. The second argument is an optional keyword 'save'. If specified, it first saves parameter changes to the current experiment in the study queue before loading the parameters for the new experiment.

Examples: `sqexp('epidw')`
`sqexp('spuls', 'save')`

See also: *VnmrJ Imaging User Guide*

Related: `apptype` Application type (P)
`execpars` Set up the exec parameters (M)

sqfilemenu Study queue file menu commands (M)

Description: A macro to perform commands for the study queue operation. Usually the macro is called from the *study queue file menu* located below the study queue area, and not from the command line.

See also: *VnmrJ Imaging User Guide*

Related: `cqinit` Initialize liquids study queue (M)
`cqreset` Reset study queue parameters (M)
`sgend` End a study queue (M)
`sqreset` Reset study queue parameters for imaging (M)
`xmunit` Initialize an imaging study queue (M)

sqmode Study queue mode (P)

Description: A global parameter that specifies the study queue mode. It is used to determine if the study queue acquisition is chained or not.

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related:	<code>startq</code>	Start a chained study queue (M)
	<code>xmnext</code>	Find next prescan or next experiment in study queue (M)
	<code>xmwexp</code>	Processing macro for end of acquisition in study queue (M)

squeue Study queue parameter template (P)

Description: Stores a string in the global tree that determines where a study is stored. It is set from the *Save data setup* dialog in the *Utilities* menu. Dollar signs (\$) are used to delimit a string to search for a parameter to be used in the study file name. Percent signs (%) are used to delimit a numeric extension, e.g. %Rn%, or time specifications. Strings from the `sampleinfo` file are not used, since studies are created in foreground, not automation. Text not delimited by dollar signs or percent signs is copied from `squeue` without any changes.

If `squeue` does not start with a slash mark (/), the study is stored in the path given by `autodir` or `globalauto`; otherwise the name is used as is. A revision number is automatically appended. Values: If `squeue` is a null string, it defaults to %R2%, and the resulting study id is a two-digit revision number. The resulting path and file name must be accessible (with read-write permission) by that user.

Examples: `squeue='s_%DATE%_%R3%' studyid='s_20040501_001'`
`squeue='s_$loc$_' studyid='s_7_01'`
`squeue='r$vrack$z$vzone$/well$loc$%R0%'`
`studyid='r1z3/well16'`

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related:	<code>autodir</code>	Automation directory absolute path (P)
	<code>autoname</code>	Prefix for automation data file (P)
	<code>globalauto</code>	Automation directory name (P)
	<code>squeue</code>	Study queue directory (P)
	<code>squeue</code>	Study queue parameter template (P)
	<code>studyid</code>	Study identification (P)
	<code>Svfname</code>	Create path for data storage (C)

squeuepars Create study queue parameters for imaging (M)

Applicability: Imaging

Description: A macro to create study queue parameters for imaging. Usually called by other macros, and not used from the command line.

See also: *VnmrJ Imaging User Guide*

Related:	<code>fixpar</code>	Correct parameter characteristics in experiment (M)

squeueprotocol Macro to create protocols (M)

Applicability: Imaging

Description: A macro to create protocols for imaging applications. Called by the *Make protocols* dialogs in the *Utilities* menu.

squeuereset Reset study queue parameters for imaging (M)

Applicability: Imaging

Description: Reset study queue parameters for imaging. Usually called by other macros, and not used from the command line.

S

- sqrt** **Return square root of a real number (O)**
- Description: A operator in MAGICAL programming that returns the square root of a real number. A negative argument to `sqrt` is evaluated to 0.0. Operator is not used from the command line.
- Examples: `a = sqrt(b)`
- See also: *User Programming*
- Related
- | | |
|---------------------|---|
| <code>asin</code> | Find arc sine of number (C) |
| <code>atan</code> | Find arc tangent of a number (C) |
| <code>cos</code> | Find cosine value of an angle (C) |
| <code>exp</code> | Find exponential value (C) |
| <code>ln</code> | Find natural logarithm of a number (C) |
| <code>tan</code> | Find tangent value of an angle (C) |
| <code>trunc</code> | Truncates real numbers (O) |
| <code>typeof</code> | Return identifier for argument type (O) |
-
- sqsavestudy** **Macro to save study parameters for imaging (M)**
- Applicability: Imaging
- Description: A macro to save study parameters in the imaging study queue. Usually called by other macros, and not used from the command line.
- See also: *VnmrJ Imaging User Guide*
- Related
- | | |
|-----------------------|-----------------------|
| <code>acquire</code> | Acquire data (M) |
| <code>sgend</code> | End a study queue (M) |
| <code>studypar</code> | Study parameters (P) |
-
- sq sinebell** **Set up unshifted sinebell-squared window function (M)**
- Syntax: `sq sinebell(<t1_inc><,t2_inc>)>`
- Description: Sets up an unshifted sinebell-squared window function in 1, 2, or 3 dimensions. The macro checks whether the data is 1D, 2D, and 3D.
- Arguments: `t1_inc` is the number of t1 increments. The default is `ni`.
`t2_inc` is the number of t2 increments. The default is `ni2`.
- See also: *NMR Spectroscopy User Guide*
- Related
- | | |
|------------------------|---|
| <code>gaussian</code> | Set up unshifted Gaussian window function (M) |
| <code>ni</code> | Number of increments in 1st indirectly detected dimension (P) |
| <code>ni2</code> | Number of increments in 2nd indirectly detected dimension (P) |
| <code>pi3ssbsq</code> | Set up pi/3 shifted sinebell-squared window function (M) |
| <code>pi4ssbsq</code> | Set up pi/4 shifted sinebell-squared window function (M) |
| <code>sq cosine</code> | Set up unshifted cosine-squared window function (M) |
-
- srate** **Spinning rate for magic angle spinning (P)**
- Applicability: Systems with solids module.
- Description: Set to the spinning speed for magic angle spinning (MAS). `srate` must be correct for the pulse sequence set up by `xpolar1` to run TOSS or dipolar dephasing correctly. If `hsrotor='y'`, the measured spinning speed is reported in `srate` for systems that have rotor synchronization.
- Values: 0 to 10⁷, in Hz.

See also: *NMR Spectroscopy User Guide*

Related: **hsrotor** Display rotor speed for solids operation (P)
xpolar1 Set up parameters for XPOLAR1 pulse sequence (M)

sread Read converted data into VnmrJ (C)

Syntax: `sread(file<,template>)`

Description: Reads 32-bit data files into VnmrJ. For Bruker data files in the AMX and AM formats, each file must first be converted using the **convertbru** command before **sread** can read the data in the file into VnmrJ.

Arguments: **file** is the name of a file containing data converted using **convertbru**.
template is the full path of a parameter template file, but without appending the **.par** extension on the file name. The default is **bruker.par**. If no parameter template is specified and **bruker.par** cannot be found in the user or system **parlib** directory, **sread** aborts with an error message.

Examples: `sread('brudata.cv', '/vnmr/parlib/bruker')`

See also: *NMR Spectroscopy User Guide*

Related: **convertbru** Convert Bruker data (M,U)

srof2 Calculate exact rof2 value for Cold Probes (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Calculates the exact value needed for **rof2** to result in a **lp=0** condition for the given **sw**. Works with either **dsp='r'** and **fsq='y'** or with **dsp='i'**. Not compatible with **qcomp**.

Related: **dsp** Type of DSP for data acquisition (P)
rof2 Receiver gating time following pulse (P)

ss Steady-state transients (P)

Description: Sets the number of complete executions of the pulse sequence not accompanied by data collection prior to the acquisition of the real data (sometimes known as *dummy scans*). If **ss** is positive, **ss** steady-state transients are applied on the first increment only, and if **ss** is negative, **-ss** steady-state transients are applied at the start of each increment.

Values: 'n', -32768 to 32767

See also: *NMR Spectroscopy User Guide; User Programming*

ssecho Set up solid-state echo pulse sequence (M)

Applicability: Systems with a solids module.

Syntax: `ssecho`

Description: Converts a standard two-pulse experiment to a ready-to-run solid-state NMR echo (SSECHO) pulse sequence.

See also: *NMR Spectroscopy User Guide*

ssecho1 Set up parameters for SSECHO1 pulse sequence (M)

Applicability: System with a wideline solids module.

Description: Sets up a parameter set for the quadrupole echo pulse sequence SSECHO1.

See also: *NMR Spectroscopy User Guide*

ssfilter Full bandwidth of digital filter to yield a filtered FID (P)

Description: Specifies the full bandwidth of the digital filter applied to the original FID to yield a filtered FID for solvent subtraction. If `ssfilter` does not exist in the current experiment, enter `addpar('ss')` to add it. The command `addpar('ss')` creates additional time-domain solvent subtraction parameters `ssfilter`, `sslsfrq`, `ssntaps`, and `ssorder`.

Values: 'n', 10 to `sw`/2, in steps of 0.1 Hz. The default is 100 Hz.

If `ssfilter` is set to a value and `ssorder` is set to some value, the zfs (zero-frequency) option of solvent subtraction is selected.

If `ssfilter` is set to 'n', ("Not Used"), both the lfs (low-frequency suppression) and zfs options are turned off.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>ft</code>	Fourier transform 1D data (C)
	<code>parfidss</code>	Create parameters for time-domain solvent subtraction (M)
	<code>ssntaps</code>	Number of coefficients in the digital filter (P)
	<code>sslsfrq</code>	Center of solvent-subtracted region of spectrum (P)
	<code>ssorder</code>	Order of polynomial to fit digitally filtered FID (P)
	<code>sw</code>	Spectral width in directly detected dimension (P)
	<code>wft</code>	Weight and Fourier transform 1D data (C)

sslsfrq Center of solvent-suppressed region of spectrum (P)

Description: Specifies the location of the center of the solvent-suppressed region of the spectrum. If `sslsfrq` does not exist in the current experiment, enter `addpar('ss')` to add it. `addpar('ss')` also creates time-domain solvent subtraction parameters `ssfilter`, `ssntaps`, and `ssorder`.

Values: 'n' (or 0) specifies solvent suppresses a region centered about the transmitter frequency. This is the default

Non-zero value shifts the solvent-suppressed region by `sslsfrq` Hz. Multiple regions may be suppressed by arraying the value of `sslsfrq`. Up to 4 values are allowed.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>parfidss</code>	Create parameters for time-domain solvent subtraction (M)
	<code>ssfilter</code>	Full bandwidth of digital filter to yield a filtered FID (P)
	<code>ssntaps</code>	Number of coefficients in the digital filter (P)
	<code>ssorder</code>	Order of polynomial to fit digitally filtered FID (P)

ssntaps Number of coefficients in digital filter (P)

Description: Specifies the number of taps (coefficients) to be used in the digital filter for solvent subtraction. If `ssntaps` does not exist in the current experiment, enter `addpar('ss')` to add it. `addpar('ss')` also creates time-domain solvent subtraction parameters `ssfilter`, `sslsfrq`, and `ssorder`.

Values: Integer from 1 to `np`/4. The default is 121. An odd number is usually best.

The more taps in a filter, the flatter the passband response and the steeper the transition from passband to stopband, giving a more rectangular filter.

For the lfs (low-frequency suppression) option, the default is suitable.

For the `zfs` (zero-frequency suppression) option, a value between 3 and 21 usually works better.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>ft</code>	Fourier transform 1D data (C)
	<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
	<code>np</code>	Number of points (P)
	<code>parfidss</code>	Create parameters for time-domain solvent subtraction (M)
	<code>ssfilter</code>	Full bandwidth of digital filter to yield a filtered FID (P)
	<code>sslsfrq</code>	Center of solvent-suppressed region of spectrum (P)
	<code>ssorder</code>	Order of polynomial to fit digitally filtered FID (P)
	<code>wft</code>	Weight and Fourier transform 1D data (C)

ssorder Order of polynomial to fit digitally filtered FID (P)

Description: Specifies the order of the polynomial to fit the digitally filtered FID if the `zfs` (zero-frequency suppression) option is selected for solvent subtraction. `ssorder` is not used if the `lfs` (low-frequency suppression) option is selected. If `ssorder` does not exist in the current experiment, enter `addpar('ss')` to add it. `addpar('ss')` also creates time-domain solvent subtraction parameters `ssfilter`, `sslsfrq`, and `ssntaps`.

The solvent subtraction option (`zfs` or `lfs`) is selected as follows:

- If `ssorder` and `ssfilter` are both set to values, `zfs` is selected.
- If `ssorder`='n' and `ssfilter` is set to a value, `lfs` is selected.
- If `ssorder`='n' and `ssfilter`='n', `zfs` and `lfs` are both turned off.

Values: 'n', integer from 1 to 20. The default is 'n'.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>parfidss</code>	Create parameters for time-domain solvent subtraction (M)
	<code>ssfilter</code>	Full bandwidth of digital filter to yield a filtered FID (P)
	<code>sslsfrq</code>	Center of solvent-suppressed region of spectrum (P)
	<code>ssntaps</code>	Number of coefficients in the digital filter (P)
	<code>wft</code>	Weight and Fourier transform 1D data (C)

stack Stacking mode for processing and plotting arrayed spectra (M)

Syntax: `stack(mode)`

Description: When processing and plotting arrayed 1D spectra, VnmrJ automatically determines if the *stacking mode* is horizontal, vertical or diagonal from the number of traces and the number of lines in the spectrum. If you do not want this automatic function (or it makes an undesirable decision), you can override it by placing the `stack` macro in the experiment startup macro or by calling `stack` before processing (or reprocessing) a spectrum. The macro `autostack` switches back to automatic determination of the stack mode by destroying the parameter `stackmode`.

Arguments: `mode` is one of the stacking modes 'horizontal', 'vertical', or 'diagonal'.

See also: *NMR Spectroscopy User Guide*

Related:	<code>autostack</code>	Automatic stacking for processing and plotting arrays (M)
	<code>procararray</code>	Process arrayed 1D spectra (M)

`plarray` Plot arrayed 1D spectra (M)
`stackmode` Stacking control for processing (P)

stackmode **Stacking control for processing arrayed 1D spectra (P)**

Description: Controls whether stacking for processing arrayed 1D spectra is automatic or nonautomatic. The *automatic stacking mode* can be overridden by creating and setting `stackmode` in the startup macro or before calling `procplot` or `procararray`. The `autostack` macro switches back to automatic determination of the stack mode by destroying this parameter.

Values: 'horizontal', 'vertical', or 'diagonal'.

See also: *NMR Spectroscopy User Guide*

Related: `autostack` Automatic stacking for processing and plotting arrays (M)
`procararray` Process arrayed 1D spectra (M)
`procplot` Automatically process FIDs (M)
`stack` Fix stacking mode for processing and plotting arrayed spectra (M)

startq **Start a chained study queue (M)**

Description: Start a chained acquisition for a study queue.

Related: `sqmode` Study queue mode (P)
`xmnext` Find next prescan or next experiment in study queue (M)

status **Display status of sample changer (C,U)**

Applicability: Systems with an automatic sample changer.

Syntax: `status<(directory<,config_file>)>`
(From UNIX) `status directory <config_file>`

Description: Displays a status window with a summary of all experiments and a scrollable list of individual experiments. Individual experiments are selected by clicking anywhere on the experiment of interest. `status` updates as the state of an automation run changes. If an experiment finishes or a new experiment is added, the `status` display is updated.

Arguments: `directory` is the path to the directory where the done queue (`doneQ`) is stored. In the UNIX shell, a directory path is required. In VnmrJ, a directory path is optional. The default is the automation mode directory.

`config_file` is the name of a user-supplied file that customizes `status` for local use. Refer to the manual *User Programming* for details.

Examples: (From VnmrJ) `status`
(From VnmrJ) `status ('/home/vnmr1/AutoRun_621')`
(From UNIX) `status /home/vnmr1/AutoRun_621 mystatus`

See also: *VnmrJ Walkup; User Programming*

Related: `autodir` Automation directory absolute path (P)
`autoname` Prefix for automation data file (P)
`enter` Enter sample information for automation run (C,U)

std1d **Apptype macro for Standard 1D experiments (M)**

Applicability: Liquids

Description: Perform the actions for Standard 1D protocols to set up, process, and plot experiments.

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related: [apptype](#) Application type (P)
[execpars](#) Set up the exec parameters (M)

stdshm Interactively create a method string for autoshimming (M)

Syntax: `stdshm`

Description: Creates a [method](#) string to be used in adjusting the spinning controls z1, z2, z3, and z4 when a sample is changed. If non-spin controls also need adjusting, further shimming operations are required.

The [method](#) string is constructed in answer to questions about the sample length, the time available for shimming, and the solvent T_1 or, in FID shimming, the T_1 of the sample. In asking about sample height, `stdshm` assumes that z3 and z4 need adjusting only with short samples; therefore, select “sample height will vary” if z3 and z4 shimming is definitely wanted.

Try lock shimming first to see if it produces a satisfactory result. Lock shimming requires a much shorter shimming time than FID shimming and usually adjusts z1 and z2 just as well. If lock shimming is unsatisfactory, try FID shimming. Again, when z3 and z4 adjustment is required, lock shimming is faster, but FID shimming is more effective. `stdshm` displays the estimated shimming time, permitting revision when the time is too long.

To shim after running `stdshm`, enter [method](#)= 'std' (for lock shimming) or [method](#)= 'fidstd' (for FID shimming). Then enter [shim](#) or set the [wshim](#) parameter to shim before the start of acquisition.

Note that the command [newshm](#) is much like `stdshm` but that [newshm](#) provides more flexibility in making [method](#) strings

See also: *NMR Spectroscopy User Guide*

Related: [dshim](#) Display a shim method string (M)
[method](#) Autoshim method (P)
[newshm](#) Interactively create a shim method with options (M)
[shim](#) Submit an Autoshim experiment to acquisition (C)
[wshim](#) Conditions when shimming is performed (P)

sth Minimum intensity threshold (P)

Description: Intensity threshold above which transitions are printed and included in the simulated spectrum. Transitions whose intensity falls below this threshold are omitted from the simulation.

Values: 0 to 1.00. A typical value is 0.05.

See also: *NMR Spectroscopy User Guide*

Related: [spins](#) Perform spin simulation calculation (C)
[spsm](#) Enter spin system (M)
[th](#) Threshold (P)

string Create a string variable (C)

Syntax: `string(variable)`

Description: Creates a string variable without a value.

Arguments: `variable` is the string variable to be created.

Examples: `string('strvar1')`

See also: *User Programming*

strtext Starting point for LP data extension in np dimension (P)

Description: Specifies inclusively the complex time-domain data point at which LP (linear prediction) data extension (alteration) is to begin in the **np** dimension. Enter **addpar**('lp') to create **strtext** and other **np** dimension LP parameters in the current experiment.

Values: 1 to **np**/2

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg LP algorithm in **np** dimension (P)
np Number of data points (P)
strtlp Starting point for LP calculation in **np** dimension (P)

strtext1 Starting point for LP data extension in ni dimension (P)

Description: Specifies inclusively the complex time-domain data point at which LP (linear prediction) data extension (alteration) is to begin in the **ni** dimension. Enter **addpar**('lp',1) to create **strtext1** and other **ni** dimension LP parameters in the current experiment.

Values: 1 to **ni**/2

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg1 LP algorithm in **ni** dimension (P)
ni Number of increments in 1st indirectly detected dimension (P)
strtlp1 Starting point for LP calculation in **ni** dimension (P)

strtext2 Starting point for LP data extension in ni2 dimension (P)

Description: Specifies inclusively the complex time-domain data point at which LP (linear prediction) data extension (alteration) is to begin in the **ni2** dimension. Enter **addpar**('lp',2) to create **strtext2** and other **ni2** dimension LP parameters in the current experiment.

Values: 1 to **ni2**/2

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg2 LP algorithm in **ni2** dimension (P)
ni2 Number of increments in 2nd indirectly detected dimension (P)
strtlp2 Starting point for LP calculation in **ni2** dimension (P)

strtlp Starting point for LP calculation in np dimension (P)

Description: Specifies the first complex, time-domain data point to be used in calculating the complex linear prediction (LP) coefficients in the **np** dimension. If **lpopt**='b', the **strtlp**-th complex time-domain data point and the ensuing $(2*\text{lpfilt}-1)$ data points are used in this calculation. If **lpopt**='f', the **strtlp**-th complex time-domain data point and the preceding $(2*\text{lpfilt}-1)$ data points are used in this calculation. Enter **addpar**('lp') to create **strtlp** and other **np** dimension LP parameters in the current experiment.

See also: *NMR Spectroscopy User Guide*

Related: **addpar** Add selected parameters to the current experiment (M)
lpalg LP algorithm in **np** dimension (P)

<code>lpfilt</code>	LP coefficients to calculate in <code>np</code> dimension (P)
<code>lpnupts</code>	LP number of data points in <code>np</code> dimension (P)
<code>lpopt</code>	LP algorithm data extension in <code>np</code> dimension (P)
<code>strtext</code>	Starting point for LP data extension in <code>np</code> dimension (P)

strtlp1 Starting point for LP calculation in `ni` dimension (P)

Description: Specifies the first complex, time-domain data point to be used in calculating the complex linear prediction (LP) coefficients in the `ni` dimension. It functions analogously to `strlp`. Enter `addpar('lp', 1)` to create `strtlp1` and other `ni` dimension LP parameters in the current experiment.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>lpalg1</code>	LP algorithm in <code>ni</code> dimension (P)
	<code>lpfilt1</code>	LP coefficients to calculate in <code>ni</code> dimension (P)
	<code>lpnupts1</code>	LP number of data points in <code>ni</code> dimension (P)
	<code>lpopt1</code>	LP algorithm data extension in <code>ni</code> dimension (P)
	<code>strtext1</code>	Starting point for LP data extension in <code>ni</code> dimension (P)

strtlp2 Starting point for LP calculation in `ni2` dimension (P)

Description: Specifies the first complex, time-domain data point to be used in calculating complex linear prediction (LP) coefficients in the `ni2` dimension. `strtlp2` functions analogously to `strlp`. Enter `addpar('lp', 2)` to create `strtlp2` and other `ni2` dimension LP parameters in the current experiment.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>lpalg2</code>	LP algorithm in <code>ni2</code> dimension (P)
	<code>lpfilt2</code>	LP coefficients to calculate in <code>ni2</code> dimension (P)
	<code>lpnupts2</code>	LP number of data points in <code>ni2</code> dimension (P)
	<code>lpopt2</code>	LP algorithm data extension in <code>ni2</code> dimension (P)
	<code>strtext2</code>	Starting point for LP data extension in <code>ni2</code> dimension (P)

studyid Study identification (P)

Applicability: Liquids

Description: Specifies the relative directory where a study is stored. In Walkup, it is relative to `autodir`. In imaging, it is relative to `globalauto`; It is set when a new study is created.

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related:	<code>autodir</code>	Automation directory absolute path (P)
	<code>globalauto</code>	Automation directory name (P)
	<code>sqdir</code>	Study queue directory (P)
	<code>sqname</code>	Study queue parameter template (P)

studypar Study parameters (P)

Applicability: Liquids, Imaging

Description: A global parameter that contains the list of parameters saved with a study. If the parameter does not exist, it is created by `cqsavestudy` for liquids or `sqsavestudy` for imaging when a study is saved.

S

See also: *NMR Spectroscopy User Guide*, *VnmrJ Walkup*, *VnmrJ Imaging User Guide*

Related: [cqsavestudy](#) Macro to save study queue parameters (M)
[sqsavestudy](#) Macro to save study parameters for imaging (M)

studystatus Study status (P)

Applicability: *VnmrJ Walkup*

Description: The status of a study for a sample. The status is set from the status of the experiments within the study by the macro [cqsavestudy](#).

See also: *VnmrJ Walkup*

Related: [cqsavestudy](#) Macro to save study queue parameters (M)
[studytime](#) Study time (P)

studytime Study time (P)

Applicability: *Walkup*

Description: The total time it takes to run a study. It is set by the `xmtime` macro when a study is created.

See also: *VnmrJ Walkup*

Related: [xmsubmit](#) Submit sample(s) to the study queue (M)
[xmtime](#) Update the study queue time (M)

su Submit a setup experiment to acquisition (M)

Description: Sets up the system hardware to match the current parameters but does not initiate data acquisition. Typical uses of `su` are to change the system frequency in preparation for probe tuning, to change the sample temperature in advance of beginning an experiment (or after a variable temperature experiment is run), and to turn the decoupler on or off. If `load= 'Y'`, `su` can be used to set shim values. `su` also sets lock parameters ([lockpower](#), [lockgain](#), [lockphase](#)) and the field offset parameter (`z0`).

`su` does *not* delete any existing data in the current experiment (only [go](#), [ga](#), and [au](#) do that). Everything that `su` does is also done by [go](#), [ga](#), and [au](#).

Shim DAC values are automatically loaded when the acquisition system boots up; if the acquisition system has been recently rebooted, `su` must be entered before [acqi](#) or [qtune](#) can be run.

See also: *NMR Spectroscopy User Guide*

Related: [acqi](#) Interactive acquisition display process (C)
[au](#) Submit experiment to acquisition and process data (C)
[change](#) Submit a change sample experiment to acquisition (M)
[ga](#) Submit experiment to acquisition and FT the result (C)
[go](#) Submit experiment to acquisition (C)
[load](#) Load status of displayed shims (P)
[lock](#) Submit an Autolock experiment to acquisition (C)
[lockgain](#) Lock gain (P)
[lockphase](#) Lock phase (P)
[lockpower](#) Lock power (P)
[qtune](#) Tune probe using swept-tune graphical tool (C)
[sample](#) Submit change sample, autoshim experiment to acquisition (M)
[shim](#) Submit an Autoshim experiment to acquisition (C)
[spin](#) Submit a spin setup experiment to acquisition (C)
[z0](#) Z0 field position (P)

sub Subtract current FID from add/subtract experiment (C)

Syntax: (1) `sub<(multiplier<,'new'>>`
 (2) `sub('new')`
 (3) `sub('trace',index)`

Description: Subtracts the last displayed or selected FID from the current contents of the add/subtract experiment (exp5). `lsfid` and `phfid` can be used to shift or phase rotate the selected FID before it is subtracted from the data in add/subtract experiment. A multi-FID add/subtract experiment can be created by using the 'new' keyword. Individual FIDs in a multi-FID add/subtract experiment can subsequently be subtracted by using the 'trace' keyword followed by the index number of the FID.

Arguments: `multiplier` is a value that the FID is to be multiplied by before being subtracted from the add/subtract experiment (exp5). The default is 1.0.
 'new' is a keyword to create a new FID element in an add/subtract experiment.
 'trace' is a keyword to use the next argument (`index`) as the number of the FID to subtract from in an add/subtract experiment. The default is to subtract from the first FID in a multi-FID add/subtract experiment.
`index` is the index number of the FID to be used as a target in a multi-FID add/subtract experiment.

Examples: `sub`
`sub(0.75)`
`sub('new')`
`sub('trace',2)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>add</code>	Add current FID to add/subtract experiment (C)
	<code>clradd</code>	Clear add/subtract experiment (C)
	<code>lsfid</code>	Number of complex points to left-shift <code>ni</code> interferogram (P)
	<code>phfid</code>	Zero-order phasing constant for <code>np</code> FID (P)
	<code>select</code>	Select a spectrum without displaying it (C)
	<code>spsub</code>	Subtract current spectra from add/subtract experiment (P)

substr Select a substring from a string (C)

Applicability: `VnmrJ`

Syntax: `substr('string',word_number):$n1<,$n2<,$n3>>`
`substr('string',index,length<,'new_string'):`
`n1<,$n2<,$n3>>`
`substr('string',word_number,'delimiter',`
`'delimiter_char'):`
`n1<,$n2<,$n3>>`

Description: Picks a substring or word out of a string, replace, or delete a set of characters from a string and returns the result to the string variable `$n1`. The position of the first character of the word and the number of characters of the word are returned to `$n2` and `$n3` if these string variables are supplied.

Arguments: 'string' string or a string variable.

`word_number` is the number of the word to select. Words are counted sequential beginning with the first word of the string as 1.

`index` is the number of characters counted from the first character of the string or a string variable containing this number.

`length` is the number of characters in the substring.

`new_string` is string or a string variable to replace the contents of `string` at the position specified by `index` and `length` and pass the resulting string to the return string variable.

'`delimiter`' is a keyword that requires the '`delimiter_char`' argument to specify that the argument that follows specifies the delimiter(s).

'`delimiter_char`' is a string of characters to use as delimiters to separate words.

Default delimiters are space and tab " \t".

`$n1` is the return string variable containing the searched for text.

`$n2` is the return variable containing the position of the first character of the word in the string.

`$num` is the return string variable containing the number of characters in the word specified by `word_number` and contained within the delimiters.

Examples: Search examples:

```
substr('There are 10 samples to be run',4):n1
string n1='samples'

substr('There are 10 samples to be run',4):n1,$f,$num
sets strings n1='samples' $f=14 and $num=7

substr('abcdefg',2,3):n1
string n1='bcd'

substr('This is;a phrase',2):n1
string n1='is;a'

substr('This is;a phrase',2,
      'delimiter',';\t'):n1,$f,$num
sets strings n1='is' $f=6 and $num=2
```

Text substitution examples:

Explicit text substitution and passing the result to the return string variable.

```
substr('abcdefg',2,3,'1234'):n1
string n1='a1234efg'
```

Text substitution in a string variable using results held in return string variable from a previous search. Start with the following text held in a string variable:

```
n1='There are 10 samples to be run'
```

```
substr(n1,4):n2,$f,$num
sets strings n2=samples, $f=14, and $num=7
```

```
substr(n1,$f,$num,'experiments'):n3
```

Counts 14 characters (`$f=14`) from the beginning of `n1`, substitutes the word `experiments` for the 7 character (`$num=7`) word in `n1`, and passes the new string to the return string variable setting

```
n3='There are 10 experiments to be run'
```

See also: *User Programming*

Related:	<code>length</code>	Determine length of a string (C)
	<code>string</code>	Create a string variable (C)

suselfrq **Select peak, continue selective excitation experiment (M)**

Syntax: `suselfrq`

Description: Sets up selective frequency pulse, power, and shape and continue with the selective excitation experiment. Used by `Noesy1d`, and `TOCSY1D`.

See also: *NMR Spectroscopy User Guide*, *VnmrJ Walkup*

Related:	<code>Noesy1d</code>	Change parameters for NOESY1D experiment (M)
	<code>setselinv</code>	Set up selective inversion (M)

`setselfrqc` Select selective frequency and width (M)
`TOCSY1D` Change parameters for TOCSY1D experiment (M)

svdat Save data (C)

Syntax: `svdat (file<, 'f' | 'm' | 'i' | 'b'>)`

Description: Outputs current data from the current experiment to a file. Integer data is scaled when it is written.

Arguments: `file` is the name of the data file. The file is created in the current directory VnmrJ is in unless a full directory path is given. If a file of the same name already exists, the user will be queried to overwrite the file. If a fully qualified filename is not given, the file will be created in VnmrJ's current directory.

'f' | 'm' | 'i' | 'b' defines how the data is to be written out: 'f' is 32-bit floating point, 'm' or 'i' is 16-bit integer scaled to 12 bits, and 'b' is 8-bit byte integer. The default is 'f'.

Floating point data is not scaled when written.

Integer data is scaled when written. A data value x is scaled as $ax+b$ where:

$$a = (vs * \text{graysl} * \text{numgray}) / 64.0$$

$$b = \text{numgray} * (0.5 - (\text{graysl} * \text{grayctr} / 64.0))$$

where `numgray` (see below) has a default of 4096 for 'm' and 'i' formats and a default of 256 for the 'b' format, `graysl` has a default of 1, and `grayctr` has a default of 32.0.

To scale 16-bit integer data other than 12-bits, the global parameter `numgray` can be created using `create (numgray, real, global)` and set to the value 2^n , where n is the number of bits desired. For example, to scale to 15-bits, set `numgray=32768`.

The display parameters `graysl` and `grayctr` are used to save data files for ImageBrowser.

Examples: `svdat (rathead, 'b')`

See also: *VnmrJ Imaging NMR*

Related: `create` Create new parameter in parameter tree (C)
`grayctr` Gray level window adjustment (P)
`graysl` Gray level slope (contrast) adjustment (P)

svf Save FIDs in current experiment (M)

Syntax: `svf<(file<, 'nolog'><, 'arch'><, 'force'><, 'nodb'>)>`

Description: Saves parameters, text, and FID data in the current experiment to a file. No data is removed from the current experiment; `svf` merely saves a copy of the data in a different file. You can enter `rt` to retrieve the complete data set, or enter `rtp` to retrieve parameters only.

Arguments: `file` is the name of the file, with the suffix `.fid` added, to be created to save the data. The default is the system prompts for a file name. You are warned if you attempt to overwrite a file that already exists. In fact, if data has been acquired with the `file` parameter set, the data does not need to be saved. It is already stored in a named file.

'nolog' is a keyword to not save the log file with the data. The default is to save the log file.

'arch' is a keyword to assume that the data goes to a database and appends to the (or creates a) `doneQ` file with information that can be used by the command `status`.

If `force` is given, you are not warned and the older parameter set is removed.

`nodb` is a keyword to prevent `svf` from adding information to a database. This prevention is useful if temporary parameter files are saved that will soon be removed.

Examples: `svf`
`svf ('/home/vnmr1/mydatafile')`

See also: *NMR Spectroscopy User Guide*

Related: `file` File name (P)
`rt` Retrieve FID (M)
`rtp` Retrieve parameters (M)
`status` Display status of all experiments (C)

svfdf Save FID data in FDF format (M)

Syntax: `svfdf(directory)`

Description: Saves raw data from the FID file of the current experiment as an FDF (Flexible Data Format) file. Data is saved in multiple files, with one trace per file. The files are named `fid0001.fdf`, `fid0002.fdf`, etc. The `procpa` file from the current experiment is also saved in the same directory.

The FDF file format is described in the manual *User Programming*. Note that the data is complex (FDF type="complex"), and the FDF ordinate = {"intensity", "intensity"}, indicating that each point consists of a pair of intensities. The FDF headers also contain the following special fields:

- `nfile` gives the sequential number of this file in the series.
- `ct` is the value of the `ct` parameter. The data should be divided by `ct` to give the average signal intensity for one scan.
- `scale` gives the power of two scaling factor for the data. The data should be multiplied by 2^{scale} to give the true values.

Arguments: `directory_name` is the directory in which to store the files. The extension `.dat` is appended to the given name.

Examples: `svfdf(curexp+'/raw')`

See also: *User Programming*

Related: `ct` Completed transients (P)

svfdir Directory for non-study data (P)

Description: Specifies the directory where data is saved when not using a study in VnmrJ.

See also: *NMR Spectroscopy User Guide*, *VnmrJ Walkup*

Related: `fidsave` Save data (M)
`save` Save data (M)
`svfname` Filename parameter template for non-study data ((P))

Svfname Create path for data storage (C)

Applicability: Automation

Syntax: `Svfname:$path`
`Svfname(name_template):$path`
`Svfname(name_template,suffix):$path`
`Svfname(name_template,suffix,excluded_suffix):$path`

```
Svfname(name_template,suffix<,'excluded_suffix',
        <'keepspace' | 'replacespace'>):$path
```

Description: Determines the name used to store data. This command provides the functionality of the autoname parameter without being in automation mode.

Svfname default naming command with alternate suffixes is *svfname* and the default directory is *svfdir*. *Svfname* does not read a sample info file. A suffix is specified as the second argument. Use a suffix of " to access ordinary files and directories. Arguments used with *Svfname* are constructed the same way arguments are constructed for *autoname*.

The name is prefixed with using the value of the parameter *autodir* or *userdir*+ '/data/' if *name_template* is a relative path.

The default suffix is *.fid*.

Arguments: *svfname* is default naming parameter.

svfdir is default directory parameter.

name_template (no quotes) is string that contains keywords separated by substitution specifiers to represent the data storage path. Substitution specifiers in this template are either a percent sign (%) or a dollar sign (\$). The keywords are obtained using % substitution specifiers or VNMR parameters using \$ substitution specifiers.

Percent sign (%) substitution specifier is used to scan for the text specified by keyword between the first percent sign in the template string and the next percent sign. The text specified by the keyword between the % substitution specifiers is passed to \$path.

The following percent substitutions (% keywords) for time and date are obtained from the system clock, not from the sample info file:

<i>Keyword</i>	<i>Format</i>	<i>Description</i>
%DATE%	YYYYMMDD	4-digit year, 2-digit month, 2-digit day
%TIME%	HHMMSS	2-digit hour, 2-digit minute, 2-digit second
%YR%	YYYY	4-digit year
%YR2%	YY	2-digit year
%MO%	MM	2-digit month
%DAY%	DD	2-digit day
%HR%	HH	2-digit hour
%MIN%	MM	2-digit month
%SEC%	SS	2-digit second

Dollar sign (\$) substitution specifier is used with the *Svfname* command to interpreted a VNMR parameter and substitute the value of this parameter a suffix.

Numeric parameters are truncated and represented as a string with the form: <optional string>parameter value<optional string>. The *name_template*, *pw=\$pw\$usec*, with *vnmr* parameter *pw* having a value of 12.3 produces *pw=12usec01* which is appended to *.fid* (or *.img*) and passed to \$path.

String parameters cannot not contain any of the following characters: ' ', '!', '"', '\$', '&', '\', '(', ')', '*', ';', '<', '>', '?', '\\', '[', ']', '^', '\', '{', '}', '|', ':', '\0'

A comma separated excluded suffix list appends a string based on the suffixes and excluded suffixes to the path. Using the keyword 'replacespace' uses underscores (_) in place of spaces ' ' in the resulting path name. The keyword 'keepspace' retains spaces in the resulting path name.

'keepspace' | 'replacespace' is an optional argument (includes quotes) that uses either of the following keywords: `replacespace` or `keepspace`. The argument is accepted if the third argument is a list of suffixes. The action is the same as described for the third argument

Version number is specified by `%Rn%` where `n` is an integer from 0 to 9 (default 2), as follows:

<i>n</i> =	Description
0	no revision digits are appended (all names must be uniquely constructed without these revision digits).
1 to 9	revision number is padded with leading zeroes to form an <i>n</i> -digit number. If more places are needed than specified, more zeroes are used.
>9 (more than one digit)	<code>Rnn</code> is still used as a search string in the sampleinfo file. <code>%Rn%</code> must be specified at the end of the <code>name_template</code> string. The revision digits are always appended except if <code>%R0%</code> is used.
no <code>%Rn%</code>	default of <code>%R2%</code> is used

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related: `autoname` Determines path for data storage during an automation run (C)
`autoname` Temple determining the path where is data stored (P)
`sqname` Study queue parameter template (P)
`svfname` Specifies the filename template (P)

svfname Filename parameter template for non-study data ((P))

Description: Specifies the filename template where data is saved when not using a study in VnmrJ. The template is constructed using the same keywords and delimiter, dollar sign (\$) and percent sign (%), as `autoname`.

Examples: If `svfdir=userdir+'/data'`, the result from `fidsave` is:
`svfname='$pslabel$_$tn$_' -> userdir+'/data/Proton_H1_01.fid'`
`svfname='%DATE%/t%TIME%%R0%' -> userdir+'/data/20040501/t113005.fid'`

See also: *NMR Spectroscopy User Guide, VnmrJ Walkup*

Related: `fidsave` Save data (M)
`Svfname` Create path for data storage (C)
`sqname` Study queue parameter template (P)
`save` Save data (M)
`svfname` Filename parameter template for non-study data ((P))

svp Save parameters from current experiment (M)

Syntax: `svp(file) <(file<,'force'><,'nodb'>)>`

Description: Saves parameters from current experiment to a file. The parameter set can be retrieved with the `rtp` and `rt` macros. `svp` reflects any changes made in parameters up to the moment of entering `svp`, including acquisition parameters (unlike macro `svf`).

Arguments: `file` is the name of the file, with the suffix `.par` added, to be created to save the parameters. The default is the system prompts for a file name. You are warned if you attempt to overwrite a parameter set that already exists.

If `force` is given, you are not warned and the older parameter set is removed.
`nodb` is a keyword to prevent `svp` from adding information to a database. This prevention is useful if temporary parameter files are saved that will soon be removed.

Examples: `svp ('/vnmr/stdpar/P31')`
`svp ('/usr/george/testdata')`

See also: *NMR Spectroscopy User Guide*

Related: `rt` Retrieve FID (M)
`rtp` Retrieve parameters (M)
`svf` Save FIDs in current experiment (M)

svs Save shim coil settings (C)

Syntax: `svs (file) <:status>`

Description: Saves all shim coil settings except Z0 to a file.

Arguments: `file` is the name of a file for saving the shim coil settings. If the file name is an absolute path, `svs` uses it with no modifications. Otherwise, `svs` saves the shim in the first application directory for which it has write permission.

The `svs` command reports where it stored the shims, unless it is requested to return the status.

`status` is a return variable with one of the following values after `svs` finishes:

- 0 indicates `svs` failed to store shim file.
- 1 indicates `svs` stored the shim file, either as an absolute path or in the `shims` directory of the first application directory.
- ≥ 2 indicates `svs` stored the file in `shims` directory of the second, third, or later application directory.

Examples: `svs ('acetone')`
`svs ('bb10mm') :r1`

See also: *NMR Spectroscopy User Guide*

Related: `rts` Retrieve shim coil settings (C)

svs Spin simulation vertical scale (P)

Description: Vertical scale for simulated spectrum.

Values: 0 to 1e10. A typical value is 200.

See also: *NMR Spectroscopy User Guide*

Related: `spins` Perform spin simulation calculation (C)
`spsm` Enter spin system (M)

svtmp Move experiment data into experiment subfile (M)

Syntax: `svtmp <(file)>`

Description: Moves the experiment data (parameters, FID, and transformed spectrum) from current experiment into a subdirectory inside `curexp+ '/subexp'`. Unlike the macro `cptmp`, the experiment data is no longer accessible in the current experiment; only a copy of the parameters is still present.

Arguments: `file` is the name of the subfile that receives the experiment data. The default name is either the transmitter nucleus (if `seqfil` = 's2pul') or the pulse sequence name.

S

Examples: `svtmp`
`svtmp('cosy')`

See also: *NMR Spectroscopy User Guide*

Related: `cptmp` Copy experiment data into experiment subfile (M)
`curexp` Current experiment directory (P)
`rttmp` Retrieve experiment data from experiment subfile (M)
`seqfil` Pulse sequence name (P)

sw

Spectral width in directly detected dimension (P)

Description: Sets the total width of the spectrum to be acquired, from one end to the other. All spectra are acquired using quadrature detection. The spectral width determines the sampling rate for data, which occurs at a rate of $2 * sw$ points per second (actually sw pairs of complex points per second). Note that the sampling rate itself is not entered, either directly or as its inverse (known on some systems as the *dwell time*).

If a value of sw is entered whose inverse is not an even multiple of the time base listed above, sw is automatically adjusted to a slightly different value to give an acceptable sampling rate.

To enter a value in ppm, append the character `p` (e.g., $sw=200p$).

If a DSP facility is present in the system (i.e., `dsp='i'` or `dsp='r'`) and oversampling in the experiment has not been turned off by setting `oversamp='n'`, then the oversampling factor will be recalculated.

Values: Number, in Hz. The range possible is based on the system:

100 Hz to 500 kHz.

solids systems: up to 5 MHz.

See also: *NMR Spectroscopy User Guide*

Related: `dp` Double precision (P)
`dsp` Type of DSP for data acquisition (P)
`oversamp` Oversampling factor for acquisition (P)
`setlp0` Set parameters for zero linear phase (M)
`sw1` Spectral width in 1st indirectly detected dimension (P)
`sw2` Spectral width in 2nd indirectly detected dimension (P)
`sw3` Spectral width in 3rd indirectly detected dimension (P)

sw1

Spectral width in 1st indirectly detected dimension (P)

Description: Analogous to the `sw` parameter except that $sw1$ applies to the first indirectly detected dimension of a multidimensional data set. The increment of the variable evolution time `d2` is automatically calculated from $sw1$. The number of increments for this dimension is set by `ni`. To create $sw1$ in the current experiment, as well as `ni` and `phase`, enter `addpar('2d')`.

See also: *NMR Spectroscopy User Guide*

Related: `addpar` Add selected parameters to the current experiment (M)
`d2` Incremented delay in 1st indirectly detected dimension (P)
`ni` Number of increments in 1st indirectly detected dimension (P)
`phase` Phase selection (P)
`sw` Spectral width in directly detected dimension (P)
`sw2` Spectral width in 2nd indirectly detected dimension (P)
`sw3` Spectral width in 3rd indirectly detected dimension (P)

sw2 Spectral width in 2nd indirectly detected dimension (P)

Description: Analogous to the **sw** parameter except that **sw2** applies to the second indirectly detected dimension of a multidimensional data set. The increment of the variable evolution time **d3** is automatically calculated from **sw2**. The number of increments for this dimension is set by **ni2**. To create **sw2** in the current experiment, as well as **d3**, **ni2**, and **phase2**, enter **addpar** (' 3d ').

See also: *NMR Spectroscopy User Guide*

Related:	addpar	Add selected parameters to the current experiment (M)
	d3	Incremented delay for 2nd indirectly detected dimension (P)
	ni2	Number of increments in 2nd indirectly detected dimension (P)
	phase2	Phase selection for 3D acquisition (P)
	sw	Spectral width in directly detected dimension (P)
	sw1	Spectral width in 1st indirectly detected dimension (P)
	sw3	Spectral width in 3rd indirectly detected dimension (P)

sw3 Spectral width in 3rd indirectly detected dimension (P)

Description: Analogous to the **sw** parameter except that **sw3** applies to the third indirectly detected dimension of a multidimensional data set. The increment of the variable evolution time **d4** is automatically calculated from **sw3**. The number of increments for this dimension is set by **ni3**. To create **sw3** in the current experiment, as well as **d4**, **ni3**, and **phase3**, enter **addpar** (' 4d ').

See also: *NMR Spectroscopy User Guide*

Related:	addpar	Add selected parameters to the current experiment (M)
	d4	Incremented delay for 3rd indirectly detected dimension (P)
	ni3	Number of increments in 3rd indirectly detected dimension (P)
	par4d	Create 4D acquisition parameters (C)
	phase3	Phase selection for 4D acquisition (P)
	sw	Spectral width in directly detected dimension (P)
	sw1	Spectral width in 1st indirectly detected dimension (P)
	sw2	Spectral width in 2nd indirectly detected dimension (P)

sysgcoil System gradient coil (P)

Description: Specially reserved string parameter that specifies which physical gradient set is currently installed, and allows convenient updating of important gradient characteristics when one gradient set is interchanged for another. The value to **sysgcoil** is assigned to the parameter **gcoil** when joining experiments or retrieving parameter sets.

This parameter is set in the Spectrometer Configuration window to the name of the gradient set in use. Once set, it is then available to all experiments and to all users.

See also: *VnmrJ Installation and Administration; VnmrJ Imaging NMR*

Related:	config	Display current configuration and possibly change it (M)
	gcoil	Current gradient coil (P)
	gmax	Maximum gradient strength (P)
	setgcoil	Assign sysgcoil configuration parameter (M)

system System type (P)

Description: A global parameter that sets the basic type of system: spectrometer or data station. The value is set using the System Type label in the Spectrometer Configuration window.

S

Values: 'spectrometer' is a spectrometer system (Spectrometer choice in Spectrometer Configuration window).
'datastation' is a system used as a data station (Data Station choice in Spectrometer Configuration window). Acquisition is not allowed in this setting.

See also: *VnmrJ Installation and Administration*

Related: [config](#) Display current configuration and possibly change it (M)
[Console](#) System console type (P)

systemdir **VnmrJ system directory (P)**

Description: Contains path to VnmrJ system directory, typically /vnmr. The UNIX environmental variable vnmrsystem initializes systemdir at bootup.

See also: *NMR Spectroscopy User Guide*

T

<code>t1</code>	T_1 exponential analysis (M)
<code>t1s</code>	T_1 exponential analysis with short output table (M)
<code>t2</code>	T_2 exponential analysis (M)
<code>t2s</code>	T_2 exponential analysis with short output table (M)
<code>tabc</code>	Convert data in table order to linear order (M)
<code>tan</code>	Find tangent value of an angle (C)
<code>tape</code>	Read tapes from VXR-style system (M,U)
<code>tape</code>	Control tape options of files program (P)
<code>target_bval</code>	Adjust <code>gdif f</code> to achieve target b-value (M)
<code>tchan</code>	RF channel number used for tuning (P)
<code>tcl</code>	Send Tcl script to Tcl version of dg window (C)
<code>temp</code>	Open the Temperature Control window (C)
<code>temp</code>	Sample temperature (P)
<code>tempcal</code>	Temperature calculation (C)
<code>tempcalc</code>	Measure approximate sample temperature in Cold Probes (M)
<code>testacquire</code>	Test acquire mode (P)
<code>testct</code>	Check ct for resuming signal-to-noise testing (M)
<code>testsn</code>	Test signal-to-noise of a spectrum (M)
<code>teststr</code>	Find which array matches a string M)
<code>text</code>	Display text or set new text for current experiment (C)
<code>textis</code>	Return the current text display status (C)
<code>textvi</code>	Edit text file of current experiment (M)
<code>th</code>	Threshold (P)
<code>th2d</code>	Threshold for integrating peaks in 2D spectra (P)
<code>thadj</code>	Adjust threshold for peak printout (M)
<code>time</code>	Display experiment time or recalculate number of transients (M)
<code>tin</code>	Temperature interlock (P)
<code>tlt</code>	First-order baseline correction (P)
<code>tmove</code>	Left-shift FID to time-domain cursor (M)
<code>tmsref</code>	Reference 1D proton or carbon spectrum to TMS (M)
<code>tn</code>	Nucleus for observe transmitter (P)
<code>tncosyps</code>	Set up parameters for TNCOSYPS pulse sequence (M)
<code>tndqcosy</code>	Set up parameters for TNDQCOSY pulse sequence (M)
<code>tnmqcosy</code>	Set up parameters for TNMQCOSY pulse sequence (M)
<code>tnnoesy</code>	Set up parameters for TNNOESY pulse sequence (M)
<code>tnroesy</code>	Set up parameters for TNROESY pulse sequence (M)
<code>tntocsy</code>	Set up parameters for TNTOCOSY pulse sequence (M)
<code>Tocsy</code>	Convert the parameters to a TOCSY experiment (M)
<code>Tocsy1d</code>	Convert the parameter set to a Tocsy1d experiment (M)
<code>tocsyHT</code>	Set up the tocsyHT experiment (M)
<code>tof</code>	Frequency offset for observe transmitter (P)
<code>tpwr</code>	Observe transmitter power level with linear amplifiers (P)
<code>tpwrf</code>	Observe transmitter fine power (P)

T

<code>tpwrm</code>	Observe transmitter linear modulator power (P)
<code>trace</code>	Mode for n -dimensional data display (P)
<code>traymax</code>	Sample changer tray slots (P)
<code>troesy</code>	Set up parameters for TROESY pulse sequence (M)
<code>trunc</code>	Truncate real numbers (O)
<code>tshift</code>	Adjust tau2 to current cursor position (M)
<code>tugain</code>	Amount of receiver gain used by qtune (P)
<code>tune</code>	Assign a frequency to a channel for probe tuning (C)
<code>tunehf</code>	Tune both H1 and F19 on an HFX probe (M)
<code>tunematch</code>	Default match target, in percent of optimum (P)
<code>tunemethod</code>	Method to use for tuning (P)
<code>tuneResult</code>	Message indicating how well the tuning succeeded (P)
<code>tunesw</code>	Width of the tuning sweep in Hz (P)
<code>tupwr</code>	Transmitter power used in tuning (P)
<code>typeof</code>	Return identifier for argument type (O)

t1 **T_1 exponential analysis (M)**

Description: Processes data obtained using an array of values of the parameter `d2` for a T_1 experiment. It runs `expfit`, which does an exponential curve fitting that determines the value of T_1 . The output is matched to the equation:

$$M(t) = (M(0) - M_0) * \exp(-t/T_1) + M_0$$

where M_0 is the equilibrium Z magnetization and $M(0)$ is the magnetization at time zero (e.g., immediately after the 180° pulse for an inversion recovery T_1 experiment). Notice that this equation will fit inversion recovery data (for which $M(0)$ is approximately equal to $-M_0$) or saturation recovery data (for which $M(0)$ is 0).

The required input is the file `fp.out` from `fp` and the values of the arrayed parameter. The T_1 analysis is done for all the peaks listed in `fp.out`. Peaks are selected for analysis by entering `fp(index1,index2,...)` before running the analysis. The output file is the `analyze.list` in the current experiment. The file `analyze.out` is used by `exp1` to display the results. The output of the analysis program shows T_1 and its standard deviation, but does not explicitly show $M(0)$, M_0 , or their standard deviations. The $M(0)$ and M_0 values can be found in “raw” form in `analyze.out` in the current experiment, but their standard deviations are not part of the program output.

See also: *NMR Spectroscopy User Guide*

Related:	<code>d2</code>	Incremented delay in 1st indirectly detected dimension (P)
	<code>expfit</code>	Make least squares fit to polynomial or exponential curve (C)
	<code>fp</code>	Find peak heights (C)
	<code>t1s</code>	T_1 exponential analysis with short output table (M)
	<code>t2</code>	T_2 exponential analysis (M)
	<code>t2s</code>	T_2 exponential analysis with short output fable (M)

t1s **T_1 exponential analysis with short output table (M)**

Description: Performs the same analysis as `t1` but produces a short output table showing only a summary of the measured relaxation times.

See also: *NMR Spectroscopy User Guide*

Related:	<code>t1</code>	T_1 exponential analysis (M)

t2 **T_2 exponential analysis (M)**

Description: Processes data obtained using an array of values for the base time parameter `bt` for a T_2 experiment. It runs `expfit`, which does an exponential curve fitting that determines the value of T_2 . The output is matched to the equation:

$$M(t) = (M(0) - M(\text{inf})) * \exp(-t/T_2) + M(\text{inf})$$

where $M(0)$ is the magnetization at time zero (i.e., the full magnetization excited by the observe pulse) and $M(\text{inf})$ is the xy-magnetization at infinite time (zero unless the peak is sitting on an offset baseline).

The required input is the file `fp.out` from `fp` and the values of the arrayed parameter. The T_2 analysis is done for all the peaks listed in `fp.out`. Peaks are selected for analysis by entering `fp(index1, index2, ...)` before running the analysis. The output file is the file `analyze.list` in the current experiment. The file `analyze.out` is used by `exp1` to display the results. The output of the analysis program shows T_2 and its standard deviation, but does not explicitly show $M(0)$, $M(\text{inf})$, or their standard deviations. The $M(0)$ and $M(\text{inf})$ values can be found in “raw” form in `analyze.out` in the current experiment, but their standard deviations are not part of the program output.

See also: *NMR Spectroscopy User Guide*

Related:	<code>expfit</code>	Make least squares fit to polynomial or exponential curve (C)
	<code>fp</code>	Find peak heights (C)
	<code>t1</code>	T_1 exponential analysis (M)
	<code>t1s</code>	T_1 exponential analysis with short output table (M)
	<code>t2s</code>	T_2 exponential analysis with short output table (M)

t2s **T_2 exponential analysis with short output table (M)**

Description: Performs the same analysis as `t2` but produces a short output table showing only a summary of the measured relaxation times.

See also: *NMR Spectroscopy User Guide*

Related:	<code>t2</code>	T_2 exponential analysis (M)

tabc **Convert data in table order to linear order (M)**

Syntax: `tabc<(dimension)>`

Description: Converts arbitrarily ordered data obtained under control of an external AP table to linear monotonic order, suitable for processing in VnmrJ. The data must have been acquired according to a table in the `tablib` directory.

Imaging and other 2D experiments are normally acquired so that the order of the incremented acquisition parameter, such as the phase-encode gradient, is linear and monotonic. For a standard imaging experiment, this linear order means that the phase-encode gradient progresses from a starting negative value monotonically up through zero to a positive value (e.g., -64, -63, -62, ..., -1, 0, 1, ..., 62, 63). The `ft2d` program assumes this structure in its operation.

Data from table-driven 2D pulse sequences is used by entering `tabc` only once before normal 2D processing and/or parameter storage. In this situation, `tabc` takes no arguments and is executed by entering `tabc` in the command window. A simple check is done by `tabc` to prevent it from being executed more than once on the same data set.

2D data is expected to be in the standard VnmrJ format, but if the 2D data is in the compressed format, setting `dimension` to 1 converts the data. `tabc` supports all 2D data types recognized by VnmrJ: arrayed, compressed multislice, and arrayed compressed multislice,

3D data is expected to be in the compressed/standard format, in which there are `ni` standard 2D planes of data (the third dimension), each consisting of `nf` compressed FIDs (the second dimension). Setting `dimension` to 3 reorders 3D data acquired with an external table.

`tabc` reads the file `fid` in the `acqfil` subdirectory of the current experiment. Before the data is reordered, this file is written to the file `fid.orig` in the same `acqfil` directory. If for any reason `tabc` fails or results in an unpredictable or undesired transformation, the original raw data can be recovered by moving `fid.orig` back to `fid`. To gain more disk space, you can delete `fid.orig` after you are satisfied that conversion is successful.

Use `tabc` on saved data that has been loaded into an experiment or on data in an experiment that has just been acquired but not yet saved. In the first case, converted data must be resaved for the saved data set to reflect conversion.

`tabc` requires that data must have the same number of “traces” as the table elements. It does not support any of the advanced features of table expansion (e.g., the entire table must be explicitly listed in the table file), and expects to find only one table in a file; whether the table is `t1` or `t60` is unimportant.

Arguments: `dimension` specifies the type of data to be converted: 1 for 2D compressed data, 2 for 2D standard data, or 3 for 3D compressed/standard data. The default is 2.

Examples: `tabc`
`tabc (1)`
`tabc (3)`

See also: *VnmrJ Imaging NMR*

Related:	<code>flashc</code>	Convert compressed 2D data to standard 2D format (C)
	<code>ft2d</code>	Fourier transform 2D data (C)
	<code>ni</code>	Number of increments in 1st indirectly detected dimension (P)
	<code>nf</code>	Number of FIDs (P)

tan Find tangent value of an angle (C)

Syntax: `tan (angle) <:n>`

Description: Finds the tangent of an angle.

Arguments: `angle` is an angle, in radians.

`n` is the return value giving the tangent of `angle`. The default is to display the tangent value in the status window.

Examples: `tan (.5)`
`tan (val) :tan_val`

See also: *User Programming*

Related:	<code>atan</code>	Find arc tangent value of a number (C)
	<code>cos</code>	Find cosine value of an angle (C)
	<code>exp</code>	Find exponential value of a number (C)
	<code>ln</code>	Find natural logarithm of a number (C)
	<code>sin</code>	Find sine value of an angle (C)

tape Read tapes from VXR-style system (M,U)

Syntax: (From VnmrJ) `tape (<-d device,><type,>option
<,file1,file2,...>)`
(From UNIX) `tape <-d device> <type> <option>
<file1> <file2>...`

Description: Displays the contents of a VXR-style (Gemini, VXR-4000, or XL) 9-track tape for use with VnmrJ or reads one or several files from the tape into the current directory. Note that the *write* option is not supported (i.e., VnmrJ only *reads* tapes in a VXR-style format and does not write to a tape).

Arguments: *device* is the tape drive device name. The default value is `/dev/rst8`. For AIX systems, *device* should be `/dev/rmt0`. If the default value is not set properly or another device name is wanted, be sure to type `-d` and a space before the device name you want to input.

type is the type of tape to be accessed. `'-q'` or `'-s'` select the 1/4-inch tape unit ("streaming" or cartridge tape); this is the default. `'-9'`, `'-h'`, or `'-n'` select the 1/2-inch tape unit (open reel tape drive).

option is one of the following:

- `'help'` is a keyword to display help on the use of the system.
- `'cat'` is a keyword to display a catalog of files on tape.
- `'read'` is a keyword to read one or more files. This option requires that the files be listed as the next argument.
- `'rewind'` is a keyword to rewind tape (1/2-inch tape only).
- `'quit'` is a keyword to release the tape drive (1/2-inch tape only).

file1, *file2*, ... are the names of one or more files to be read. Wildcard characters (`*` and `?`) can be used.

Examples: `tape('cat')`
`tape('-h','read','mydata')`
`tape -h read mydata`
`tape -d /dev/rmt/0lb read mydata`

Related: `decomp` Decompose a VXR-style directory (C)
`vxr_unix` Convert VXR-style text files to UNIX format (M,U)

tape Control tape options of files program (P)

Description: Defines device that `files` program accesses when it is instructed to read or write to a tape. The parameter `tape` is in the user's global parameter tree.

Values: Name of a device. The default device is `/dev/rst8`. If `tape` does not exist or is set to the null string (two single quotes with no space between), `files` uses its default device value. Notice that different computers define tape drives differently. For VnmrSGI, `tape='/dev/tapens'` is appropriate. For Solaris, `tape='/dev/rmt/0mb'`.

Related: `files` Interactively handle files (C)

target_bval Adjust gdiff to achieve target b-value (M)

Applicability: Imaging Systems

Syntax: `target_bval(value)`

Description: This macro iteratively adjusts `gdiff` and calls the sequence `(go('check'))` to achieve the target b-value. The sequence is evoked because the contributions from the imaging gradients must be taken into account backwards calculation of b is not possible because the relationship between `gdiff` and b-value is not simple. The macro defaults to getting within 1 s/mm² of the target or maximum of 20 iterations and exits if either condition is met.

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Arguments: value, the target b-value in s/mm2.

Examples: `target_bval(1000)`

See also: *VnmrJ Imaging User's Guide*

tchan RF channel number used for tuning (P)

Description: Set by the protune macro.

See also: *NMR Spectroscopy User Guide*

Related:	<code>protune</code>	Macro to start ProTune (M)
	<code>atune</code>	ProTune Present (P)
	<code>mtune</code>	Tune probe using swept-tune graphical display (M)
	<code>tugain</code>	Receiver gain used in tuning (P)
	<code>tunesw</code>	Width of the tuning sweep in Hz (P)
	<code>tupwr</code>	Transmitter power used in tuning (P)

tcl Send Tcl script to Tcl version of dg window (C)

Syntax: `tcl(script)`

Description: Sends a Tcl (Tool Command Language) script to the Tcl version of the `dg` window. If this window is not active, this command does nothing.

Arguments: `script` is any legal Tcl script.

See also: *User Programming*

Related: `dg` Display group of acquisition/processing parameters (C)

temp Open the Temperature Control window (C)

Applicability: Systems with a variable temperature (VT) controller.

Description: Opens the Temperature Control window, which has the following capabilities:

- Turn temperature control off.
- Set temperature control on at a specified temperature in degrees C.
- Enable temperature control from within an experiment using the `temp` parameter and the `su`, `go`, `ga`, or `au` macros. This mode is the default.
- Alternatively, turn off experiment control of the temperature and allow only the Temperature Control window (and `sethw`) to set the temperature. This mode has the advantage that, often times, `temp` is different between experiments. Joining a different experiment and entering `go` can unexpectedly change the temperature. This mode prevents this problem.
- Resetting the temperature controller when the temperature cable is reconnected to a probe.

See also: *NMR Spectroscopy User Guide*

Related:	<code>acqi</code>	Interactive acquisition display process (C)
	<code>au</code>	Submit experiment to acquisition and process data (M)
	<code>ga</code>	Submit experiment to acquisition and FT the result (M)
	<code>go</code>	Submit experiment to acquisition (M)
	<code>readhw</code>	Read current values of acquisition hardware (C)
	<code>sethw</code>	Set values for hardware in acquisition system (C)
	<code>su</code>	Submit a setup experiment to acquisition (M)
	<code>temp</code>	Sample temperature (P)
	<code>tin</code>	Temperature interlock (P)

temp Sample temperature (P)

Applicability: Systems with a variable temperature (VT) module.

Description: Sets the temperature of sample.

Values: 'n' or -150 to +200, in steps of 0.1°C. 'n' instructs the acquisition system not to change the VT controller and to ignore temperature regulation throughout the course of the experiment.

See also: *NMR Spectroscopy User Guide*

Related:

<code>readhw</code>	Read current values of acquisition hardware (C)
<code>temp</code>	Open the Temperature Control window (C)
<code>tempcal</code>	Temperature calculation (C)
<code>tin</code>	Temperature interlock (P)
<code>vtc</code>	Variable temperature cutoff point (P)

tempcal Temperature calculation (C)

Applicability: Systems with a variable temperature (VT) module.

Syntax: `tempcal(solvent)<:temperature>`

Description: For exact determination of sample temperature when using the VT unit, a temperature calibration curve must be made for each probe used. All data, such as gas flow, must be noted. Use samples of ethylene glycol for high-temperature calibration, and use samples of methanol for low-temperature calibration. To make the calculation:

- Bring the sample to the desired temperature and allow sufficient time for equilibration, then obtain a spectrum.
- Next, align two cursors on the two resonances in the spectrum, then enter `tempcal('e')` for ethylene glycol, or enter `tempcal('m')` for methanol. The temperature is calculated based on the difference frequency between the cursors.

Arguments: `solvent` is the sample solvent: 'glycol', 'e', or 'g' for ethylene glycol, or 'methanol' or 'm' for methanol.

`temperature` returns the calculated value of the sample temperature. The default is the system displays the value.

Examples: `tempcal('glycol')`
`tempcal('m'):temp`

See also: *NMR Spectroscopy User Guide*

tempcalc Measure approximate sample temperature in Cold Probes (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Measure the approximate sample temperature and the actual sample temperature gradient and generate a report. Requires a ~1% HOD CH₃CN sample.

testacquire Test acquire mode (P)

Description: Allows test acquisitions to be done while a study queue is active, without using the study queue. When this mode is enabled, acquisitions do not update the status of the currently loaded experiment in the study queue, and data is not saved in the study queue. This mode is set from the Test mode check box in the Acquisition menu or from the command line.

T

Syntax: `testacquire=<'y' or 'n'>`

Values: `'y'` test acquire mode enabled

`'n'` test acquire mode disabled

Related: `acquire` Acquire data (M)
`save` Save data (M)

testct Check ct for resuming signal-to-noise testing (M)

Description: Used by the `testsn` macro to decide when to resume testing of signal-to-noise. See the description of `testsn` for details.

See also: *NMR Spectroscopy User Guide*

Related: `ct` Completed transients (P)
`testsn` Test signal-to-noise of a spectrum (M)

testsn Test signal-to-noise of a spectrum (M)

Description: Part of the automatic periodic signal-to-noise testing that occurs during various automated acquisitions, most notably `c13`. Transforms the data using `fn=16000`, and then baseline corrects, setting the left-most 10% of the spectrum and the right-most 2% as baseline. After the baseline correction, `testsn` uses `getsn` to calculate the signal-to-noise.

- If signal-to-noise exceeds the desired goal in parameter `sn` (found in the standard carbon parameter set `/vnmr/stdpar/c13`), `testsn` aborts the experiment using the command `halt`, which initiates processing according to the `wexp` parameter.
- If signal-to-noise is not reached, `testsn` estimates the signal-to-noise ratio at the end of the experiment. If signal-to-noise target will not be reached by then, it cancels subsequent signal-to-noise testing, but allows the experiment to proceed.
- If the signal-to-noise target will be reached before the end of the experiment, it saves the estimated number of transients required to reach the goal in the parameter `r7` (using a conservative estimate), and then sets the processing at future blocks to be only `testct`, which simply tests if `ct` is greater than `r7`, and, if so, resumes testing of signal-to-noise with `testsn`.

See also: *NMR Spectroscopy User Guide*

Related: `c13` Automated carbon acquisition (M)
`fn` Fourier number in directly detected dimension (P)
`getsn` Get signal-to-noise estimate of a spectrum (M)
`halt` Abort acquisition with no error (C)
`r1-r7` Real parameter storage for macros (P)
`sn` Signal-to-noise ratio (P)
`testct` Check ct for resuming signal-to-noise testing (M)
`wexp` Specify action when experiment completes (C)

teststr Find which array matches a string M)

Syntax: `teststr(parameter,string <,tree>):$ret`

Description: The `teststr` command requires at least two arguments. The first is the name of a string parameter. The first argument must generally be enclosed in single quotes. The `teststr` command needs the name of the parameter, not its

values. The second is a string. The optional third argument is the parameter tree. The default is current.

Macro parameters can be used as the first argument. In this case, the third argument must be 'local'.

This command sets \$ret to the index of the array element that matches the second argument. If none of the array values of the parameter match the second argument, a zero is returned.

Examples: `n1='hello','labas','giddy','hola','bonjour','ciao'`
`teststr('n1','labas'):r1`
 sets `r1=2`, since 'labas' matches element 2 of the `n1` array.

The elements do not need to be single words. For example,
`n1='good night','labanaktis','bonne nuit','gute Nacht','boa noite','buonas nocces'`

`teststr('n1','boa noite'):r1`
 sets `r1=5`. The strings must match exactly, including upper and lower case
`teststr('n1','gute nacht'):r1`
 sets `r1=0`, since the lower case n in nacht does not match the upper case N in Nacht.

For local dollar variables, the 'local' argument must be used. Again, enclose the name of the local parameter in single quotes.

`$greet='hello','labas','giddy','hola','ciao'`
`teststr('$greet','labas','local'):r1`

text

Display text or set new text for current experiment (C)

Syntax: `text<(text_string)><:string_variable>`

Description: Associated with each experiment is a text file, consisting of a block of text, that can be used to describe the sample and experiment. `text` allows displaying the text file and changing the text file for the current experiment. A UNIX text editor, such as `vi`, or the macro `textvi` can also be used to edit the text file of the current experiment.

Arguments: `text_string` is a string of text that replaces the existing text file. The default is to display the text file in the current experiment. The characters `\` or `\n` can be used in the string to denote a new line, and the characters `\t` can be used to denote a tab (see example below).

`string_variable` returns the text in `text_string` as a string variable. Thus, for example, the `text:n1` and `text(n1+'cosy experiment')` commands, where `n1` is a string, can be used in a macro to add a "cosy experiment" to the text. An equivalent operation using the `atext` command would be `atext('cosy experiment')`.

Examples: `text('Sample 101\tCDC13\\13 February')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>atext</code>	Append string to the current experiment text (M)
	<code>ctext</code>	Clear the text of the current experiment (C)
	<code>curexp</code>	Current experiment directory (P)
	<code>dtext</code>	Display a text file in the graphics window (C)
	<code>puttxt</code>	Put text file into another file (C)
	<code>textvi</code>	Edit text file of current experiment (M)
	<code>vnmrprint</code>	Print text files (U)

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textis **Return the current text display status (C)**

Syntax: (1) `textis(command):$yes_no`
 (2) `textis:$display_command`

Description: Determines if a command given by the user currently controls the text window (syntax 1) or returns the name of the command currently controlling the text window (syntax 2).

Arguments: `command` is the name of a command that potentially may be controlling the text window.

`$yes_no` returns 1 if `command` controls the text window, or 0 if it does not.

`$display_command` returns the name of the command currently controlling the text window.

Examples: `textis:$display`
`if ($display = 'dg') then . . . endif`

See also: *User Programming*

Related: [graphis](#) Return the current graphics display status (C)

textvi **Edit text file of current experiment (M)**

Description: Edits the text file of the current experiment using the UNIX text editor `vi`. `textvi` is equivalent to the command `vi(curexp+'text')`.

See also: *NMR Spectroscopy User Guide*

Related: [edit](#) Edit a file with user-selectable editor (M)
[text](#) Display text or set new text for current experiment (C)
[vi](#) Edit text file with `vi` editor (M)

th **Threshold (P)**

Description: Sets threshold for printout of peak frequencies so that peaks greater than `th` on the plot appear on any peak listings. `th` is always bipolar (i.e., negative peaks greater in magnitude than `th` also appear in peak listings).

Values: 0 to 1e9, in mm.

See also: *NMR Spectroscopy User Guide*

Related: [thadj](#) Adjust threshold for peak printout (M)

th2d **Threshold for integrating peaks in 2D spectra (P)**

Description: Used by [l12d](#) when determining the bounds of a peak and calculating its volume. To create the 2D peak picking parameters `th2d` and `xdiag` in the current experiment, enter `addpar('l12d')`.

Values: From 0.0 to 1.0. If `th2d=1.0`, [l12d](#) integrates all points in the peak that are above the current threshold for the spectrum (i.e., the portion of the peak that can be seen in a contour plot of the spectrum). A smaller value causes [l12d](#) to integrate a larger area when determining the volume of a peak. If `th2d=0.5`, for example, [l12d](#) integrates all points in a peak that are above 0.5 times the current threshold.

See also: *NMR Spectroscopy User Guide*

Related: [addpar](#) Add selected parameters to the current experiment (M)
[l12d](#) Automatic and interactive 2D peak picking (C)
[xdiag](#) Threshold for excluding diagonal peaks when peak picking (P)

thadj Adjust threshold for peak printout (M)

Syntax: `thadj<(max_peaks<,noise_mult<,llarg1<,llarg2>>>>>`

Description: Adjusts the threshold **th** so that no more than a specified maximum number of peaks are found in a subsequent line listing (see **nll**) and so that **th** is at least a specified noise multiplier times the root-mean-square noise level.

Arguments: **max_peaks** is the maximum number of peaks in the displayed spectral range. The default is **wc**/4 (i.e., the threshold is adjusted such that **ppf** will produce a “reasonable” number of lines with any width of plot).

noise_mult is a noise multiplier used to calculate the minimum value for **th** from the size of the root-mean-square noise.

llarg1 is the **noise_mult** argument (the default is 3) to the **nll** command used inside this macro

llarg2 is the keyword argument ('pos', 'neg', 'all'; the default is 'all'.) to the **nll** command used inside this macro.

Examples: `thadj`
`thadj(50)`
`thadj(200,4)`
`thadj(200,4,2)`
`thadj(200,4,2,'pos')`

See also: *NMR Spectroscopy User Guide*

Related:	nll	Find line frequencies and intensities (C)
	ppf	Plot peak frequencies over spectrum (M)
	th	Threshold (P)
	vsadj	Automatic vertical scale adjustment (M)
	vsadj2	Automatic vertical scale adjustment by powers of two (M)
	vsadjc	Automatic vertical scale adjustment for ¹³ C spectra (M)
	vsadjh	Automatic vertical scale adjustment for ¹ H spectra (M)
	wc	Width of chart (P)

time Display experiment time or recalculate number of transients (M)

Syntax: `time<(<hours,>minutes)>`

Description: Estimates the acquisition time or recalculates the number of transients so that the total acquisition time is approximately the requested time. The parameters looked at when calculating the time per transient are **d1**, **d2**, **d3**, **at**, **ni**, **sw1**, **ni2**, and **sw2**.

Arguments: **hours** and **minutes** are numbers making up a time to be used by the system to recalculate the parameter **nt** so that the total acquisition time is approximately the time requested; the default (no arguments) is for the system to estimate the acquisition time for a 1D, 2D, or 3D experiment using the parameters in the current experiment.

Examples: `time`
`time(2,45)`

See also: *NMR Spectroscopy User Guide*

Related:	at	Acquisition time (P)
	d1	First delay (P)
	d2	Incremented delay in 1st indirectly detected dimension (P)
	d3	Incremented delay in 2nd indirectly detected dimension (P)
	exptime	Display experiment time (C)
	ni	Number of increments in 1st indirectly detected dimension (P)
	ni2	Number of increments in 2nd indirectly detected dimension (P)

T

<code>nt</code>	Number of transients (P)
<code>sw1</code>	Spectral width in 1st indirectly detected dimension (P)
<code>sw2</code>	Spectral width in 2nd indirectly detected dimension (P)

`tin` **Temperature interlock (P)**

Description: Controls error handling based on temperature regulation. If temperature regulation is lost, `tin` can be used to select whether an error is generated and acquisition is halted or whether a warning is generated and acquisition continues. In both cases, the lost regulation will cause `werr` processing to occur, thus providing a user-selectable mechanism to respond to VT failure.

Values: 'n' turns off the temperature interlock feature
 'w' indicates the variable temperature regulation light is monitored during the course of the experiment and, if it starts to flash (regulation lost), a warning is generated; however, acquisition is not stopped.
 'y' indicates the variable temperature regulation light is monitored during the course of the experiment and, if it starts to flash (regulation lost), the current data acquisition is stopped. The acquisition will not resume automatically if regulation is regained.

See also: *NMR Spectroscopy User Guide*

Related: `in` Lock and spin interlock (P)
`werr` When error (P)

`t1t` **First-order baseline correction (P)**

Description: When spectral display is active, the command `dc` turns on a linear drift correction (baseline correction). The result of this operation includes calculating a first-order baseline correction parameter `t1t`. The calculation is made by averaging of a small number of points at either end of the display and drawing a straight line baseline between them.

See also: *NMR Spectroscopy User Guide*

Related: `cdc` Cancel drift correction (C)
`dc` Calculate spectral drift correction (C)
`lv1` Zero-order baseline correction (P)

`tmove` **Left-shift FID to time-domain cursor (M)**

Description: Provides an alternative method of left shifting time-domain data. To use this method, position the right time cursor at the place that should be the start of the FID, then enter `tmove`. This adjusts `lsfid` to left-shift the FID.

See also: *NMR Spectroscopy User Guide*

Related: `lsfid` Number of complex points to left-shift *np* FID (P)

`tmsref` **Reference 1D proton or carbon spectrum to TMS (M)**

Syntax: `tmsref:tms_found`

Description: Tries to locate a TMS line. If found, `tmsref` re-references the spectrum to the TMS line and returns a 1 to the calling macro; if not found, `tmsref` returns 0 and the referencing is left as it was. In the case of other signals (e.g., from silicon grease) immediately to the left of the TMS line (even if they are higher than the reference line), `tmsref` tries avoiding those by taking the rightmost line in that area, as long as it is at least 10% of the main Si-CH₃ signal. Large signals within

0.6 ppm for ^1H (or 6 ppm for ^{13}C) to the right of TMS may lead to misreferencing.

Arguments: `tms_found` returns 1 if a TMS line was located or returns 0 if not.

See also: *NMR Spectroscopy User Guide*

Related: `c13` Automated carbon acquisition (M)

`h1` Automated proton acquisition (M)

tn Nucleus for observe transmitter (P)

Description: Changing the value of `tn` causes a macro (`_tn`) to be executed that extracts values for `sfrq` and `tof` from lookup tables. The tables, stored in the directory `/vnmr/nuctables`, are coded by atomic weights.

Values: In the lookup tables, typically given by `'H1'`, `'C13'`, `'P31'`, etc. The value `tn='lk'` sets the deuterium frequency, and also holds the lock current and switches the relay in the automated deuterium gradient shimming module, if present, so that deuterium signal may be observed without disturbing lock. The frequency is the same as `tn='H2'`.

See also: *NMR Spectroscopy User Guide*

Related: `dn` Nucleus for first decoupler (P)

`dn2` Nucleus for second decoupler (P)

`dn3` Nucleus for third decoupler (P)

`sfrq` Transmitter frequency of observe nucleus (P)

`tof` Frequency offset for observe transmitter (P)

tncosyps Set up parameters for TNCOSYPS pulse sequence (M)

Description: Sets up a homonuclear correlation experiment (phase-sensitive version) with water suppression.

See also: *NMR Spectroscopy User Guide*

tndqcosy Set up parameters for TNDQCOSY pulse sequence (M)

Applicability: Systems with a linear amplifier on the observe channel and a T/R switch.

Description: Sets up a 2D J-correlation experiment with water suppression.

See also: *NMR Spectroscopy User Guide*

tnmqcosy Set up parameters for TNMQCOSY pulse sequence (M)

Applicability: Systems with hardware digital phaseshifter for transmitting with direct-synthesis rf; otherwise, software small-angle phaseshifter for transmitting with the old-style rf is used.

Description: Sets up a multiple-quantum filtered COSY experiment with water suppression.

See also: *NMR Spectroscopy User Guide*

tnnoesy Set up parameters for TNNOESY pulse sequence (M)

Applicability: Systems with a linear amplifier on the observe channel and a T/R switch.

Description: Sets up a 2D cross-relaxation experiment with water suppression.

See also: *NMR Spectroscopy User Guide*

T

tnroesy Set up parameters for TNROESY pulse sequence (M)

Description: Sets up a rotating-frame NOE experiment with water suppression.

See also: *NMR Spectroscopy User Guide*

tntocsy Set up parameters for TNTOCSY pulse sequence (M)

Applicability: Systems with T/R switch, computer-controlled attenuators, and linear amplifiers on observe channel.

Description: Sets up a total-correlation spectroscopy experiment (HOHAHA) with water suppression.

See also: *NMR Spectroscopy User Guide*

Tocsy Convert the parameters to a TOCSY experiment (M)

Description: Convert parameters to a TOCSY experiment.

See also: *NMR Spectroscopy User Guide*

Related:	ft1dac	Combined arrayed 2D FID matrices (M)
	ft2dac	Combined arrayed 2D FID matrices (M)
	wft1dac	Combined arrayed 2D FID matrices (M)
	wft2dac	Combined arrayed 2D FID matrices (M)

Tocsy1d Convert the parameter set to a Tocsy1d experiment (M)

Description: Convert the parameter set to a Tocsy1d experiment.

See also: *NMR Spectroscopy User Guide*

Related:	Proton	Set up parameters for ¹ H experiment (M).
	sel1d	Selective 1D protocols to set up (M).

tocsyHT Set up the tocsyHT experiment (M)

Description: Sets up parameters for a Hadamard-encoded tocsy experiment.

See also: *NMR Spectroscopy User Guide*

Related:	htofs1	Hadamard offset in ni (P)
	fn1	Fourier number in 1st indirectly detected dimension (P)
	ni	Number of increments in 1st indirectly detected dimension (P)
	ft2d	Fourier transform 2D data (C)
	sethtfrq1	Set Hadamard frequency list from a line list (M)
	Tocsy	Set up parameters for a TOCSY pulse sequence (M)
	htfrq1	Hadamard frequency list in ni (P)

tof Frequency offset for observe transmitter (P)

Description: Controls the exact positioning of the transmitter. As the value assigned to **tof** increases, the transmitter moves to a higher frequency (toward the left side of the spectrum). The minimum step size of **tof** is determined by the type of rf hardware in the spectrometer. The limit is specified using the Step Size label in the Spectrometer Configuration window. Systems with broadband style rf (**rf****type**= 'b ') generally have 100-Hz resolution; all other systems have 0.1 Hz resolution.

Values: Approximate, depends on frequency—100000 to 100000, in Hz.

See also: *NMR Spectroscopy User Guide*

Related:	<code>config</code>	Determine current configuration and possibly change it (M)
	<code>dof</code>	Frequency offset for first decoupler (P)
	<code>dof2</code>	Frequency offset for second decoupler (P)
	<code>dof3</code>	Frequency offset for third decoupler (P)
	<code>rftype</code>	Type of rf generation (P)

tpwr **Observe transmitter power level with linear amplifiers (P)**

Applicability: Systems with a linear amplifier on the observe channel.

Description: Controls transmitter power. The value of the attenuator upper safety limit is set using the Upper Limit label in the Spectrometer Configuration window. Depending on hardware adjustments, the system may saturate at a given value of `tpwr` (i.e., values above a certain value may give equal output).

Values: On systems with 63-dB attenuator installed: 0 to 63 (63 is maximum power), in units of dB. About 55 to 60 is normal. Lower values (e.g., 49) might be used for water suppression experiments like 1-3-3-1.

On systems with 79-dB attenuator installed: -16 to 63 (63 is maximum power), in units of dB.

CAUTION: Continuous power greater than 2 watts in a switchable probe will damage the probe. Always carefully calibrate power to avoid exceeding 2 watts. The maximum value for `tpwr` on a 200-MHz, 300-MHz, or 400-MHz system with a linear amplifier on the decoupler channel has been set to 49, corresponding to about 2 watts of power. Before using `tpwr=49` for continuous decoupling, ensure safe operation by measuring the output power. This should be done during system installation and checked periodically by the user.

See also: *NMR Spectroscopy User Guide*

Related:	<code>cattn</code>	Coarse attenuator (P)
	<code>config</code>	Determine current configuration and possibly change it (M)
	<code>dpwr</code>	Power level for first decoupler with linear amplifiers (P)
	<code>dpwr2</code>	Power level for second decoupler (P)
	<code>dpwr3</code>	Power level for third decoupler (P)
	<code>dpwrf</code>	First decoupler fine power (P)
	<code>fattn</code>	Fine attenuator (P)
	<code>tpwrf</code>	Observe transmitter fine power (P)

tpwrf **Observe transmitter fine power (P)**

Applicability: Systems with a fine attenuator on the observe transmitter channel.

Description: Controls the transmitter fine attenuator. Systems with this attenuator are designated using the Fine Attenuator label in the Spectrometer Configuration window. The fine attenuator is linear and spans 60 dB or 6 dB. If `tpwrf` is not present, enter `create('tpwrf','integer')`
`setlimit('tpwrf',4095,0,1)` to create it.

Values: 0 to 4095, where 4095 is maximum power. If `tpwrf` does not exist in the parameter table, a value of 4095 is assumed.

See also: *NMR Spectroscopy User Guide*

Related:	<code>config</code>	Determine current configuration and possibly change it (M)
	<code>dpwr</code>	Power level for first decoupler with linear amplifiers (P)
	<code>dpwrf</code>	First decoupler fine power (P)
	<code>fattn</code>	Fine attenuator (P)

T

`tpwr` Observe transmitter power level with linear amplifier (P)
`tpwrm` Observe transmitter linear modulator power (P)

tpwrm Observe transmitter linear modulator power (P)

Description: Controls the power level on the observe transmitter linear modulator. The fine power control is linear and spans 0 to `tpwr`.

Values: 0 to 4095, where 4095 is maximum power. If `tpwrm` does not exist in the parameter table, a value of 4095 is assumed.

See also: *NMR Spectroscopy User Guide*

Related: `config` Determine current configuration and possibly change it (M)
`dpwrf` First decoupler fine power (P)
`fatten` Fine attenuator (P)

trace Mode for *n*-dimensional data display (P)

Description: Sets the multidimensional data display mode.

Values: 'f1' displays the f_1 axis horizontally and allows f_1 traces to be displayed.
'f2' displays the f_2 axis horizontally and allows f_2 traces to be displayed.
'f3' displays the f_3 axis horizontally and allows f_3 traces to be displayed if the data set is 3D.

See also: *NMR Spectroscopy User Guide*

traymax Sample changer tray slots (P)

Applicability: Systems with an automatic sample changer.

Description: Specifies the type of sample changer. It also can be used to disable the sample changer. The value is set using the Sample Changer label in the Spectrometer Configuration window.

Values: 0 is setting for no sample changer present or, if a sample changer is attached, to disable the changer (None choice in the Spectrometer Configuration window).
9, 50, 100, 96, 48 are `traymax` values that indicate the number of sample slots for the corresponding sample changer (9 is for Carousel, 50 is for SMS/ASM 50 Sample, 100 is for SMS/ASM 100 Sample, 96 is for VAST, and 48 is for NMS, 768 for 768AS).

See also: *VnmrJ Installation and Administration; VnmrJ Walkup*

Related: `config` Display current configuration and possibly change it (M)

troesy Set up parameters for TROESY pulse sequence (M)

Description: Sets up parameters for the transverse cross-relaxation experiment in a rotating frame.

See also: *NMR Spectroscopy User Guide*

trunc Truncate real numbers (O)

Description: In MAGICAL programming, an operator that truncates real numbers.

Examples: `$3 = trunc(3.6)`

See also: *User Programming*

Related: `acos` Find arc cosine of number (C)
`asin` Find arc sine of number (C)

<code>atan</code>	Find arc tangent of a number (C)
<code>cos</code>	Find cosine value of an angle (C)
<code>exp</code>	Find exponential value (C)
<code>ln</code>	Find natural logarithm of a number (C)
<code>tan</code>	Find tangent value of an angle (C)
<code>sqrt</code>	Return square root of a real number (O)
<code>typeof</code>	Return identifier for argument type (O)

tshift Adjust tau2 to current cursor position (M)

Applicability: Systems with a solids module.

Description: Adjusts `tau2` to make the current time cursor position the start of acquisition. As the time-domain cursor can move between points, this macro allows the accurate adjustment of `tau2` so as to start another acquisition exactly at the top of an echo.

See also: *User Guide: Solid-State NMR*

tugain Receiver gain used in tuning (P)

Description: Used internally by the `protune` macro to set the receiver gain.

See also: *NMR Spectroscopy User Guide*

Related:	<code>protune</code>	Macro to start ProTune (M)
	<code>atune</code>	ProTune Present (P)
	<code>mtune</code>	Tune probe using swept-tune graphical display (M)
	<code>tchan</code>	RF channel number used for tuning (P)
	<code>tunematch</code>	Default match target, in percent of optimum (P)
	<code>tunesw</code>	Width of the tuning sweep in Hz (P)
	<code>tupwr</code>	Transmitter power used in tuning (P)

tune Assign a frequency to a channel for probe tuning (C)

Syntax: (1) `tune(freq1,<freq2,freq3,freq4>)`
(2) `tune(chan1,freq1,<chan2,freq2,...>)`

Description: Assigns a frequency to a channel when tuning the probe. The frequency assignment remains in effect (as a tune frequency) until the next `su` or `go` command is executed. Although only the first synthesizer is connected to the tuning system, the console is programmed to set this synthesizer to the desired frequency based on the channel shown on the CHAN readout on the TUNE INTERFACE unit.

The `tune` program has two formats. If syntax 1 is used, frequencies are assigned to channels based on the order of the arguments. The first argument is interpreted and assigned to the first (observe) channel, the second argument is assigned to the second (decoupler) channel. A third or fourth argument would be interpreted and assigned in a similar manner.

If syntax 2 is used, the arguments are entered in pairs, with the first argument specifying the rf channel and the next argument specifying the frequency.

`tune` selects the format based on the first argument. If the first argument is a name for an rf channel, syntax 2 is assumed; otherwise, syntax 1 is used.

Arguments: `freq1`, `freq2`, `freq3`, and `freq4` specify the frequency of the rf channel as a value in MHz (e.g., 200 or 300) or indirectly using the nucleus for tuning the probe (e.g., 'H1' or 'C13'). If a nucleus is entered, it must be found in the nucleus table. The frequency of any channel without an argument is unaffected. For example, `tune('H1','C13','N15')` sets the first channel to tune at

the ^1H , the second channel at ^{13}C , and the third channel at ^{15}N . If a fourth channel is present, it is not affected. Entering `tune('H1','C13',200)` assigns the same frequencies for the first and second channels but the third channel tunes to 200 MHz, regardless of the proton frequency.

`chan1`, `chan2`, `chan3`, and `chan4` specify the channel directly:

- `'todev'` or `'ch1'` specify channel 1 (observe transmitter).
- `'dodev'` or `'ch2'` specify channel 2 (first decoupler).
- `'do2dev'` or `'ch3'` specify channel 3 (second decoupler).
- `'do3dev'` or `'ch4'` specify channel 4 (third decoupler).

Only one of these keywords is used per channel (do not enter the channel using just its number). If a channel does not have a keyword entered as an argument, that channel is not affected (e.g., `tune('ch4','P31')` selects the frequency corresponding to ^{31}P on the fourth channel, but leaves the first three channels unaffected).

Examples: `tune('H1','C13','N15')`
`tune('H1','C13',200)`
`tune('ch4','P31')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>dfrq</code>	Transmitter frequency of first decoupler (P)
	<code>dfrq2</code>	Transmitter frequency of second decoupler (P)
	<code>dfrq3</code>	Transmitter frequency of third decoupler (P)
	<code>go</code>	Submit experiment to acquisition (C)
	<code>mtune</code>	Tune probe using swept-tune graphical display (M)
	<code>qtune</code>	Tune probe using swept-tune graphical tool (C)
	<code>sfrq</code>	Transmitter frequency of observe nucleus (P)
	<code>spcfrq</code>	Display frequencies of rf channels (M)
	<code>su</code>	Submit a setup experiment to acquisition (C)
	<code>tune</code>	Assign frequencies (C)

tunehf **Tune both H1 and F19 on an HFX probe (M)**

Syntax: `tunehf(<'x'>)`

Description: Tune both H1 and F19 on an HFX probe. Including the optional argument, `tunehf('x')` also tunes the low band channel to `dn(dfrq)`.

Arguments: `'x'` — low band channel to `dn(dfrq)`

See also: *NMR Spectroscopy User Guide*

Related: `protune` Macro to start ProTune (M)

tunematch **Default match target, in percent of optimum (P)**

Description: The default match target, in percent of optimum. This local real parameter must be created. It is used as the match criterion in calls of the form `protune(599.96)`

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related:	<code>protune</code>	Macro to start ProTune (M)
	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>atune</code>	ProTune Present (P)
	<code>mtune</code>	Tune probe using swept-tune graphical display (M)
	<code>tchan</code>	RF channel number used for tuning (P)
	<code>tugain</code>	Receiver gain used in tuning (P)

`tunesw` Width of the tuning sweep in Hz (P)
`tupwr` Transmitter power used in tuning (P)

tunemethod Method to use for tuning (P)

Applicability: Liquids, VnmrJ Walkup, Automation

Description: Specify probe tuning method. Methods are located in:
`$home/vnmrsys/tune/methods` for local user or
`/vnmr/tune/methods` for access by all users.
The method determines the nucleus to tune and how coarse or fine the probe is
tuned as a percentage of the optimal pw.

Values: `'lohi'` –tune low band to medium criterion then tune high band to medium
criterion

`'<name>'` – user defined method.

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `atune` ProTune Present (P)
`protune` Macro to start ProTune (M)
`wtune` Specify when to tune (P)

tuneResult Message indicating how well the tuning succeeded (P)

Description: Message indicating how well the tuning succeeded. This local string parameter
is created by ProTune and set to a string describing the result of the tuning. The
first word of the message will be "ok" if tuning is successful, "failed" if it fails,
and "Warning;" if tuning was not done but the experiment should proceed.

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `protune` Macro to start ProTune (M)

tunesw Width of the tuning sweep in Hz (P)

Description: Sets the width of the tuning sweep in Hz and is set by the `protune` macro.

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `protune` Macro to start ProTune (M)
`atune` ProTune Present (P)
`mtune` Tune probe using swept-tune graphical display (M)
`tchan` RF channel number used for tuning (P)
`tugain` Receiver gain used in tuning (P)
`tunematch` Default match target, in percent of optimum (P)
`tupwr` Transmitter power used in tuning (P)

tupwr Transmitter power used in tuning (P)

Description: The transmitter power used in tuning. The `aptune` pulse sequence uses this to
set the transmitter power. Set by the `protune` macro.

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `protune` Macro to start ProTune (M)
`atune` ProTune Present (P)
`mtune` Tune probe using swept-tune graphical display (M)
`tchan` RF channel number used for tuning (P)
`tugain` Receiver gain used in tuning (P)
`tunematch` Default match target, in percent of optimum (P)
`tunesw` Width of the tuning sweep in Hz (P)

T

typeof **Return identifier for argument type (O)**

Syntax: `typeof`

Description: In MAGICAL programming, an operator that returns an identifier (0 or 1) for the type (real or string) of an argument.

Examples: `if typeof('$1') then $arg=1 else $arg=$1 endif`

See also: *User Programming*

Related	<code>isreal</code>	Utility macro to determine a parameter type (M)
	<code>isstring</code>	Utility macro to determine a parameter type (M)
	<code>on</code>	Make a parameter active or test its state (C)
	<code>size</code>	Return number of elements in an arrayed parameter (O)

U

ultra8	Selects the Ultra 8 shim configuration (M)
ultra18	Selects the Ultra 18 shim configuration (M)
undospins	Restore spin system as before last iterative run (M)
undosy	Restore original 1D NMR data from sub experiment (M)
unit	Define conversion units (C)
unlock	Remove inactive lock and join experiment (C)
updatepars	Update all parameter sets saved in a directory (M)
updateprobe	Update probe file (M)
updaterev	Update after installing new VnmrJ version (M)
updtgcoil	Update gradient coil (M)
updtparam	Update specified acquisition parameters (C)
usemark	Use “mark” output as deconvolution starting point (M)
userdir	VnmrJ user directory (P)
usergo	Experiment setup macro called by go, ga, and au (M)
userfixpar	Macro called by fixpar (M)

ultra8 **selects the Ultra 8 shim configuration (M)**

Syntax: `ultra8`

Description: The `ultra8` macro selects the Ultra 8 shim configuration and selects an appropriate template for the `dgs` command and manual shim panel.
Administrator privilege is required to change the shim configuration. The shims are: `z1c z2c x1 y1 xz yz xy x2y2`.

Related: `ultra18` selects the Ultra 18 shim configuration (M)

ultra18 **Select 18 shim configuration for Ultra 18 shim power supply (M)**

Syntax: `ultra18`

Description: Selects the 18 shim configuration for the Ultra 18 shim power supply and selects an appropriate template for the `dgs` command and manual shim panel.
Administrator privilege is required to change the shim configuration.
The shims are: `z1 z1c z2 z2c z3c z4c x1 y1 xz yz xy x2y2 x3 y3 xz2 yz2 zxy zx2y2`

Related: `ultra8` selects the Ultra 8 shim configuration (M)

undospins **Restore spin system as before last iterative run (M)**

Description: Returns the values of the line assignments and the chemical shifts and coupling constants existing before the last iterative adjustment with `spins('iterate')`, and then runs `spins`. The parameters are returned from the file `spini.inpar` and the transitions from the file `spini.savela` in the current experiment.

U

See also: *NMR Spectroscopy User Guide*

Related: [spins](#) Perform spin simulation calculation (C)

undosy Restore original 1D NMR data from sub experiment (M)

Description: Restores the 1D DOSY data stored by the [dosy](#) macro (if data exists) by recalling the data stored in the file `subexp/dosy2Ddisplay` in the current experiment. `undosy` and [redosy](#) enable easy switching between the 1D DOSY data (spectra as a function of `gzlv11`) and the 2D DOSY display (signal as a function of frequency and diffusion coefficient).

See also: *NMR Spectroscopy User Guide*

Related: [dosy](#) Process DOSY experiments (M)
[redosy](#) Restore 2D DOSY display from subexperiment (M)

unit Define conversion units (C)

Syntax: `unit<(suffix,label,m<,tree><,'mult'|'div'> \`
`,b<,tree><,'add'|'sub'>)>`

Description: Defines a linear relationship that can be used to enter parameters with units. The unit is applied as a suffix to the numerical value (e.g., 10k, 100p). The definition of the linear relations follows the traditional $y=mx+b$ equation, where x is the input value and y is the converted result.

Entering the `unit` command with no arguments displays all currently defined units. To remove a unit, define the unit with a 0 for the slope.

A convenient place to put `unit` commands for all users is in the [bootup](#) macro. Put private `unit` commands in a user's `login` macro.

Arguments: `suffix` is a string identifying the name for the unit. The length of the string is limited to 12 characters.

`label` is a string for the name to be displayed when the [axis](#) parameter is set to the value of the suffix (if the suffix is only a single character). The length of the string is limited to 12 characters.

`m` is the slope of the linear relationship, defined either as a numerical value or as the name of a parameter. If a parameter name is used, it may be optionally followed with the parameter tree to use (argument `tree`) and by another optional keyword that specifies whether the parameter value should be a multiplier (keyword `'mult'`) or divisor (keyword `'div'`).

`tree` is the parameter tree to use (i.e., `'current'`, `'processed'`, `'global'`, or `'systemglobal'`). The default tree is `'current'`.

`'mult'` is a keyword that specifies that a parameter value used for the slope should be a multiplier. This is the default for the slope.

`'div'` is a keyword that specifies that a parameter value used for the slope should be a divisor.

`b` is the intercept of the linear relationship, defined either as a numerical value or as the name of a parameter. If a parameter name is used, it may be optionally followed with the parameter tree to use (argument `tree`) and by another optional keyword that specifies whether the parameter value should be added (keyword `'add'`) or subtracted (keyword `'sub'`).

`'add'` is a keyword that specifies that a parameter value used for the intercept should be added. This is the default for the intercept.

`'sub'` is a keyword that specifies that a parameter value used for the intercept should be subtracted.

Examples: `unit`
 Displays all currently defined units
`unit('k','kHz',1000)`
`r1=10k` will set `r1` to 10000
`unit('p','ppm','reffrq','processed')`
`r1=10p` will set `r1` to `10*reffrq`, where `reffrq` from processed tree
`unit('p','',0)`
`r1=10p` will set `r1` to 10 and give an error "unknown unit p"
`unit('F','degF',5/9,-32*5/9)`
`r1=212F` will set `r1` to 100 (degrees C)
`unit('C','degC',9/5,32)`
`r1=100C` will set `r1` to 212 (degrees F)

See also: *NMR Spectroscopy User Guide, User Programming*

Related: `axis` Axis label for displays and plots (P)
`bootup` Macro executed automatically when VnmrJ is activated (M)

unlock Remove inactive lock and join experiment (C)

Syntax: `unlock(exp_number, 'force')`

Description: In attempting to join another experiment, the `jexp` command may abort claiming the experiment is locked. This feature prevents two users from processing the same experimental data at the same time, which could corrupt the data (a "user" can also be a background operation invoked by the same user, such as in `wexp` processing). This lock can be left behind if the program or the computer crashes.

The `unlock` command removes the lock if it is inactive and joins the unlocked experiment. The command will fail if the lock is still active (i.e., the process that made the lock is still executing) or if the lock was placed on the experiment by a remote host. The latter situation can only occur when one or more nodes are sharing the same file system (and experimental data).

Arguments: `exp_number` is the number of the experiment from 1 to 9 to be unlocked.
`force` unlocks an experiment under all circumstances and joins the unlocked experiment.

Examples: `unlock(3)`

See also: *NMR Spectroscopy User Guide*

Related: `jexp` Join existing experiment (C)

updatepars Update all parameter sets saved in a directory (M)

Syntax: `updatepars(directory)`

Description: Corrects saved parameter sets. Starting with VNMR version 4.2, all parameters, upper limit, lower limit, and step sizes have been tightened. Further additions were made in VNMR 4.3. `updatepars` searches a directory for parameter and FID files and corrects the `procpars` files found. This macro overwrites parameters in the current experiment. The corrections applied to the parameter sets are defined by the `parfix` macro. Because `updatepars` uses the current experiment to process the parameter sets, the experiment chosen for running `updatepars` should not contain a valuable data set.

Arguments: `directory` is the name of the directory to be searched.

Examples: `updatepars('myparlib')`
`updatepars('mydata')`

U

See also: *NMR Spectroscopy User Guide*

Related: `parfix` Update parameter sets (M)
`parversion` Version of parameter set (P)

updateprobe Update probe file (M)

Syntax: `updateprobe (<probe|'tmplt'>,<'system'>)`

Description: Updates the current existing probe file or probe template.

Arguments: `probe` is the probe parameter to update. The default is the current probe parameter value.

'`tmplt`' is a keyword to update the local probe template. The default is the current probe file.

'`system`' is a keyword to update the system template or probe file, providing you have write permission to the file. The default is to update the local template or probe file.

Examples: `updateprobe`
`updateprobe ('autosw')`
`updateprobe ('autosw', 'system')`
`updateprobe ('tmplt')`

See also: *NMR Spectroscopy User Guide*

Related: `addparams` Add parameter to current probe file (M)
`getparam` Receive parameter from probe file (M)
`setparams` Write parameter to current probe file (M)

updaterev Update after installing new VnmrJ version (M)

Description: Updates experiment parameters and the global file following installation of a new VNMR software version. `updaterev` is called by the `makeuser` command during the installation process.

See also: *VnmrJ Installation and Administration*

updtgcoil Update gradient coil (M)

Applicability: Systems with three-axis gradients.

Description: Creates the `gcoil` parameter, if it does not exist, and sets it to the current value of the system gradient coil `sysgcoil`. `updtgcoil` only executes if gradients are configured in the system.

The `updtgcoil` macro is called when a new experiment is joined or new parameters are read into an experiment; however, it is only called at these times if the `gcoil` parameter exists. If `sysgcoil` is set to a gradient table name and if the values of `sysgcoil` and `gcoil` are different, a message is displayed in the Status window to let the user know that the gradient coil parameters have been updated.

`updtgcoil` can be called directly if the user wants to update the parameter set with the `gcoil` and gradient table parameters.

See also: *NMR Spectroscopy User Guide; User Programming; VnmrJ Imaging NMR*

Related: `gcoil` Read data from gradient calibration tables (P)
`sysgcoil` System gradient coil (P)

updtparam Update specified acquisition parameters (C)

Description: Enables interactive updating of specified acquisition parameters.

See also: *SpinCAD*

Related: `psgupdateoff` Prevent update of acquisition parameters (C)
`psgupdateon` Enable update of acquisition parameters (C)

usemark Use “mark” output as deconvolution starting point (M)

Description: In some cases it is not possible to produce a line list that is a suitable starting point for a deconvolution (e.g., lines may overlap so severely that a line list does not find them). In this case, or in any case, the results of a “mark” operation during a previous spectral display (`ds`) may be used to provide a starting point. If the “mark” has been made with a single cursor, the information in the file `mark1d.out` contains only a frequency and intensity, and the starting linewidth is taken from the parameter `slw`.

If the “mark” is made with two cursors, placed symmetrically about the center of each line at the half-height point, `mark1d.out` contains two frequencies and an intensity. In this case, the starting frequency is taken as the average of the two cursor positions; the starting linewidth is taken as their difference (thus allowing different starting linewidths for each line).

See also: *NMR Spectroscopy User Guide*

Related: `ds` Display a spectrum (C)
`slw` Spin simulation linewidth (P)

userdir VnmrJ user directory (P)

Description: Stores the full UNIX path of the directory that contains a user's private VnmrJ files. These include a user's private `maclib`, `menulib`, `shims`, `psglib`, `experiments`, etc. This parameter is initialized at bootup by the UNIX environmental variable `vnmruser`.

Values: Typical value is `/home/vnmr2/vnmrsys`

See also: *NMR Spectroscopy User Guide*

Related: `curexp` Current experiment directory (P)
`systemdir` VnmrJ system directory (P)

usergo Experiment setup macro called by go, ga, and au (M)

Description: Called by macros `go`, `ga`, or `au` before starting an experiment. The user typically creates `usergo` as a means to set up general experiment conditions.

See also: *NMR Spectroscopy User Guide*

Related: `au` Submit experiment to acquisition and process data (M)
`ga` Submit experiment to ac acquisition and FT the result (M)
`go` Submit experiment to acquisition (M)
`go_` Pulse sequence setup macro called by `go`, `ga`, and `au` (M)

userfixpar Macro called by fixpar (M)

Description: Called by the macro `fixpar` to provide an easy mechanism to customize parameter sets.

See also: *NMR Spectroscopy User Guide*

Related: `fixpar` Correct parameter characteristics in experiment (M)

V

<code>vast1d</code>	Set up initial parameters for VAST experiments (M)
<code>vastget</code>	Selects and displays VAST spectra (M)
<code>vastglue</code>	Assemble 1D datasets into a 2D (or pseudo-2D) datasets (M)
<code>vastglue2</code>	Assemble 1D datasets into a 2D (or pseudo-2D) datasets (M)
<code>vastgo</code>	Turn off LC stop flow automation, start VAST automation (M)
<code>vbg</code>	Run VNMR processing in background (U)
<code>vf</code>	Vertical scale of FID (P)
<code>vi</code>	Edit text file with vi text editor (M)
<code>vibradd</code>	Display relative amplitudes of Cold Probe vibrations (M)
<code>vjhelp</code>	Display VnmrJ help (U)
<code>vn</code>	Start VNMR directly (U)
<code>vnmr</code>	Start VNMR in current windowing system (U)
<code>vnmr2sc</code>	VNMR to SpinCAD pulse sequence translator (M)
<code>vnmr_accounting</code>	Open Accounting window (U)
<code>vnmrexit</code>	Exit from the VNMR system (C)
<code>vnmrj</code>	Start VnmrJ (U)
<code>vnmrjcmd()</code>	Commands to invoke the GUI popup (C)
<code>vnmrplot</code>	Plot files (U)
<code>vnmrprint</code>	Print text files (U)
<code>vo</code>	Vertical offset (P)
<code>vp</code>	Vertical position of spectrum (P)
<code>vpaction</code>	Set initial state for multiple viewports (M)
<code>vpf</code>	Current vertical position of FID (P)
<code>vpfi</code>	Current vertical position of imaginary FID (P)
<code>vpset3def</code>	Set the viewport state to three default viewports (M)
<code>vpsetup</code>	Set new viewports (M)
<code>vs</code>	Vertical scale (P)
<code>vs2d</code>	Vertical scale for 2D displays (P)
<code>vsadj</code>	Automatic vertical scale adjustment (M)
<code>vsadj2</code>	Automatic vertical scale adjustment by powers of 2 (M)
<code>vsadjc</code>	Automatic vertical scale adjustment for ^{13}C spectra (M)
<code>vsadjh</code>	Automatic vertical scale adjustment for ^1H spectra (M)
<code>vsproj</code>	Vertical scale for projections and traces (P)
<code>vtairflow</code>	Variable Temperature Air Flow (P)
<code>vtairlimits</code>	Variable Temperature Air Flow Limits (P)
<code>vtc</code>	Variable temperature cutoff point (P)
<code>vtcomplvl</code>	Variable temperature compensation for gradient shimming (P)
<code>vttype</code>	Variable temperature controller present (P)
<code>vtwait</code>	Variable temperature wait time (P)
<code>vxr_unix</code>	Convert VXR-style text files to UNIX format (M,U)

vast1d Set up initial parameters for VAST experiments (M)

Applicability: Systems with VAST accessory.

Description: Sets up initial VAST parameters from the `/vnmr/stdpar` directory or from the user's `stdpar` directory if the appropriate file exists there. Any changes made to the files in these directories are reflected in the setup. The file `/vnmr/stdpar/vast1d.par` contains the “default” parameters for VAST spectra and should be modified as needed to produce spectra under desirable conditions. After running `vast1d`, the solvent parameter can be set by choosing it from the list of solvents listed in `/vnmr/solvents`.

See also: *NMR Spectroscopy User Guide*

vastget Selects and displays VAST spectra (M)

Applicability: Systems with VAST accessory.

Syntax: `vastget (<well>, <well>, ... ) >`

Description: Selects and displays the spectra from any arbitrary well or wells using the well label(s) as arguments. the spectra are displayed in a `dss` stacked plot.

Arguments: `well` is the well label from which you want to select and display spectra. The wells are labeled [A->H][1-8].

Examples: `vastget ( 'B6' , 'B7' , 'C11' , 'G3' )`

See also: *NMR Spectroscopy User Guide*

vastglue Assemble 1D datasets into a 2D (or pseudo-2D) datasets (M)

Applicability: Systems with the VAST accessory.

Syntax: `vastglue (<rack>, <zone>)`

`vastglue (<glue order>, <plate>)`

Description: Used to artificially reconstruct a 2D datasets from a series of 1D data sets having similar filenames. It is crucial to ensure that the format of the file names of each of the 1D data sets is identical. `vastglue` reads in each 1D file, in succession, and adds it to the previous data, but in a 2D format. It assumes that file names are of the format obtained when using the default setting of `autoname` (`autoname= ' '`). If `autoname` has been redefined, use a macro like `vastglue2`. Save the resulting reconstructed 2D datasets in the normal manner using `svf`.

Arguments: `rack` is the rack number; the default is 1. If you enter a `rack` number, you must also enter a `zone` number.

`zone` is the zone number; the default is 1. If you want to specify a `zone` number, you must enter a `rack` number.

`glue order` is the specific glue order to be defined based on the order defined in a `plate_glue` file. If `glue order` is specified, you can provide a `plate` number as the second argument and used with the `glue order` argument.

See also: *NMR Spectroscopy User Guide*

Related: `autoname` Prefix for automation data file (P)

`vastglue2` Assemble related 1D datasets into a 2D (or pseudo-2D) datasets (M)

vastglue2 Assemble 1D datasets into a 2D (or pseudo-2D) datasets (M)

Applicability: Systems with the VAST accessory

Syntax: `vastglue2<(number)>`

Description: Used to artificially reconstruct a 2D data set from a series of 1D datasets having similar filenames. It is crucial to ensure that the format of the file names of each of the 1D datasets is identical. `vastglue2` reads in each 1D file, in succession, and adds it to the previous data, but in a 2D format. It assumes that file names are of the format obtained using a nondefault setting of `autoname` (`autoname='filename_R%RACK:%_Z%ZONE:%_S%SAMPLE#:%_'`). This definition must be hard coded into the macro by the user. If `autoname` has not been redefined, use a macro like `vastglue`. Save the resulting reconstructed 2D data set in the normal manner using `svf`.

Arguments: `number` is used to specify that only spectra from 1 through `number` are to be glued. The default is to glue all the spectra stored in the current directory that have the proper file name format (from 1 through `arraydim`).

See also: *NMR Spectroscopy User Guide*

Related: `autoname` Prerix for automation data file (P)
`vastglue` Assemble related 1D datasets into a 2D (or pseudo-2D) data set (M)

vastgo Turn off LC stop flow automation, start VAST automation (M)

Applicability: Systems with the LC-NMR and VAST accessory

Description: Turns off LC stopped flow use of automation and starts VAST automation run.

vbg Run VNMR processing in background (U)

Syntax: (From UNIX) `vbg exp_number command_string <prefix>`

Description: Enables user to perform VNMR tasks in the background. `vbg` (for “VNMR background processing”) must be run from within a UNIX shell, and *no* foreground or other background processes can be active in the designated experiment (e.g., if you are working in `exp2` in VNMR (in the foreground), you cannot execute background processing in `exp2` as well).

Foreground processing causes a lock file to be placed in the appropriate experiment. The file has a format such as `f.1268`, where 1268 indicates the process number in the process table (accessed in UNIX by entering the command `ps -e`). Background processing causes a lock file to be in the appropriate experiment as well. This file has a format such as `b.4356`, where 4356 indicates the process number. By displaying the files within an experiment, the user can readily determine whether any foreground or background processes are active in that experiment.

Arguments: `exp_number` is the number of the experiment, from 1 to 9, in the user’s directory in which the background processing is to take place.

`command_string` is the command string to be executed by VNMR in the background. Double quotes enclosing the string are mandatory (e.g., `"fn=4096 fn1=2048 wft2da"`).

`prefix` is a prefix to be added to the name of the log file, making the name `prefix_bgf.log`. The default name is `exp_number_bgf.log`, where `exp_number` is the experiment number. The log file is placed in the experiment in which the background processing takes place.

Examples: (From UNIX) `vbg 1 "wft2da bc('f1')"`

(From UNIX) `vbg 3 "vsadj pl pscale pap page" plotlog`

See also: *User Programming*

vf Vertical scale of FID (P)

Description: In normalized intensity (**nm**) mode, **vf** is the height of the largest FID. In absolute intensity (**ai**) mode, **vf** is a multiplier that is adjusted to produce a desired vertical scale, using the appearance on the display screen as a guide (full scale on the screen gives full scale on the plotter).

vf can be entered in the usual way or interactively controlled by clicking the middle mouse button in the graphics window during a FID display (click above the FID to increase **vf** or below the FID to decrease it).

Values: 1e-6 to 1e9, in mm (in **nm** mode) or as a multiplier (in **ai** mode).

See also: *NMR Spectroscopy User Guide*

Related:	ai	Select absolute intensity mode (C)
	df	Display a single FID (C)
	nm	Select normalized intensity mode (C)
	sf	Start of FID (P)
	wf	Width of FID (P)

vi Edit text file with vi text editor (M)

Syntax: **vi** (file)

Description: Invokes the UNIX text editor **vi** for editing the file name given. On the Sun workstation, a popup screen contains the editing window. On the GraphOn terminal, the main screen becomes the editing window. **vi** is a powerful text editor, but its user interface is limited: the mouse is not used, menus are not available, and status information is virtually nonexistent.

vi operates in three modes: the *command mode* (for moving the cursor and editing text), the *insert mode* (for inserting text into the file), and the *last line mode* (for special operations). Each mode is described below.

Command mode

vi starts up in the command mode. In this mode, user commands consist mostly of a single character, sometimes in combination with another character, or a number, or both. A number preceding a command typically defines how many times a command should be executed (e.g., 3dd means delete three lines). The commands available include the following:

G	go to the start of the last line in the file
3G	go to the start of line 3
0	(zero) go to the start of the current line
\$	go to the end of the current line
Return or +	go to start of next line
-	(hyphen) go to start of previous line
Ctrl-d	scroll down (forward) half a screen
Ctrl-f	scroll forward by a full screen
Ctrl-u	scroll up (back) half a screen
Ctrl-b	scroll back by a full screen
/expression	find next expression and jump to its first character
?expression	find previous expression, jump to its first character
n	find next expression (from the last search)
N	find previous expression (from the last search)
dd	delete one line and put it into the buffer
3dd	delete three lines and put them into the buffer
dw	delete word

x	erase one character forward (under cursor)
X	erase one character backwards (before cursor)
3x	erase three characters forward
rcharacter	erase character and replace with character
ZZ	write if necessary and quit vi
.	(period) repeat the last command
u	undo the last command
J	join the next line to the current line
yy or Y	yank one line and put into a buffer (called yank buffer)
p	put contents of yank buffer after the cursor
P	put contents of yank buffer before the cursor
"aY	yank line into buffer a (buffers b to z also available)
"ap	put contents of buffer a below current line
"aP	put contents of buffer a above current line

Because there is no command line, these commands do not show up on the screen but are *executed immediately* (without pressing the Return key).

Insert mode

In the insert mode, characters typed on the keyboard (except for the Esc key) show up in the text. The insert mode is entered by typing one of the following commands from the command mode:

a text Esc	append text after the current cursor position
A text Esc	append text to the end of current line
i text Esc	insert text before current cursor position
cw word Esc	change word from current cursor position to end
2cw words Esc	change two words from current cursor position to end
o text Esc	open line below current line and append text
O text Esc	open line above current line and append text

The only way to exit the insert mode is by pressing the Esc key, which leads back to the command mode. Unfortunately, there is no indication on the screen whether vi is in the command mode or in the insert mode. Inexperienced users often press the Esc key to make sure they are still in the command mode. The Esc key can also be used to avoid execution of commands that have been typed partially (e.g., the number has been typed, but not the last character).

You can insert special (normally nondisplayable) characters into the text if they are preceded by a Ctrl-v (e.g., entering Ctrl-v Ctrl-q is displayed in the text as ^Q).

Changing selected occurrences

The following actions find one or more occurrences of a particular word and change it to another word:

- First, type /word and press Return, where / is a forward slash and word is word you want to change.
- Next, press n as necessary until you reach the occurrence of the word you want to change.
- Finally, type cw newword and press Esc, where newword is replacement word.
- To repeat for another occurrence of word, press n as necessary to scan forward, and then type . (a period) to repeat cw newword (or whatever was the last change)

Changing selected occurrences of an expression (one or more words) is similar. To change two words, for example, take the same actions as above but use the command `2cw` (or `c2w`) instead.

Last line mode

The last line mode is initiated with a colon; thereafter, commands such as the following can be used (press Return to execute these commands):

```
:r filename      read file named filename (insert in currently open file)
:w              write (save) file
:w filename      write under a new file named filename
:e filename      edit a different file named filename
:q              quit vi (only possible if file has been written back)
:wq             write back file (save changes) and quit vi
:q!             quit vi without saving changes
```

Exiting from `vi` is accomplished by using the `ZZ` command in the command mode, or with the `:q`, `:wq`, or `:q!` commands in the last line mode.

This description lists only a selection of the most important commands. For more information on `vi`, refer to UNIX books and manuals.

Examples: `vi (userdir+'/psglib/apt.c')`
`vi (curexp+'text')`

See also: *User Programming*

Related:	<code>edit</code>	Edit a file with user-selectable editor (M)
	<code>paramvi</code>	Edit a parameter and its attributes with <code>vi</code> text editor (M)
	<code>macrovi</code>	Edit a user macro with the <code>vi</code> text editor (C)
	<code>menuvi</code>	Edit a menu with the <code>vi</code> text editor (M)
	<code>textvi</code>	Edit text file of current experiment (M)

vibradd Display relative amplitudes of Cold Probe vibrations (M)

Applicability: Systems with Varian, Inc. Cold Probes

Description: Display the relative amplitudes of the vibrations reaching the probe. Requires a doped HOD sample.

vjhelp Display VnmrJ help (U)

Syntax: `vjhelp file:///vnmr/jhelp/jhelp.html`

Description: Displays the VnmrJ help in a Web browser.

vn Start VNMR directly (U)

Syntax: (From UNIX) `vn <-display Xserver> <-fn font> &`

Description: Starts the VNMR application directly without checking the operating system and attempting to run the window manager.

Arguments: `-display Xserver` specifies X server display (e.g., `hostname:0.0`). The default is the environment set by the `DISPLAY` variable.

`-fn font` specifies the size of the font displayed (e.g., `9x15`, `8x13`, or `7x13`). The default is the font set in the `.Xdefaults` file. Note that the size of the font affects the size of the VNMR window.

Examples: `vn &`
`vn -display hostname:0.0 &`
`vn -font 8x13 &`

See also: *NMR Spectroscopy User Guide*

Related: [vnmr](#) Start VNMR (U)

vnmr Starts VnmrJ (U)

Applicability: VnmrJ

Syntax: `vnmr`

Description: Starts the VnmrJ application

See also: *NMR Spectroscopy User Guide*

Related: [vnmrj](#) Start VnmrJ (U)

vnmr2sc VNMR to SpinCAD pulse sequence translator (M)

Syntax: `vnmr2sc<('sequence_name'<,rfchannels<,gradchannels>>>)>`

Description: Converts the pulse sequence pointed to by the [seqfil](#) parameter in the current VNMR parameter set from a C program into a SpinCAD pulse sequence. The conversion result is stored in the local `spincad/psglib` under the same name as the C pulse sequence (i.e., the name stored in the `seqfil` parameter), but without the `.c` extension.

`vnmr2sc` uses [dps](#) output to generate the SpinCAD code, i.e., the pulse sequence must be compiled and must be displayable with `dps`. Pulse sequences that do not compile with the `dps` option cannot be translated. For the same reason, `vnmr2sc` cannot translate features that do not show up in `dps`. This means that [go](#)-time decisions (such as flag-based `C if` constructs) will *not* show up in the translated SpinCAD sequence. In such cases, you have two options:

- Translate the sequence several times, once for each of the relevant flag settings. That is, generate several (simpler) SpinCAD pulse sequences from a single C sequence.
- Translate the sequence once (preferably with all options turned on), then manually insert the necessary `if` statements and other missing elements using SpinCAD.

Arguments: `sequence_name` is an optional argument that permits the name of the resulting SpinCAD pulse sequence to be specified. By default, `vnmr2sc` creates a SpinCAD sequence with the name specified in the `seqfil` parameter (i.e., the SpinCAD sequence has the same name as the C pulse sequence). `sequence_name` is particularly useful if a C sequence is to be translated into multiple SpinCAD sequences; see the examples.

`rfchannels` is an optional numeric argument specifying the number of rf channels. Use it when you want the SpinCAD sequence to address more rf channels. By default, `vnmr2sc` determines the number of rf channels from the source sequence. You can only *increase* the number of rf channels. If you specify 0 rf channels, the number of rf channels is left unchanged.

`gradchannels` is a second optional numeric argument specifying the number of gradient channels or axes. Use it when you want to convert a nongradient sequence to a gradient sequence or when you want the SpinCAD sequence to address more gradient axes than the source sequence. By default, `vnmr2sc` determines the number of gradient axes from the source sequence. You can only *increase*, not decrease, the number of gradient axes.

Examples: `vnmr2sc`
`setup('H1','CDCl3') hmqc null=0.2 vnmr2sc`
`null=0 mbond='y' vnmr2sc('hmbc')`

```

vnmr2sc('gcosy',2,3)
nt=256 vnmr2sc
vnmr2sc(4,1)
vnmr2sc(0,1)

```

See also: *SpinCAD Manual*

Related: `dps` Display pulse sequence (C)
`spincad` Run SpinCAD program (C)

vnmr_accountingOpen Accounting window (U)

Description: Opens a window for creating and maintaining cost accounting data for groups of users on a spectrometer system. The program accommodates multiple rate schedules for spectrometer usage. A calendar tool can be used to define holidays for holiday rates. There is no limit on the number of rates that can be defined. Multiple printers can be selected.

Any user can view the accounting information (enter `cd /vnmr/bin` followed by `./vnmr_accounting`), but to update information, the user must have root privileges.

See also: *System Installation and Administration*

Related: `operator` Operator name (P)
`operatorlogin` Sets work space and parameters for the operator (M)

vnmrjcmd() Commands to invoke the GUI popup (C)

Syntax: `vnmrjcmd('command1','command2',..., parametername)`
`vnmrjcmd('command1','command2',...<, callback>)`

Description: The `vnmrjcmd()` commands are needed in order to invoke the GUI popup in which the user enters the parameters.

Note that `vnmrbg` and `VnmrJ` cannot be easily synchronized. When a macro invokes `VnmrJ` via `vnmrjcmd`, the `VnmrJ` thread runs independently and the macro continues on and takes action without otherwise having knowledge of `VnmrJ`. In order to have events associated with required parameters occur in the proper order, a callback strategy was devised. In simple terms, the `vnmrj` commands can have a `callback` string such that when the required parameters are established in `VnmrJ`, `vnmrbg` can be re- invoked - the foremost example of this is re-entering the 'go' macro after the parameters are established in `VnmrJ`.

Examples: Sends parameters one at a time to `VnmrJ` to be eventually displayed in an entry popup:

```

vnmrjcmd('reqpar','warngui','set','real',
parametername)
vnmrjcmd('reqpar','warngui','set','string',
parametername)

```

Display a GUI panel listing required parameters sent from `vnmrbg` in the previous 'set' option above:

```

vnmrjcmd('reqpar','warngui','show')
vnmrjcmd('reqpar','warngui','show', callback)

```

The callback is a command string to be sent back to `vnmrbg`, if needed. See the `reqpartest` macro source code for examples of how to use callback.

See also: *VnmrJ User Programing*

Related `go` Submit experiment to acquisition (M)
`reqpartest` Tests whether required parameters are set (M)

vnmr`exit` Exit from the VNMR system (C)

Description: Exits from the VNMR system in a graceful manner by writing parameters and data to the disk, removing lock files, and restoring the terminal (if on a GraphOn). To provide flexibility when exiting VNMR, the macro `exit` calls `vnmrexit` to exit from VNMR.

CAUTION: When you exit from the VNMR user interface on your X display system, whether you are using an X terminal or a Sun computer, and whether you are using OpenWindows, CDE, or Motif, you must first exit from any copy of VNMR running on your system. Failure to do this can cause current parameter values and even current data to be lost.

vnmr`j` Start VnmrJ (U)

Applicability: VnmrJ

Syntax: `vnmrj`

Description: Starts the VnmrJ application

See also: *NMR Spectroscopy User Guide; VnmrJ Walkup*

Related: `vnmr` Starts VnmrJ (U)

vnmr`plot` Plot files (U)

Syntax: (From UNIX) `vnmrplot <file>`

Description: A UNIX command that plots files from inside VNMR commands. To plot a file, you should use the `page` command, which uses `vnmrplot` internally.

Arguments: `file` is the name of the file to be plotted.

See also: *NMR Spectroscopy User Guide*

Related: `vnmrprint` Print text files (U)

vnmr`print` Print text files (U)

Syntax: (From UNIX) `vnmrprint printfile <printcap>
 <printer_type <clear|file>>`

Description: A UNIX command installed as part of the VNMR system to print text files. The `printon` and `printoff` commands use `vnmrprint` to print files. `vnmrprint` can also be used to delete a print file or save a print file to a different name.

Arguments: `printfile` is the name of the text file to be printed.

`printcap` is a UNIX printcap entry (e.g. LaserJet_300) for the printer to print the text file. The default is the printer selected by the `-p` option of the UNIX `lp` command.

`printer_type` is the type of printer from the list of VNMR printers (e.g., LaserJet_300). `printer_type` is required as an argument when it is desired to clear the printer file or save the printer file to another name.

`clear` is a keyword to delete the current print file. Deleting this file also requires that the `printfile`, `printcap`, and `printer_type` arguments be entered so that `clear` is the fourth argument.

file is the name of the file to use in saving the printfile. If a file with the name specified already exists, it is overwritten. Saving the file also requires that the printfile, printcap, and printer_type arguments be entered so that file is the fourth argument.

Examples: `vnmrprint /vnmr/psglib/tocsy.c LaserJet_300`
`vnmrprint myfile LaserJet_300 LaserJet_300 clear`
`vnmrprint myfile ps PS_AR yourfile`

See also: *NMR Spectroscopy User Guide*

Related: `printoff` Stop sending text to printer and start print operation (C)
`printon` Direct text output to printer (C)
`vnmrplot` Plot files (U)

vo Vertical offset (P)

Description: Sets the vertical offset, for 1D data sets, of the each spectrum in a *stacked display* with respect to the previous spectrum. The parameter `ho` sets the horizontal offset. For a “left-to-right” presentation, `ho` is typically negative; for a “bottom-to-top” presentation, `vo` is positive.

For 2D data sets, the parameter `wc2` sets the distance between the first and last trace and the `vo` parameter is inactive.

Values: Number, in mm.

See also: *NMR Spectroscopy User Guide*

Related: `ho` Horizontal offset (P)
`wc2` Width of chart in second direction (P)

vp Vertical position of spectrum (P)

Description: Contains vertical position of spectrum with respect to the bottom of the display or plotter.

Values: –200 to +200, in mm.

See also: *NMR Spectroscopy User Guide*

Related: `vpf` Current vertical position of FID (P)
`vpfi` Current vertical position of imaginary FID (P)

vpaction Set initial state for multiple viewports (M)

Applicability: *VnmrJ Walkup*

Description: Sets the initial state for multiple viewports. Used by the viewport editor dialog under **Edit -> Viewports**.

See also: *User Programming*

Related: `jcurwin` Work space numbers of all viewports (P)
`jviewportlabel` Work space labels for all viewport buttons (P)
`jviewports` Viewport layout (P)

vpf Current vertical position of FID (P)

Description: Contains the current vertical position of an FID. To create this parameter and the other FID display parameters `axisf`, `crf`, `deltaf`, `dotflag`, and `vpfi` (if the parameter set is older and lacks these parameters), enter `addpar('fid')`.

Values: Number, in mm. If `vpf=0`, the FID is positioned in the middle of the screen.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>axisf</code>	Axis label for FID displays and plots (P)
	<code>crf</code>	Current time-domain cursor position (P)
	<code>deltaf</code>	Difference of two time-domain cursors (P)
	<code>dotflag</code>	Display FID as connected dots (P)
	<code>vp</code>	Vertical position of spectrum (P)
	<code>vpfi</code>	Current vertical position of imaginary FID (P)

vpfi **Current vertical position of imaginary FID (P)**

Description: Contains the current vertical position of the imaginary part of an FID. To create this parameter and the other FID display parameters `axisf`, `crf`, `deltaf`, `dotflag`, and `vpf` (if the parameter set is older and lacks these parameters), enter `addpar('fid')`.

Values: Number, in mm. In `vpfi=0`, the imaginary part is positioned in the middle of the screen.

See also: *NMR Spectroscopy User Guide*

Related:	<code>addpar</code>	Add selected parameters to the current experiment (M)
	<code>axisf</code>	Axis label for FID displays and plots (P)
	<code>crf</code>	Current time-domain cursor position (P)
	<code>deltaf</code>	Difference of two time-domain cursors (P)
	<code>dotflag</code>	Display FID as connected dots (P)
	<code>vp</code>	Vertical position of spectrum (P)
	<code>vpf</code>	Current vertical position of FID (P)

vpset3def **Set the viewport state to three default viewports (M)**

Description: Sets the number of viewports to three, and resets the viewport button labels.

See also: *User Programming*

Related:	<code>jcurwin</code>	Work space numbers of all viewports (P)
	<code>jviewportlabel</code>	Work space labels for all viewport buttons (P)
	<code>jviewports</code>	Viewport layout (P)

vpsetup **Set new viewports (M)**

Description: Sets the viewports from the selections made in the viewport editor dialog. For each viewport, it checks the work space number to join, then joins the appropriate work space.

See also: *User Programming*

Related:	<code>jcurwin</code>	Work space numbers of all viewports (P)
	<code>jviewportlabel</code>	Work space labels for all viewport buttons (P)
	<code>jviewports</code>	Viewport layout (P)

vs **Vertical scale (P)**

Description: In normalized (`nm`) mode, `vs` is the height of the largest peak in the spectrum. In absolute intensity (`ai`) mode, `vs` is a multiplier that is adjusted to produce a desired vertical scale, using the appearance on the display screen as a guide (full scale on the screen gives full scale on the plotter). `vs` can be entered in the usual way or interactively controlled by clicking the middle mouse button.

Values: 1e-6 to 1e9, in mm (in `nm` mode) or as a multiplier (in `ai` mode).

See also: *NMR Spectroscopy User Guide*

Related:	ai	Select absolute intensity mode (C)
	isadj	Adjust integral scale (M)
	nm	Select normalized intensity mode (C)
	thadj	Adjust threshold for peak printout (M)
	vsadj	Automatic vertical scale adjustment (M)
	vsadj2	Automatic vertical scale adjustment by powers of two (M)
	vsadjc	Automatic vertical scale adjustment for ¹³ C spectra (M)
	vsadjh	Automatic vertical scale adjustment for ¹ H spectra (M)

vs2d Vertical scale for 2D displays (P)

Description: Sets a multiplier for 2D spectra and images that is adjusted to produce a desired vertical scale for display or plotting. **vs2d** takes the place of **vs** for 2D data display and can be adjusted by explicitly setting it to a value or by clicking the middle mouse button when pointing to a point on a 2D display. If **vs2d** does not exist, it can be created by running **par2d**.

See also: *NMR Spectroscopy User Guide*

Related:	par2d	Create 2D acquisition, processing, and display parameters (M)
	vs	Select vertical scale (C)
	vsproj	Adjust vertical scale for projections and traces (M)

vsadj Automatic vertical scale adjustment (M)

Syntax: **vsadj**<(height)>

Description: Automatically sets the vertical scale **vs** in the absolute intensity (**ai**) mode so that the largest peak is at the requested height.

Arguments: **height** is the desired height, in mm, of the largest signal in the displayed portion of the spectrum. The default is $0.9 * (wc2max - vp - sc2)$.

Examples: **vsadj**
vsadj (100)

See also: *NMR Spectroscopy User Guide*

Related:	ai	Select absolute intensity mode (C)
	isadj	Adjust integral scale (M)
	thadj	Adjust threshold for peak printout (M)
	vs	Vertical scale (P)
	vsadj2	Automatic vertical scale adjustment by powers of two (M)
	vsadjc	Automatic vertical scale adjustment for ¹³ C spectra (M)
	vsadjh	Automatic vertical scale adjustment for ¹ H spectra (M)
	wc2max	Maximum width of chart in second direction (P)

vsadj2 Automatic vertical scale adjustment by powers of 2 (M)

Syntax: **vsadj2**<(height)>:scaling_factor

Description: Adjusts the vertical scale by powers of two as required for expansion plots (see **aexpp1** for more information).

Arguments: **height** is desired height of largest (or largest relevant) signal in displayed portion of the spectrum. The default is $0.9 * (wc2max - vp - sc2)$.
scaling_factor returns to the calling macro the ratio of the new compared to the old value of **vs**.

Examples: `vsadj2`
`vsadj2(50):r1`

See also: *NMR Spectroscopy User Guide*

Related: `aexppl` Automatic expansions plot (M)
`isadj` Adjust integral scale (M)
`sc2` Start of chart in second direction (P)
`thadj` Adjust threshold for peak printout (M)
`vp` Vertical position of spectrum (P)
`vs` Vertical Scale (P)
`vsadj` Automatic vertical scale adjustment (M)
`vsadjc` Automatic vertical scale adjustment for ¹³C spectra (M)
`vsadjh` Automatic vertical scale adjustment for H1 spectra (M)
`wc2max` Maximum width of chart in second direction (P)

vsadjc Automatic vertical scale adjustment for ¹³C spectra (M)

Syntax: `vsadjc<(height)>`

Description: Functionally the same as the macro `vsadj`, except excludes solvent and TMS signals from the carbon spectra for the adjustment of `vs`.

Arguments: `height` is desired height of largest (or largest relevant) signal in displayed portion of the spectrum. The default is $0.9 * (wc2max - vp - sc2)$.

Examples: `vsadjc`
`vsadjc(wc2max-sc2-wc2-5)`

See also: *NMR Spectroscopy User Guide*

Related: `isadj` Adjust integral scale (M)
`thadj` Adjust threshold for peak printout (M)
`vs` Vertical Scale (P)
`vsadj` Automatic vertical scale adjustment (M)
`vsadj2` Automatic vertical scale adjustment by powers of two (M)
`vsadjh` Automatic vertical scale adjustment for H1 spectra (M)

vsadjh Automatic vertical scale adjustment for ¹H spectra (M)

Syntax: `vsadjh<(height<,do_not_ignore_solvent>)>`

Description: Works as the same as the macro `vsadj`, except disregards solvent and TMS signals from proton spectra and, if from the remaining spectrum the highest line is more than three times as high as the second highest line, the spectrum is scaled to this second highest signal (otherwise the highest signal is taken as relevant).

Arguments: `height` is desired height of largest (or largest relevant) signal in displayed portion of the spectrum. If `height` is 0 or a negative value, it defaults to $0.9 * (wc2max - vp - sc2)$, which is also the default with no arguments.
`do_not_ignore_solvent` is any second argument. If present, it signals `vsadjh` to not ignore the solvent line and regard the solvent line as normal signal (i.e., only exclude the TMS line). This argument was added for the situation where frequently there are high “real” signals at the position of the solvent line. Such signals could otherwise be regarded as solvent line and would then be ignored. This could then lead to overscaling in the result.

Examples: `vsadjh`
`vsadjh(0.7*wc2max)`

See also: *NMR Spectroscopy User Guide*

Related:	<code>isadj</code>	Adjust integral scale (M)
	<code>sc2</code>	Start of chart in second direction (P)
	<code>thadj</code>	Adjust threshold for peak printout (M)
	<code>vs</code>	Vertical scale (P)
	<code>vsadj</code>	Automatic vertical scale adjustment (M)
	<code>vsadj2</code>	Automatic vertical scale adjustment by powers of two (M)
	<code>vsadjc</code>	Automatic vertical scale adjustment for ¹³ C spectra (M)

vsproj Vertical scale for projections and traces (P)

Description: Sets a multiplier that is adjusted to produce a desired vertical scale for projections or traces of 2D data sets. `vsproj` can be explicitly adjusted by setting it to a value or by clicking the middle mouse button when pointing at the projection or trace. When interactively adjusting the scale with the mouse, the higher the pointer is in the trace display, the larger the vertical scale. If the parameter does not exist, it can be created by running the `par2d` macro.

See also: *NMR Spectroscopy User Guide*

Related:	<code>par2d</code>	Create 2D acquisition, processing, and display parameters (M)
	<code>vs</code>	Select vertical scale (C)
	<code>vs2d</code>	Adjust vertical scale for 2D displays (M)

vtairflow Variable Temperature Air Flow (P)

Description: This global parameter sets the VT air flow, in l/min. The adjustment is coarse, +/- 1 l/min. If there is not enough air flow available it may not reach the requested value.

Values: 0 - 25

Related:	<code>pin</code>	Pneumatics router interlock (P)
	<code>vtairlimits</code>	Variable temperature air flow limits (P)

vtairlimits Variable Temperature Air Flow Limits (P)

Description: This global parameter determines the range of safe VT air flow, as indicated by the LEDs on the flow meter. It sets the LEDs on the air flow meter, upper and lower LEDs are orange, in between are green. As long as the ball in the air flow meter is next to a green LED the air flow is considered safe. If the air flow drops or increases such that the ball is next to an orange LED, the pneumatics box will turn the VT Controller off and notify the experiment, provided the switch is in the 'run' position. A bit value of 1 sets an unsafe orange state, a bit value of 0 sets a safe green state.

To create the parameter:

```
create('vtairlimits','integer','global')
setlimit('vtairlimits',1023,0,1,'global')
```

Examples: a value of 775 or 0x307 will set the two lower and the three upper LEDs (orange) and clear the remaining 5 in between (green). Note that the upper bits determine the lower LEDs. If the parameter does not exist the value defaults to 0x307 for liquids; 0x200 for solids.

Values: 0 - 1023

Related:	<code>pin</code>	Pneumatics router interlock (P)

`tin` Temperature interlock (P)
`vtairflow` Variable temperature air flow (P)

vtc Variable temperature cutoff point (P)

Applicability: Systems with a variable temperature (VT) module.

Description: Sets a VT cutoff point. Above this temperature, VT air flows straight into the probe, past the heater, then past the sample. Below this temperature, air goes first through the heat exchange bucket, for cooling by the heat exchange fluid, and then into the probe and past the heater.

Values: 0 to 50, in degrees celsius. `vtc` is typically set 5°C higher than the supply gas used for VT regulation.

See also: *NMR Spectroscopy User Guide*

Related: `temp` Sample temperature (P)
`tin` Temperature interlock (P)

vtcomp1vl Variable temperature compensation for gradient shimming (P)

Description: Specifies the level of VT compensation used by gradient shimming.

Values: 0, disable VT compensation.
 1, enable VT compensation
 2, enable VT compensation with extra gradient dephasing.

Related: `gmapz` Get parameters and files for `gmapz` pulse sequence (M)
`gmapsys` Run gradient autoshimming, set parameters, map shims (M)
`gzsize` Number of z-axis shims used by gradient shimming (P)
`temp` Sample temperature (P)
`vttype` Variable temperature controller present (P)

vttype Variable temperature controller present (P)

Description: In the Spectrometer Configuration window, this parameter specifies whether a variable temperature (VT) controller is present or not on the system. The value is set using the VT Controller label in the Spectrometer Configuration window.

When entered from command line in VNMR, control of the variable temperature (VT) controller from the current experiment is either engaged (`vttype=2`) or disengaged (`vttype=0`). The current state of the variable temperature (VT) controller is not changed when `vttype` is set in the command window.

The variable temperature (VT) controller setting in Spectrometer Configuration is not affected by entering `vttype` on the command line.

Values: 2 is setting for VT controller (Present choice in Spectrometer Configuration window).

0 is setting for no VT controller (Not Present choice in Spectrometer Configuration window).

Examples: If `temp='some temperature'` while `vttype=2` and `vttype` is then changed to `vttype=0` on the command line, the variable temperature (VT) controller will continue regulate the sample at the value set by `temp`. While `vttype=0` changes to `temp` will have no effect.

See also: *VnmrJ Installation and Administration; NMR Spectroscopy User Guide*

Related: `config` Display current configuration and possibly change values (M)
`masvt` Type of variable temperature system (P)

V

vtwait **Variable temperature wait time (P)**

Applicability: Systems with a variable temperature (VT) module.

Description: Sets a time for establishing temperature regulation. If temperature interlock **tin** is set and regulation is not established after the time set by **vtwait**, VNMR displays the message “VT FAILURE” and aborts the experiment.

Values: Number, in seconds, A typical value is 180 seconds.

See also: *NMR Spectroscopy User Guide*

Related: **pad** Preacquisition delay (P)
tin Temperature interlock (P)

vxr_unix **Convert VXR-style text files to UNIX format (M, U)**

Syntax: (From VNMR) **vxr_unix** (VXR_file<,UNIX_file>)
(From UNIX) **vxr_unix** VXR_file UNIX_file

Description: Converts a VXR-style text file (from a Gemini, VXR, or XL system) to the UNIX format.

Arguments: **VXR_file** is the name of the input file, which must be a text file.
UNIX_file is the name of the output file after conversion. The names of the input and output files must be different.

Examples: (From VNMR) **vxr_unix** ('oldtextfile', 'newtextfile')
(From UNIX) **vxr_unix** oldtextfile newtextfile

See also: *NMR Spectroscopy User Guide*

Related: **convert** Convert data set from a VXR-style system (C,U)
decomp Decompose a VXR-style directory (C)

W

w	Who is using system (C)
walkup	Walkup automation (M)
waltz	WALTZ decoupling present (P)
wbs	Specify action when bs transients accumulate (C)
wbs	When block size (P)
wc	Width of chart (P)
wc2	Width of chart in second direction (P)
wcmax	Maximum width of chart (P)
wc2max	Maximum width of chart in second direction (P)
wdone	Specify action when experiment is done (C)
wdone	Specify action when experiment is done (P)
werr	Specify action when error occurs (C)
werr	When error (P)
wet	Flag to turn on or off wet solvent suppression ((P)
Wet1d	Set up parameters for wet ^1H experiment (M)
wetdqcosy	Set up parameters for a WETDQCOSY pulse sequence (M)
wetgcosy	Set up parameters for a WETGCOSY pulse sequence (M)
wetghmqcps	Set up parameters for a WETGHMQCPS pulse sequence (M)
wetghsqc	Set up parameters for a WETGHSQC pulse sequence (M)
wetgmqcosy	Set up parameters for a WETGHSQC pulse sequence (M)
wetit	Set up and create pulse shapes for Wet1d experiment (M)
wetnoesy	Set up parameters for a WETNOESY pulse sequence (M)
wetpeaks	Number of peaks for wet solvent suppression (P)
wetpwxcal	Set up parameters for a WETPWXCAL pulse sequence (M)
wettntocsy	Set up parameters for a WETTNTOCYSY pulse sequence (M)
wetshape	Shape for pwwet pulses (P)
wexp	Specify action when experiment completes (C)
wexp	When experiment completes (P)
wf	Width of FID (P)
wf1	Width of interferogram in 1st indirectly detected dimension (P)
wf2	Width of interferogram in 2nd indirectly detected dimension (P)
wfgtest	Waveform generator test (M)
wft	Weight and Fourier transform 1D data (C)
wft1d	Weight and Fourier transform f_2 for 2D data (C)
wft1da	Weight and Fourier transform phase-sensitive data (M)
wft1dac	Combine arrayed 2D FID matrices (M)
wft2d	Weight and Fourier transform 2D data (C)
wft2da	Weight and Fourier transform phase-sensitive data (M)
wft2dac	Combine arrayed 2D FID matrices (M)
wftt3	Process f_3 dimension during 3D acquisition (M)
which	Display which command or macro is used (M)
wnt	Specify action when nt transients accumulate (C)
wnt	When number of transients (P)

W

<code>wp</code>	Width of plot in directly detected dimension (P)
<code>wp1</code>	Width of plot in 1st indirectly detected dimension (P)
<code>wp2</code>	Width of plot in 2nd indirectly detected dimension (P)
<code>write</code>	Write formatted text to a device (C)
<code>writefid</code>	Write numeric text file using a FID element (C)
<code>writeparam</code>	Write one of more parameters to a file (C)
<code>writespectrum</code>	Write a spectrum to a binary file (C)
<code>wrtpr</code>	Command string executed after rtp command (P)
<code>wsram</code>	Send hardware configuration to acquisition console (C)
<code>wshim</code>	Conditions when shimming is performed (P)
<code>wtfile</code>	User-defined weighting in directly detected dimension (P)
<code>wtfile1</code>	User-defined weighting in 1st indirectly detected dimension (P)
<code>wtfile2</code>	User-defined weighting in 2nd indirectly detected dimension (P)
<code>wtgen</code>	Compile user-written weighting functions (M,U)
<code>wti</code>	Interactive weighting (C)
<code>wtia</code>	Interactive weighting for 2D absorptive data (M)
<code>wtune</code>	Specify when to tune (P)
<code>wtunedone</code>	What to do after ProTune tuning is done (P)
<code>wysiwyg</code>	Set plot display or full display (P)

w

Who is using system (C)

Description: Displays information about users currently on the system. It functions like the UNIX command of the same name.

See also: *User Programming*

walkup

Walkup automation (M)

Description: Enables using sample changers for continuous “walk-up” operation. Click on Utilities -> New automation run to run this macro from the VnmrJ Walkup interface. The macro creates a new automation directory each day with the name `auto_yyyy.mm.dd`, where `yyyy` is the year, `dd` is the day of the month, and `mm` is the month (e.g., `auto_20040601`). The automation directory is saved in a directory specified by the global parameter `globalauto`. `walkup` creates the directory `globalauto` and the parameter `globalauto`, and then sets the `globalauto` parameter.

See also: *VnmrJ Walkup*

Related: `enter` Enter sample information for automation run (M,U)
`globalauto` Automation directory name (P)

waltz

WALTZ decoupling present (P)

Description: Sets whether system is equipped for WALTZ decoupling. The value is changed by normal parameter entry rather than using the Spectrometer Configuration window.

Values: 'n' sets WALTZ decoupling not present.

'y' sets WALTZ decoupling present.

See also: *VnmrJ Installation and Administration*

- wbs** **Specify action when bs transients accumulate (C)**
- Syntax: `wbs (string)`
- Description: Specifies what action to take when **bs** transients accumulate. The *command* **wbs** sets the corresponding *parameter* **wbs**. Using the command, rather than setting the parameter value explicitly, notifies the acquisition process that the associated parameter value has changed. Thus, the desired operation can be effected even if the experiment has already started.
- Arguments: `string` is a string argument containing the command or macro to be executed when this event happens. The string must be enclosed in single quotes. If single quotes are required *within* the text string, place a backslash character before each of the interior single quotes (`\'`). Maximum length of the string is 256 characters. To turn off **wbs** processing, enter `wbs ( ' ' )`, where the argument is two single quotes with no space between.
- Syntax: `wbs ( 'dg wft' )`
`wbs ( 'mf (3) ' )`
`wbs ( ' ' )`
- See also: *NMR Spectroscopy User Guide*
- Related: **bs** Block size (P)
makefid Make a FID element using numeric text input (C)
phfid Zero-order phasing constant for np FID (P)
wbs When block size (P)
werr Specify action when error occurs (C)
wexp Specify action when experiment completes (C)
wnt Specify action when nt transients accumulate (C)
- wbs** **When block size (P)**
- Description: Invokes an action to occur automatically after each **bs** block of transients is completed. For example, `wbs= ' wft '` results in an automatic weighting and Fourier transformation after each **bs** transients. To specify no **wbs** processing, set **wbs** to the null string. If the acquisition has already started, the **wbs** *command* must be used to change this parameter.
- Values: Command, macro, or null string (`wbs= ' '` , where the value is given by two single quotes with no space between them).
- See also: *NMR Spectroscopy User Guide*
- Related: **bs** Block size (P)
wbs Specify action when bs transients accumulate (C)
- wc** **Width of chart (P)**
- Description: Specifies the width of the chart (plotting or printing area).
- Values: 5 to **wcmax**, in mm.
- See also: *NMR Spectroscopy User Guide*
- Related: **wc2** Width of chart in second direction (P)
wcmax Maximum width of chart (P)
- wc2** **Width of chart in second direction (P)**
- Description: Specifies width of chart (plotting or printing area) along the second axis (or y axis) of a 2D contour plot or 2D “stacked display.” For plots made in the **cutoff** mode, **wc2** specifies the width of the plotted area along the y-axis.

W

Values: Width, in mm.

See also: *NMR Spectroscopy User Guide*

Related: `cutoff` Data truncation limit (P)
`ho` Horizontal offset (P)
`sc2` Start of chart in second direction (P)
`wcmax` Maximum width of chart (P)
`wc2max` Maximum width of chart in second direction (P)

wcmax Maximum width of chart (P)

Description: Specifies the maximum width of a chart (plotting or printing area). Set when plotter or printer is installed.

Values: Width, in mm.

See also: *NMR Spectroscopy User Guide*

Related: `wc` Width of chart (P)
`wc2` Width of chart in second direction (P)

wc2max Maximum width of chart in second direction (P)

Description: Specifies the maximum width of a chart (plotting or printing area) in the second direction (*y*-axis). Set when the plotter or printer is installed.

Values: Width, in mm.

See also: *NMR Spectroscopy User Guide*

Related: `wc2` Width of chart in second direction (P)
`wcmax` Maximum width of chart (P)

wdone Specify action when experiment is done (C)

Syntax: `wdone (string)`

Description: Specifies the action to take when the experiment is done, after `wexp` has been executed. The `wdone` command sets the corresponding parameter `wdone`. Using the command, rather than setting the parameter value explicitly, notifies the acquisition process that the associated parameter value has changed and the desired operation is effected even if the experiment has already started.

Arguments: The `string` argument contains the command or macro to be executed when the experiment is done. The string must be enclosed in single quotes. If single quotes are required within the text string, place a backslash character before each of the interior single quotes (`\ '`). Maximum length of the string is 256 characters.

`' '` (null string) turns off `wdone` processing.

Related: `wexp` Specify action when experiment completes (C)

wdone Specify action when experiment is done (P)

Syntax: `wdone '<command, macro, or null string >'`

Description: Invokes a single action to occur just after `wexp` is executed. As with `wexp`, it is executed automatically after the experiment is finished, which can occur at the end of a single FID or after the last fid in a multi-FID experiment. To specify no `wdone` processing, set `wdone` to the null string. If the acquisition has already started, the `wdone` command must be used to change the `wdone`

parameter. For `wdone` to execute after an experiment finishes and after `wexp` has executed, start the experiment with the `au` command.

If the `wexp` action sets the `wdone` parameter, the new value of the `wdone` parameter will be executed and the old value will be ignored.

Arguments: Any command, macro, or null string (e.g. `wdone= ' '`).

Related:	<code>acquire</code>	Acquire data (M)
	<code>au</code>	Submit experiment to acquisition and process data (M)
	<code>wexp</code>	When experiment completes (P)

werr Specify action when error occurs (C)

Syntax: `werr(string)`

Description: Specifies what action to take if an error occurs during acquisition. The *command* `werr` sets the corresponding *parameter* `werr`. Using the command, rather than setting the parameter value explicitly, notifies the acquisition process that the associated parameter value has changed. Thus, the desired operation can be effected even if the experiment has already started.

Arguments: `string` is a string argument containing the command or macro to be executed when this event happens. The string must be enclosed in single quotes. If single quotes are required *within* the text string, place a backslash character before each of the interior single quotes (`\ '`). Maximum length of the string is 256 characters. To turn off `werr` processing, enter `werr( ' ' )`, where the argument is two single quotes with no space between them.

Examples: `werr('react')`
`werr(' ')`

See also: *NMR Spectroscopy User Guide*

Related:	<code>wbs</code>	Specify action when <code>bs</code> transients accumulate (C)
	<code>werr</code>	When error (P)
	<code>wexp</code>	Specify action when experiment completes (C)
	<code>wnt</code>	Specify action when <code>nt</code> transients accumulate (C)

werr When error (P)

Description: Specifies a macro (e.g., `werr='react '`) that will take appropriate action when an error occurs during acquisition. To specify no `werr` processing, set `werr` to the null string. If the acquisition has already been started, the `werr` *command* must be used to change the `werr` *parameter*. Arrayed parameter `acqstatus` provides the error code to `werr` in `acqstatus[1]` and `acqstatus[2]`. For a list of error codes, refer to the description of `acqstatus` or view the file `acq_errors` in directory `/vnmr/manual`.

Values: Macro or null string (`werr= ' '`, where the value is given by two single quotes with no space between them).

See also: *NMR Spectroscopy User Guide*

Related:	<code>acqstatus</code>	Acquisition status (P)
	<code>react</code>	Recover from error conditions during <code>werr</code> processing (M)
	<code>werr</code>	Specify action when error occurs (C)

W

wet	Flag to turn on or off wet solvent suppression ((P)
Description:	Specifies if wet solvent suppression is turned on or off. It is now a standard option in many liquids pulse sequences, including Wet1d and sequences of apptype hetero2d and homo2d.
Related:	apptype Application type (P) hetero2d Execute protocol actions of apptype hetero2d (M) homo2d Execute protocol actions of apptype homo2d (M) std1d Execute protocol actions of apptype std1d (M) Wet1d Set up parameters for a WET1D pulse sequence (M)
Wet1d	Set up parameters for wet ¹H experiment (M)
Description:	Set up parameters for wet ¹ H experiment.
wetdqcocy	Set up parameters for a WETDQCOSY pulse sequence (M)
Applicability:	Systems with LC-NMR accessory.
Description:	Sets up for a WETDQCOSY LC-NMR experiment.
See also:	<i>NMR Spectroscopy User Guide</i>
wetgcocy	Set up parameters for a WETGCOSY pulse sequence (M)
Applicability:	Systems with LC-NMR accessory.
Description:	Sets up for a WETGCOSY LC-NMR experiment.
See also:	<i>NMR Spectroscopy User Guide</i>
wetghmqcps	Set up parameters for a WETGHMQCPS pulse sequence (M)
Applicability:	Systems with LC-NMR accessory.
Description:	Sets up for a WETHMQCPS LC-NMR experiment.
See also:	<i>NMR Spectroscopy User Guide</i>
wetghsqc	Set up parameters for a WETGHSQC pulse sequence (M)
Applicability:	Systems with LC-NMR accessory.
Syntax:	wetghsqc('nucleus')
Description:	Sets up for a WETGHSQC LC-NMR experiment.
See also:	<i>NMR Spectroscopy User Guide</i>
wetgmqcocy	Set up parameters for a WETGHSQC pulse sequence (M)
Applicability:	Systems with LC-NMR accessory.
Description:	Sets up for a WETGMQCOSY LC-NMR experiment.
See also:	<i>NMR Spectroscopy User Guide</i>
wetit	Set up and create pulse shapes for Wet1d experiment (M)
Applicability:	VnmrJ Walkup
Description:	A macro to set up and create pulse shapes for a Wet1d experiment. It is based on suppressing the largest N peaks found in a spectrum.

Related: [wetpeaks](#) (P)

wetnoesy **Set up parameters for a WETNOESY pulse sequence (M)**

Applicability: Systems with LC-NMR accessory.

Description: Sets up for a WETNOESY LC-NMR experiment.

See also: *NMR Spectroscopy User Guide*.

wetpeaks **Number of peaks for wet solvent suppression (P)**

Applicability: *Walkup*

Description: Sets the number of peaks to be suppressed by wet solvent suppression for the [Wet1d](#) protocol. The [wetit](#) macro suppresses the N tallest peaks found in the scout spectrum, where N is specified by [wetpeaks](#). The parameter is set by the *Number of peaks to suppress menu* on the Prescan page.

Values: 1 to 7 for DirectDrive or UnityInova systems; 3 for Mercury systems are the default values.

Related: [Wet1d](#) Set up parameters for wet 1H experiment (M)
[wetit](#) Set up and create pulse shapes for Wet1d experiment (M)

wetpwxcal **Set up parameters for a WETPWXCAL pulse sequence (M)**

Applicability: Systems with LC-NMR accessory.

Description: Sets up for a WETPWXCAL LC-NMR pulse width calibration.

See also: *NMR Spectroscopy User Guide*

wettntocsy **Set up parameters for a WETTNTOCYSY pulse sequence (M)**

Applicability: Systems with LC-NMR accessory.

Description: Sets up for a WETTNTOCYSY LC-NMR experiment.

See also: *NMR Spectroscopy User Guide*

wetshape **Shape for pwwet pulses (P)**

Applicability: Systems with LC-NMR accessory.

Description: Sets the name of the shape used for pwwet pulses (e.g., `wetshape='wet'`).

See also: *NMR Spectroscopy User Guide*

wexp **Specify action when experiment completes (C)**

Syntax: `wexp(string)`

Description: Specifies what action to take when the experiment completes. The `wexp` command sets the corresponding parameter [wexp](#). Using the command, rather than setting the parameter value explicitly, notifies the acquisition process that the associated parameter value has changed. Thus, the desired operation can be effected even if the experiment has already started.

Arguments: `string` is a string argument containing the command or macro to be executed when the experiment completes. The string must be enclosed in single quotes. If single quotes are required *within* the text string, place a backslash character

before each of the interior single quotes (\ '). Maximum length of the string is 256 characters. To turn off `wexp` processing, enter `wexp ( ' ' )`, where argument is two single quotes with no space between them.

Examples: `wexp ('wft (\ 'all\ ') calcT1')`
`wexp ( ' ' )`

See also: *NMR Spectroscopy User Guide*

Related:	<code>wbs</code>	Specify action when bs transients accumulate (C)
	<code>werr</code>	Specify action when error occurs (C)
	<code>wexp</code>	When experiment completes (P)
	<code>wnt</code>	Specify action when nt transients accumulate (C)

wexp

When experiment completes (P)

Description: Invokes a single action to occur automatically after the experiment is finished, which can occur after a single FID or after a number of FIDs in a multi-FID experiment. To specify no `wexp` processing, set `wexp` to the null string. If the acquisition has already started, the `wexp` command must be used to change the `wexp` parameter. For `wexp` to execute after an experiment finishes, start the experiment with the `au` command.

`wexp` processing occurs after `wnt` processing in a single FID experiment, and both can be used. `wexp` also occurs after `wnt` during the last FID of a multi-FID experiment. Thus, `wnt='wft (\ 'all\ ') ' wexp='calcT1'` and `wexp='wft (\ 'all\ ') calcT1'` transforms each FID in a T_1 experiment as it is performed, and when each of the FIDs has been collected, performs the calculation of the T_1 using a hypothetical macro command `calcT1`. Notice the use of the backslash to include a single quotation mark inside the string.

Values: Command, macro, or null string (`wexp= ' '`, where the value is given by two single quotes with no space between them). If the command or macro uses a file name as an argument, specifying an absolute path is best. Be sure the path is valid and you have the appropriate write permission.

See also: *NMR Spectroscopy User Guide*

Related:	<code>wexp</code>	Specify action when experiment completes (C)
	<code>wnt</code>	When number of transients (P)
	<code>au</code>	Submit experiment to acquisition and process data (C)

wf

Width of FID (P)

Description: Width of the FID display. This parameter can be entered in the usual way or interactively controlled by selecting the `sf wf` button during a FID display.

Values: 0 to the value of `at`, in seconds.

See also: *NMR Spectroscopy User Guide*

Related:	<code>at</code>	Acquisition time (P)
	<code>dcon</code>	Display noninteractive color intensities map (C)
	<code>dconi</code>	Interactive 2D data display (C)
	<code>df</code>	Display a single FID (C)
	<code>sf</code>	Start of FID (P)
	<code>vf</code>	Vertical scale of FID (P)
	<code>wf1</code>	Width of interferogram in 1st indirectly detected dimension (P)
	<code>wf2</code>	Width of interferogram in 2nd indirectly detected dimension (P)

- wf1** **Width of interferogram in 1st indirectly detected dimension (P)**
- Description: Sets the width of the interferogram display in the first indirectly detected dimension.
- Values: 0 to $(2 \times \text{ni})/\text{sw1}$, in seconds.
- See also: *NMR Spectroscopy User Guide*
- Related: **ni** Number of increments in 1st indirectly detected dimension (P)
sf1 Start of interferogram in 1st indirectly detected dimension (P)
sw1 Spectral width in 1st indirectly detected dimension (P)
wf Width of FID (P)
- wf2** **Width of interferogram in 2nd indirectly detected dimension (P)**
- Description: Sets the width of the interferogram display in the second indirectly detected dimension.
- Values: 0 to $(2 \times \text{ni2})/\text{sw2}$, in seconds.
- See also: *NMR Spectroscopy User Guide*
- Related: **ni2** Number of increments in 2nd indirectly detected dimension (P)
sf2 Start of interferogram in 2nd indirectly detected dimension (P)
sw2 Spectral width in 2nd indirectly detected dimension (P)
wf Width of FID (P)
- wfgtest** **Waveform generator test (M)**
- Applicability: Systems with a waveform generator.
- Description: Retrieves a parameter set and pulse sequence, and compiles the sequence, in order to set up an experiment to test the waveform generators.
- See also: *Waveform Generator Kit Installation*
- wft** **Weight and Fourier transform 1D data (C)**
- Syntax: (1) `wft(<options>,<<'nf'><,start><,finish><,step>)>`
(2) `wft('inverse',exp_number,expansion_factor)`
- Description: Performs a Fourier transform on one or more 1D FIDs with weighting applied to the FID. The command executes a left-shift, zero-order phase rotation, and a frequency shift according to the parameters **lsfid**, **phfid**, and **lsfrq**, respectively, on the time-domain data prior to the weighting and Fourier transformation. The type of Fourier transformation to be performed is determined by **proc**. **wft** uses the same arguments as the command **ft**, and except for weighting, it functions the same as the **ft** command.
- See also: *NMR Spectroscopy User Guide*
- Related: **ft** Fourier transform 1D data (C)
lsfid Number of points to left-shift np FID (P)
lsfrq Frequency shift of the fn spectrum in Hz (P)
phfid Zero-order phasing constant for np FID (P)
proc Type of processing on np FID (P)
- wft1d** **Weight and Fourier transform f₂ for 2D data (C)**
- Syntax: (1) `wft1d(element_number)`
(2) `wft1d(<options>,<coefficients>)>`

Description: Performs the first Fourier transformation along the dimension defined by **sw**, with weighting and matrix transposition. This allows the display of t_1 interferograms with the **dcon** and **dconi** commands.

Except for weighting, **wft1d** functions the same as the **ft1d** command. See the description of **ft1d** for further information.

Arguments: Same as the arguments to **ft1d**. See the **ft1d** command for details.

See also: *NMR Spectroscopy User Guide*

Related:

dcon	Display noninteractive color intensity map (C)
dconi	Interactive 2D data display (C)
ft1d	Fourier transform along f_2 dimension (C)
sw	Spectral width in directly detected dimension (P)

wft1da **Weight and Fourier transform phase-sensitive data (M)**

Values: **wft1da**<(options)>

Description: Processes 2D FID data as well as 2D planes at particular t_1 or t_2 times from a 3D data set for a pure absorptive display.

wft1da differs from **ft1da** only in that weighting of the time-domain data is performed prior to the Fourier transform. See the description of **ft1da** for further information.

Arguments: Same as arguments to **ft2da**. See the **ft2da** command for details.

See also: *NMR Spectroscopy User Guide*

Related:

ft1da	Fourier transform phase-sensitive data (M)
ft2da	Fourier transform phase-sensitive data (M)
wft2da	Weight and Fourier transform phase-sensitive data (M)

wft1dac **Combine arrayed 2D FID matrices (M)**

Syntax: **wft1dac**<(<mult1>,<mult2> , ...<multn>)>

Description: Allows the ready combination of 2D FID matrices within the framework of the 2D Fourier transform program. Weighting is performed. This command requires that the data be acquired either without f_1 quadrature or with f_1 quadrature using the TPPI method. **wft1dac** is used with TOCSY (with multiple mixing times).

Arguments: **mult1**, **mult2**, ..., **multn** are multiplicative coefficients. The n th argument is a real number and specifies the multiplicative coefficient for the n th 2D FID matrix.

See also: *NMR Spectroscopy User Guide*

Related:

ft1dac	Combine arrayed 2D FID matrices (M)
Tocsy	Set up parameters for TOCSY pulse sequence (M)
wft2dac	Combine arrayed 2D FID matrices (M)

wft2d **Weight and Fourier transform 2D data (C)**

Syntax: **wft2d**<(<options>,>coefficients)>

Description: Performs a complete 2D transformation with weighting after 2D data has been acquired. If the first Fourier transformation has already been done using **ft1d**, **wft1d**, **ft1da**, or **wft1da**, then the **wft2d** command performs only the second transform.

For arrayed 2D experiments, a single array element can be transformed and weighted using the array element number as an argument. Interferograms can

be constructed explicitly using the following coefficient table:

```
wft2d(rr1,ir1,rr2,ir2,...,ri1,ii1,ri2,ii2,...).
```

`wft2d('ptype',...)` transforms P-type spectra, and

`wft2d('ntype',...)` transforms N-type spectra. The default is N-type.

`wft2d` also *completes* a 2D transform that has been started with `wft1d` (or related commands such as `wft1da`). The first transform will not be done again if it has already been performed. For phase-sensitive 2D experiments, the coefficients must be applied as part of the first transform (e.g., with `wft1da`) since the interferograms are formed at that stage. These coefficients need not be repeated when invoking the subsequent transform: a simple `wft2d` or `ft2d` can suffice.

See the `ft2d` command description for further information.

Arguments: Same as the arguments to `ft2d`. See the `ft2d` command for details.

Examples: `wft2d(1,0,0,0)`

```
wft2d(2)
```

```
wft2d(1,0,1,0,0,1,0,1)
```

```
wft2d(.67,0,.33,0,0,.67,0,.33)
```

See also: *NMR Spectroscopy User Guide*

Related:	<code>dconi</code>	Interactive 2D data display (C)
	<code>ft1d</code>	Fourier transform along f_2 dimension (C)
	<code>ft1da</code>	Fourier transform “halfway” for pure absorption 2D data (M)
	<code>ft2d</code>	Fourier transform 2D data (C)
	<code>wft1d</code>	Weight and Fourier transform f_2 for 2D data (C)
	<code>wft1da</code>	Weight and FT “halfway” for pure absorption 2D data (M)
	<code>wft2da</code>	Weight and transform for pure absorption 2D data (M)

wft2da Weight and Fourier transform phase-sensitive data (M)

Syntax: `wft2da<(options)>`

Description: Processes 2D FID data, as well as 2D planes at particular t_1 or t_2 times, from a 3D data set for a pure absorptive display.

`wft2da` differs from `ft2da` only in that weighting of the time-domain data is performed prior to the Fourier transform. See the description of `ft2da` for further information.

Arguments: Same as used with `ft2da`. See the `ft2da` command for details.

See also: *NMR Spectroscopy User Guide*

Related:	<code>ft1da</code>	Fourier transform phase-sensitive data (M)
	<code>ft2da</code>	Fourier transform phase-sensitive data (M)
	<code>wft1da</code>	Weight and Fourier transform phase-sensitive data (M)

wft2dac Combine arrayed 2D FID matrices (M)

Syntax: `wft2dac(<mult1><,mult2>,...<,multn>)>`

Description: Allows the ready combination of 2D FID matrices within the framework of the 2D Fourier transform program. Weighting is performed. This command requires that the data be acquired either without f_1 quadrature or with f_1 quadrature using the TPPI method. `wft2dac` is used with TOCSY (with multiple mixing times).

Arguments: `mult1`, `mult2`, ..., `multn` are multiplicative coefficients. The n th argument is a real number and specifies the multiplicative coefficient for the n th 2D FID matrix.

See also: *NMR Spectroscopy User Guide*

Related:	<code>ft1dac</code>	Combine arrayed 2D FID matrices (M)
	<code>ft2dac</code>	Combine arrayed 2D FID matrices (M)
	<code>Tocsy</code>	Set up parameters for TOCSY pulse sequence (M)
	<code>wft1dac</code>	Combine arrayed 2D FID matrices (M)

wftt3 **Process f_3 dimension during 3D acquisition (M)**

Description: Allows f_3 processing of 3D data to be performed concurrently with data acquisition. To invoke this function, set `wnt='wftt3'` and use `au` to start the acquisition of the 3D data. When `wftt3` detects that all the FIDs comprising a (t_1, t_2) block have been acquired, it starts up the `ft3d` program in background to process that block of FIDs in f_3 .

The 3D processing information file, created by entering `set3dproc` within VnmrJ, does not need to contain valid f_1 and f_2 processing information but only valid f_3 processing information. Once the f_3 processing is complete, a new 3D information file can be created for the f_1 - f_2 processing stages that contains valid f_1 and f_2 processing information.

The non-standard string parameter `path3d` can be used to specify the directory into which the f_3 processed 3D data is to be stored. Normally, `path3d` is absent in the parameter set. If this is the case or if `path3d=''`, the f_3 -processed 3D data is stored in the directory `curexp/datadir`. `path3d` can be created by entering `create('path3d','string')` or `setgroup('path3d','display')`.

See also: *NMR Spectroscopy User Guide*

Related:	<code>au</code>	Submit experiment to acquisition and process data (C)
	<code>create</code>	Create new parameter in a parameter tree (C)
	<code>ft3d</code>	Perform a 3D Fourier transform (M,U)
	<code>getplane</code>	Extract planes from a 3D spectral data set (M)
	<code>path3d</code>	Path to currently displayed 2D planes from a 3D data set (P)
	<code>select</code>	Select a spectrum or 2D plane without displaying it (C)
	<code>set3dproc</code>	Set 3D processing (C)
	<code>setgroup</code>	Set group of a parameter in a tree (C)
	<code>wnt</code>	When number of transients (P)

which **Display which command or macro is used (M)**

Syntax: `which(name)`

Description: Searches VnmrJ libraries and then displays on line 3 which VnmrJ command or macro with the given name will be executed. For macros, `which` displays the type of macro (user, local, application, or Varian) and the path to the library.

Arguments: `name` is the name of a command or macro.

Examples: `which('wft')`

See also: *User Programming*

Related:	<code>exists</code>	Determine if a parameter, file, or macro exists (C)
	<code>hidecommand</code>	Execute macro instead of command with same name (M)

wnt **Specify action when nt transients accumulate (C)**

Syntax: `wnt(string)`

Description: Specifies what action to take when `nt` transients accumulate. The `wnt` command sets the corresponding parameter `wnt`. Using the command, rather than setting the parameter value explicitly, notifies the acquisition process that

the associated parameter value has changed. Thus, the desired operation can be effected even if the experiment has already started.

Arguments: `string` is a string argument containing the command or macro to be executed when this event happens. The string must be enclosed in single quotes. If single quotes are required within the text string, place a backslash character before each of the interior single quotes (`\ '`). Maximum length of the string is 256 characters. To turn off `wnt` processing, enter `wnt ( ' ' )`, where the argument is two single quotes with no space between them.

Examples: `wnt ( 'wft (\ 'all\ ' ) ' )`
`wnt ( ' ' )`

See also: *NMR Spectroscopy User Guide*

Related:	<code>nt</code>	Number of transients (P)
	<code>wbs</code>	Specify action when <code>bs</code> transients accumulate (C)
	<code>werr</code>	Specify action when error occurs (C)
	<code>wexp</code>	When experiment completes (P)
	<code>wnt</code>	When number of transients (P)

wnt **When number of transients (P)**

Description: Invokes a single action to occur automatically after the FID is finished (`ct=nt`) or after each FID in a multi-FID experiment involving an arrayed parameter. The most common processing to occur after an FID is an automatic weighting and Fourier transformation (i.e., `wnt= 'wft '`); however, this is normally not needed because the command `ga` is the exact equivalent of `wnt= 'wft (\ 'acq\ ' ) ' au` (i.e., `ga` sets the `wnt` action automatically). To specify no `wnt` processing, set `wnt` to the null string. If the acquisition has already been started, the `wnt command` must be used to change this parameter.

Values: Command, macro, or null string (`wnt= ' '` , where the value is given by two single quotes with no space between them).

See also: *NMR Spectroscopy User Guide*

Related:	<code>nt</code>	Number of transients (P)
	<code>wnt</code>	Specify action when <code>nt</code> transients accumulate (C)

wp **Width of plot in directly detected dimension (P)**

Description: Sets the width of the displayed or plotted region of the spectrum.

Values: Always stored in Hz, but can be entered in ppm by using the `p` suffix (e.g., `wp=6p` sets the width of plot to 6 ppm).

See also: *NMR Spectroscopy User Guide*

Related:	<code>wp1</code>	Width of plot in 1st indirectly detected dimension (P)
	<code>wp2</code>	Width of plot in 2nd indirectly detected dimension (P)

wp1 **Width of plot in 1st indirectly detected dimension (P)**

Description: Analogous to the `wp` parameter except that `wp1` applies to the first indirectly detected dimension of a multidimensional data set.

See also: *NMR Spectroscopy User Guide*

Related:	<code>wp</code>	Width of plot in directly detected dimension (P)
	<code>wp2</code>	Width of plot in 2nd indirectly detected dimension (P)

W

wp2	Width of plot in 2nd indirectly detected dimension (P)
Description:	Analogous to the wp parameter except that wp2 applies to the second indirectly detected dimension of a multidimensional data set.
See also:	<i>NMR Spectroscopy User Guide</i>
Related:	wp Width of plot in directly detected dimension (P) wp1 Width of plot in 1st indirectly detected dimension (P)

write	Write formatted text to a device (C)
Syntax:	<pre>(1) write('keywords'><,color pen> <,'reverse'>,x,y<,template>) <:height> (2) write('alpha' 'printer' 'line3' 'error',template) (3) write('reset' 'file' 'fileline',file<,template>) (4) write('net',host,port, template) `</pre>
Description:	Writes text to a graphics screen or plotter in a given format (syntax 1), writes formatted text to another device (syntax 2), clears a file (syntax 3), or writes to a file (syntax 3). The input to the command comes from arguments in template , which can be parameters such as n1 or pw .
Arguments:	'keywords' identify the output device ('graphics' 'plotter') and the drawing mode ('xor' 'normal' 'newovly' 'ovly' 'ovlyC'). 'graphics' 'plotter' is a keyword selecting the output device. The default is 'plotter'. The output selected is passed to subsequent pen, move, or draw commands and remains active until a different mode is specified. 'xor', 'normal' is a keyword for the drawing mode when using the 'graphics' output device. The default is 'normal'. In the 'xor' mode, if a line is drawn such that one or more points of the line are in common with a previous 'xor' line, the common points are erased. In the normal mode, the common points remain. The mode selected is passed to subsequent pen, move, and draw commands and remains active until a different mode is specified. 'newovly', 'ovly', and 'ovlyC' are keywords that specify an interactive drawing capability that is slightly slower than the 'xor' mode but more consistent in color. 'newovly' clears any previous draws, boxes, and writes made with the 'ovly' modes and draws the figure. 'ovly' draws without clearing so that multi-segment figures can be created. 'ovlyC' clears without drawing. color is the color of the text on a color display: 'red', 'yellow', 'green', 'cyan', 'blue', 'magenta', and 'white'. The default is 'yellow'. pen is the plotter pen: 'pen1', 'pen2', etc. 'reverse' is a keyword specifying a sideways orientation of the output. x and y are coordinates on the screen or plotter, in mm. template is a string of formatting characters along with arguments to those characters. The format is the same as used with the UNIX printf command (for details, see any basic UNIX manual or enter man printf in UNIX). For example, 'pw = %12.5f' is a template to format the parameter pw as fixed point with a field width of 12 spaces and 5 decimal places. The following format characters are implemented:

character	%c
integer	%d
hexadecimal	%h
exponential:	%e
fixed point	%f
exponential/fixed point	%g
octal	%o
string	%s
write a % character	use <code>write(...'%s','%')</code>

`height` returns the height of the characters on the screen or plotter. This is useful for positioning multiple-line displays. See the source code of the macro `dttext` in the `maclib` directory for an example of usage.

'alpha' is a keyword to write text to the alphanumeric screen.

'printer' is a keyword to print text on the printer

'line3' is a keyword to write text as a message on line 3.

'error' is a keyword to write text as an error on line 3 and sound a beep.

'reset' is a keyword to clear the file specified.

'file' is a keyword to append data to the file specified. Existing data in the file is not overwritten. By writing repeated 'file' calls, a formatted data file can be created (see the fifth example below). Each `write` command automatically appends a carriage return (line feed) to the end of the string defined by the `template` argument. To append data without the automatic line feed, use the 'fileline' keyword instead of 'file'. Also, two backslashes (\\) are interpreted as a new line.

'fileline' is a keyword to append data to the file specified, the same as using the 'file' keyword, but without automatically appending a carriage return (line feed) to the end of the data. Any line feeds desired must be explicitly defined (using \n) by the `template` argument (see the sixth example below). Furthermore, two backslashes (\\) output a single backslash into the file.

`file` is the name of the file used with the 'reset', 'file', and 'fileline' keywords.

'net' is a keyword for writing to a network program. The host name and port number must be supplied. The host name may also be an IP address, such as 10.190.x.y. The hostname of the local computer is stored in the `instrument` parameter. The command `serverport` may be used to get the port number for the currently executing VnmrJ program.

Examples:

```
write('graphics',100,100):$ys
write('plotter',20,180, 'pw = %12.5f',pw)
write('line3', 'Too many arguments')
write('reset','templ')
write('file','templ','%10f %10.1f',n1,pw)
write('fileline','templ','\nEnd of data\n\n')
serverport:$port
write('net',instrument,$port,'banner(`hello`'))
```

See also: *User Programming*

Related: `dttext` Display a text file in the graphics window (M)
`serverport` Returns the value of the VnmrJ network listening port (C)

writefid Write numeric text file using a FID element (C)

Syntax: `writefid(file<,element_number>)`

Description: Writes a text file using data from the selected FID element. The program writes two values per line—the first is the value from the X (or real) channel and the second is the value from the Y (or imaginary) channel. `writefid` writes the raw FID data (i.e., FID data processing based on the parameters `phfid`, `lsfid`, and `lsfrq` does not occur).

Arguments: `file` is the name of a text file to store the data.
`element_number` is an integer larger than 0 for the number of a FID element. The default is 1.

See also: *NMR Spectroscopy User Guide, User Programming*

Related:	<code>lsfid</code>	Number of complex points to left-shift <code>np</code> FID (P)
	<code>lsfrq</code>	Frequency shift of <code>fn</code> spectrum in Hz (P)
	<code>makefid</code>	Make a FID element using numeric text input (C)
	<code>phfid</code>	Zero-order phasing constant for <code>np</code> FID (P)
	<code>writespectrum</code>	Write a spectrum to a binary file (C)

writeparam Write one of more parameters to a file (C)

Syntax: `writeparam(file,parlist[,tree] ['add' | 'replace'])`

Description: The `writeparam` command will write one or more parameters to a specified file. The first argument is the name of the file. The second argument is a list of the names of the parameters to be written. It is a string parameter and the names can be separated either by a space or a comma. The optional third argument is the tree from which the parameters are copied.

The variable trees are 'current', 'global', 'processed' and 'systemglobal'.

An optional final argument is the keyword 'add' or 'replace'. The add keyword will cause the parameters to be appended to the specified file.

If they already exists in the file, their values will be updated. The replace keyword will replace the values in the file with the current values from the tree. The parameters must exist in both the file and the tree

A special case for the replace option occurs when the parameter list is an empty string. In this case, all the parameters in the file will be updated with the current values in the tree. If the parameter does not exist in the tree, no change will be made for that parameter.

This command may be used to store temporary values. For example, you may want to save `wexp`, `wbs`, `wnt`, etc. in order to run a setup acquisition. When it is done, you want to reset the original values. The `fread` command can be used to read the parameters back into an appropriate parameter tree.

Examples: `writeparam(curexp+'/mypar','in')`
 writes the parameter `in` into the file `mypar` in the current experiment directory.
`writeparam(curexp+'/mypar','sw ct np','processed')`
 writes the parameters `sw`, `ct`, and `np` from the processed tree into the file `mypar` in the current experiment directory.

writespectrum write a spectrum to a binary file (C)

Description: Writes out the current spectrum as a binary file. The file has no header information and is written in the native format (little-endian on Linux; big-endian on Solaris).

writespectrum scales the data by `vs`, determines the mode selected, `ph`, `av`, or `pwr`, and writes whatever is displayed by `ds`. The file is written in the current experiment as `specN`, where `N` is the element number.

Examples: Write files `spec1`, `spec2`, `spec3` ... `spec{arraydim}` in the current experiment directory:

```
wft $i=0 while ($i < arraydim) do $i = $i + 1
select($i) writespectrum endwhile
```

Write the real and imaginary components if phase mode is selected.

```
wft
ph
$i=0
$index=''
while ($i < arraydim) do
    $i = $i + 1
    format($i,0,0):$index
    select($i)
    writespectrum
    mv(curexp+' /spec'+$index, curexp+' /
    spec'+$index+'.re')
    rp = rp + 90
    writespectrum
    mv(curexp+' /spec'+$index, curexp+' /
    spec'+$index+'.im')
    rp = rp - 90
endwhile
```

Related: `writefid` Write numeric text file using a FID element (C)

wrtpr Command string executed after rtp command (P)

Description: Holds the command string that is executed after an `rtp` command finishes. It is mostly used to set frequency-dependent parameter values, such as `sw`, so that one parameter set can be used on all spectrometers.

Examples: `wrtpr='setsw(13p,-2p)'`

wsram Send hardware configuration to acquisition console (C)

Syntax: `wsram<:$success>`

Description: Sends new hardware configuration information to the acquisition console when `config` is used (e.g., to set `lockfreq`). `wsram` (write to static RAM) is not normally entered directly by the user.

Arguments: `success` returns 1 if `wsram` is successful, or 0 otherwise.

See also: *VnmrJ Installation and Administration*.

Related: `config` Display current configuration and possibly change it (M)
`lockfreq` Lock frequency (P)

wshim Conditions when shimming is performed (P)

Description: Specifies when automatic shimming is to be used, according to the method specified by the parameter `method`.

Values: `'n'` sets that no automatic shimming is performed. Even with `wshim` set to this value, the shimming procedure specified by the parameter `method` can be activated by using the `shim` command.

'e' or 'exp' sets that automatic shimming is done before data acquisition.

's' or 'samp' sets that automatic shimming is done only at the beginning of the first experiment, following the change of a sample using the automatic sample changer.

'g' sets that automatic shimming using gradient shimming is done only at the beginning of the first experiment, following the change of a sample using the automatic sample changer. The parameter `method` is ignored. This option is only available in automation and is not used with the `go`, `ga`, or `au` commands.

'f' or 'fid' set automatic shimming is done prior to the data collection of each new array member in a multi-FID experiment.

'fn', where *n* is an integer, sets shimming is done prior to data collection of every *n*th FID (e.g., `wshim='f16'` shims prior to acquiring FIDs 1, 17, 33, etc.). This method is only relevant to arrayed or 2D experiments.

See also: *NMR Spectroscopy User Guide*

Related: `gf` Prepare parameters for FID/spectrum display in `acqi` (M)
`method` Autoshim method (P)

wtfile User-defined weighting in directly detected dimension (P)

Description: Set to name of the file containing the user-written weighting function along the directly detected dimension. This dimension is referred to as the f_2 dimension in 2D data sets, the f_3 dimension in 3D data sets, etc. The shellscript `wtgen` is used to compile the user-written weighting module into an executable program. The source file is stored in the directory `vnmruser+'wtlib'` with a `.c` file extension. The executable file is in the same directory and has the same name as the source file but has no file extension.

Values: `file` is the name of the executable weighting function or the name of the weighting function text file.

' ' (two single quotes with no space in between) indicates `wtfile` is inactive and VnmrJ should not look for a user-written weighting function.

See also: *NMR Spectroscopy User Guide; User Programming*

Related: `wtfile1` User-defined weighting in 1st indirectly detected dimension (P)
`wtfile2` User-defined weighting in 2nd indirectly detected dimension (P)
`wtgen` Compile user-written weighting functions (C,U)

wtfile1 User-defined weighting in 1st indirectly detected dimension (P)

Description: Set to the name of the file containing the user-written weighting function for the first indirectly detected dimension. This dimension is often referred to as the f_1 dimension of a multidimensional data set. Otherwise, `wtfile1` is analogous to `wtfile`.

See also: *NMR Spectroscopy User Guide; User Programming*

Related: `wtfile` User-defined weighting in directly detected dimension (P)
`wtfile2` User-defined weighting in 2nd indirectly detected dimension (P)

wtfile2 User-defined weighting in 2nd indirectly detected dimension (P)

Description: Set to the name of the file containing the user-written weighting function along the second indirectly detected dimension. This dimension is often referred to as the f_2 dimension of a multidimensional data set. `wtfile2` can be set with `wti` on the 2D interferogram data. Otherwise, `wtfile2` is analogous to `wtfile`.

See also: *NMR Spectroscopy User Guide; User Programming*

Related: **wtfile** User-defined weighting in directly detected dimension (P)
wtfile1 User-defined weighting in 1st indirectly detected dimension (P)
wti Interactive weighting (C)

wtgen Compile user-written weighting functions (M,U)

Syntax: (From VnmrJ) `wtgen (file<.c>)`
 (From UNIX) `wtgen file<.c>`

Description: Allows compilation of a user-written weighting function that subsequently can be executed from within VnmrJ. `wtgen` performs the following functions:

- Checks for the existence of the `/vnmr/bin` directory and aborts if the directory is not found.
- Checks for files `usrwt.o` and `weight.h` in the `/vnmr/bin` directory and aborts if either of these two files cannot be found there.
- Checks for the existence of the user's directory and creates this directory if it does not already exist.
- Establishes in the `wtlib` directory soft links to `usrwt.o` and `weight.h` in the `/vnmr/bin` directory.
- Compiles the user-written weighting function, which is stored in the `wtlib` directory, link loads it with `usrwt.o`, and places the executable program in the same directory; any compilation and/or link loading errors are placed in the file `errmsg` in `wtlib`.
- Removes the soft links to `usrwt.o` and `weight.h` in the `/vnmr/bin` directory.

The name of the executable program is the same as that for the source file without a file extension (e.g., `testwt.c` is the source file for the executable file `testwt`).

Examples: (From VnmrJ) `wtgen ('testwt')`
 (From UNIX) `wtgen testwt.c`

See also: *User Programming*

Related: **wtfile** User-defined weighting for t_2 (P)
wtfile1 User-defined weighting for t_1 (P)
wtfile2 User-defined weighting in $ni2$ dimension (P)

wti Interactive weighting (C)

Syntax: `wti<(element_number)>`

Description: Allows weighting parameters to be set interactively for both t_2 FIDs and t_1 interferograms. `wti` responds appropriately to **phfid** and **lsfid** for t_2 FIDs and to **phfid1** and **lsfid1** for t_1 interferograms. The following parameters can be interactively weighted:

- **awc**, **awc1**, and **awc2** set the additive weighting constant; added in to the weighting function after the **lb** and **sb** (or **sbs**) contributions but before the **gf** (or **gfs**) contributions.
- **gf**, **gf1**, and **gf2** set the Gaussian apodization constant, in seconds.
- **gfs**, **gfs1**, and **gfs2** set the Gaussian function shift, in seconds; shifts the origin of the Gaussian function; active only if **gf** (or **gf1**) is active.

- **lb**, **lb1**, and **lb2** set the line broadening factor, in Hz; a positive value gives sensitivity enhancement; a negative value gives resolution enhancement.
- **sb**, **sb1**, and **sb2** set the sinebell time period, in seconds; a negative value give a sine squared bell.
- **sbs**, **sbs1**, and **sbs2** set the sinebell shift, in seconds; shifts the origin of the sine bell; active only if **sb** (or **sb1**) is active.

These parameters can be typed in or changed with the left mouse button in the proper field. The right mouse button turns off the spectrum for a faster response to changes in the weighting function.

Arguments: **element_number** specifies which FID element or interferogram trace is to be used in adjusting the weighting parameters. The default is the currently active element or trace.

Examples: `wti`
`wti (3)`

See also: *NMR Spectroscopy User Guide*

Related:	lsfid	Number of complex points to left-shift np FID (P)
	lsfid1	Number of complex points to left-shift ni interferogram (P)
	phfid	Zero-order phasing constant for np FID (P)
	phfid1	Zero-order phasing constant for ni interferogram (P)
	wtia	Interactive weighting for 2D absorptive data (C)

wtia Interactive weighting for 2D absorptive data (M)

Syntax: `wtia<(element_number)>`

Description: Allows weighting parameters to be set interactively for both **t2** FIDs and **t1** interferograms in 2D absorptive data. Refer to the description of the **wti** command for further information.

Arguments: **element_number** specifies which FID element or interferogram trace is to be used in adjusting the weighting parameters. The default is the currently active trace.

See also: *NMR Spectroscopy User Guide*

Related:	lsfid	Number of complex points to left-shift np FID (P)
	lsfid1	Number of complex points to left-shift ni interferogram (P)
	phfid	Zero-order phasing constant for np FID (P)
	wti	Interactive weighting (C)

wtune Specify when to tune (P)

Applicability: Liquids, VnmrJ Walkup, Automation

Description: Specify when automatic probe tuning will happen.

Syntax: `wtune = 'value1<value2>...'`

Values: 's' – when a new sample is inserted
 'e' – before each experiment
 'o' – change of operator
 'v' – change of solvent
 't' – change of temperature
 '1' – change of high band frequency (tn or dn)
 '2' – change of low band frequency (dn or tn)

'n' – do not tune, if 'n' is included in argument list, no tuning will occur.

Examples: `wtune = 'st12'`

The system will tune when a new sample is inserted (s) or the temperature changes for the current or new sample (t) or there is a change in the high band frequency (tn or dn) (1) or there is a change of low band frequency (dn or tn) (2).

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `tunemethod` Method to use for tuning (P)
`protune` Macro to start ProTune (M)
`wtunedone` What to do after ProTune tuning is done (P)

wtunedone What to do after ProTune tuning is done (P)

Description: Specific what to do after ProTune tuning is done. This is a local string parameter that does not exist by default and must be created to specify a command to be executed after tuning is finished.

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `protune` Macro to start ProTune (M)
`create` Create new parameter in a parameter tree (C)
`wtune` Specify when to tune (P)

wysiwyg Set plot display or full display (P)

Description: Sets whether the window display is the same as the plot (“what you see is what you get,” or WYSIWYG) or is expanded to fill the window. This allows the user to scale the image to the full window, making it easier to view. This parameter is in the user’s global parameter file.

Values: 'y' makes the window picture size depend on the current plotter setting. Scaling the window does not change the ratio of the picture. This value is the default display condition.

'n' makes the window display expand, giving a full display.

See also: *NMR Spectroscopy User Guide*

X

<code>x0</code>	X-zero position of HP pen plotter or Postscript device (P)
<code>x1</code>	X1 shim gradient (P)
<code>x2y2</code>	X2Y2 shim gradient (P)
<code>x3</code>	X3 shim gradient (P)
<code>x4</code>	X4 shim gradient (P)
<code>xdiag</code>	Threshold for excluding diagonal peaks when peak picking (P)
<code>xgate</code>	Load time counter (M)
<code>xml</code>	Utility macro for study queue experiment manager (M)
<code>xmaction</code>	Perform study queue action (M)
<code>xmactionw</code>	Perform study queue action for walkup (M)
<code>xmaddreq</code>	Add a required protocol before the main protocol (M)
<code>xmcheckreq</code>	Check required protocol name (M)
<code>xmconvert</code>	Convert a temporarily stored study into a submitted study (M)
<code>xmcopy</code>	Copy protocols in a study queue (M)
<code>xmdelete</code>	Delete nodes in a study queue (M)
<code>xmenablepanel</code>	Enable or disable a parameter panel (M)
<code>xmendq</code>	End a chained study queue (M)
<code>xmgetatts</code>	Get study queue attributes (M)
<code>xmHprescan</code>	Set up and process Proton prescans (M)
<code>xminit</code>	Initialize an imaging study queue (M)
<code>xmlockup</code>	Move a study queue node up and lock it (M)
<code>xmmakenode</code>	Make a new study queue node (M)
<code>xmnext</code>	Find next prescan or next experiment in study queue (M)
<code>xmprescan</code>	Run prescans in study queue (M)
<code>xmreact</code>	Recover from error conditions during automation study (M)
<code>xmreadnode</code>	Read attributes from a study queue node (M)
<code>xmrtpar</code>	Retrieve parameters from a study queue node (M)
<code>xmsample</code>	Write enterQ entry for a sample for study queue – automation (M)
<code>xmsara</code>	Write sample enterQ entry for study queue– imaging (M)
<code>xmsatfrq</code>	Processing for Presat experiment (M)
<code>xmselect</code>	Action when study queue node is selected (M)
<code>xmsetattr</code>	Set an attribute for a study queue node (M)
<code>xmsetatts</code>	Set an attribute for a study queue node (M)
<code>xmshowdata</code>	Show data from a study queue node (M)
<code>xmstartnightq</code>	Start the night queue (M)
<code>xmsubmit</code>	Submit sample(s) to the study queue (M)
<code>xmtime</code>	Update the study queue time (M)
<code>xmtune</code>	Check tune parameter during automation (M)
<code>xmwerr</code>	Recover from acquisition error in study queue (M)
<code>xmwexp</code>	Processing macro for end of acquisition in study queue (M)
<code>xmwritenode</code>	Write study queue node attributes (M)
<code>xmwritesq</code>	Write study queue node order (M)
<code>xpol</code>	Cross-polarization (P)

xpolar1	Set up parameters for XPOLAR1 pulse sequence (M)
xy	XY shim gradient (P)
xz	XZ shim gradient (P)
xz2	XZ2 shim gradient (P)

x0 X-zero position of HP pen plotter or Postscript device (P)

Applicability: Systems with a Hewlett-Packard pen plotter or a Postscript output device.

Description: Adjusts the x-zero position on the chart. Use **hpa** to adjust **x0** (and **y0**) to place the numbers in a pleasing position when filled in on the blank lines. **x0** is part of `vnmr/sys/global` and hence common to all experiments.

Values: Number, in mm.

See also: *NMR Spectroscopy User Guide*

Related: **hpa** Plot parameters on special preprinted chart paper (C)
y0 Y-zero position of HP plotter or Postscript device (P)

x1 X1 shim gradient (P)

Description: Holds current setting of the X1 radial shim gradient.

Values: If **shimset** is 1, 2, 8, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

x2y2 X2Y2 shim gradient (P)

Description: Holds current setting of the X2Y2 radial shim gradient.

Values: If **shimset** is 1, 2, 8, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

x3 X3 shim gradient (P)

Description: Holds current setting of the X3 radial shim gradient.

Values: If **shimset** is 1, 2, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

x4 X4 shim gradient (P)

Description: Holds current setting of the X4 radial shim gradient.

Values: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

- xdiag** **Threshold for excluding diagonal peaks when peak picking (P)**
- Description: Used by the **l12d** program to exclude diagonal peaks when peak picking. To create the 2D peak picking parameters **xdiag** and **th2d** in the current experiment, enter **addpar** (' l12d ').
- Values: Peaks within **xdiag** Hz of the diagonal will not be picked by **l12d**. Setting **xdiag** to 0 . 0 will cause **l12d** to pick all peaks, including diagonal peaks.
- See also: *NMR Spectroscopy User Guide*
- Related: **addpar** Add selected parameters to the current experiment (M)
 l12d Automatic and interactive 2D peak picking (C)
 th2d Threshold for integrating peaks in 2D spectra (P)
-
- xgate** **Load time counter (M)**
- Applicability: Systems with a solids module.
- Syntax: **xgate** (counts)
- Description: Loads the (12-bit) time counter on the pulse programmer with the specified number of counts and switches the counter to the external time base (the external trigger). On each trigger, the counter counts one unit down, and the next pulse sequence event starts when the count reaches zero. Often that time count will be just 1 (1.0, as the argument must be a floating point number). If the final pulse is to be performed after a longer delay, two options are available:
- Perform a normal delay, followed by the **xgate** (1 . 0) call.
 - Calculate how many rotor cycles that delay would be (calculation is typically done based on a parameter **srate**) and then perform **xgate** with that calculated number of rotor triggers. Be aware that the only number of rotor cycles that can be counted this way is 4096, because the pulse programmer uses a 12-bit counter). At typical rotor speeds of 5 to 10 kHz, the “counted” delay is limited to 0.8 to 0.4 seconds.
- Arguments: **counts** is the number of counts to load into the time counter. The value must be a floating point number.
- Examples: **xgate** (5 . 0)
- See also: *User Guide: Solid-State NMR; VNMR Pulse Sequences*
- Related: **srate** Spinning rate for magic angle spinning (P)
-
- xm1** **Utility macro for study queue experiment manager (M)**
- Description: A utility macro for setting study queue attributes and other study queue operations. Usually called from other macros, and not from the command line.
-
- xmaction** **Perform study queue action (M)**
- Applicability: *VnmrJ Walkup*, Imaging
- Description: Perform an action on an experiment node in the study queue. Usually called from study queue actions, and not from the command line.
-
- xmactionw** **Perform study queue action for walkup (M)**
- Applicability: *VnmrJ Walkup*
- Description: Perform an action on an experiment node in the study queue. Usually called from other macros, and not from the command line.

X

- xmaddreq** **Add a required protocol before the main protocol (M)**
- Applicability: *VnmrJ Walkup, Imaging*
- Description: Add a required protocol before the main protocol, when adding a protocol to the study queue. Usually called from other macros, and not from the command line.
- See also: *VnmrJ Walkup, VnmrJ Imaging User's Guide*
- Related: [xmmakenode](#) Make a new study queue node (M)
-
- xmcheckreq** **Check required protocol name (M)**
- Applicability: *VnmrJ Walkup, Imaging*
- Description: Check if a required protocol exists in the study queue, and return the full path filename to data, if data has been acquired. Usually called from plotting macros, and not from the command line.
- See also: *VnmrJ Walkup, VnmrJ Imaging User's Guide*
- Related: [cqplot](#) Macro to perform generic 2D plot (M)
[plot2D](#) Plot 2D spectra (M)
-
- xmconvert** **Convert a temporarily stored study into a submitted study (M)**
- Applicability: *VnmrJ Walkup, Imaging*
- Description: Convert a temporarily stored study into a submitted study. Usually only called from other macros.
- See also: *VnmrJ Walkup, VnmrJ Imaging User's Guide*
- Related: [xmsubmit](#) Submit sample(s) to the study queue (M)
-
- xmcopy** **Copy protocols in a study queue (M)**
- Applicability: *VnmrJ Walkup, Imaging*
- Description: Copy protocols within a study queue. Usually only called from other macros.
- See also: *VnmrJ Walkup, VnmrJ Imaging User's Guide*
- Related: [xmaction](#) Perform study queue action (M)
[xmactionw](#) Perform study queue action for walkup (M)
-
- xmdelete** **Delete nodes in a study queue (M)**
- Applicability: *VnmrJ Walkup, Imaging*
- Description: Delete nodes within a study queue. Usually only called from other macros.
- See also: *VnmrJ Walkup, VnmrJ Imaging User's Guide*
- Related: [sqfilemenu](#) Study queue file menu commands (M)
[xmaction](#) Perform study queue action (M)
[xmactionw](#) Perform study queue action for walkup (M)
-
- xmenablepanel** **Enable or disable a parameter panel (M)**
- Description: Enable or disable a parameter panel. Usually used to disable the Acquire panel for Imaging applications. Usually called only from a panel.
-
- xmendq** **End a chained study queue (M)**
- Applicability: *VnmrJ Walkup*

Description: End a chained study queue in the Walkup interface. Usually called by other macros.

See also: *VnmrJ Walkup*

Related: [xmnext](#) Find next prescan or next experiment in study queue (M)

xmgetatts Get study queue attributes (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: Get study queue attributes.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [xmaction](#) Perform study queue action (M)

xmHprescan Set up and process Proton prescans (M)

Applicability: *VnmrJ Walkup*

Description: A macro to set up and process prescans for Proton-type experiments (Proton, Presat, or Wet1d protocols). Usually called from other macros, and not from the command line.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [Hprescan](#) Proton prescan (P))
[std1d](#) Apttype macro for Standard 1D experiments (M)

xminit Initialize an imaging study queue (M)

Applicability: Imaging

Description: Initialize an imaging study queue. Usually called from other macros, and not from the command line.

See also: *VnmrJ Imaging User's Guide*

Related: [sqfilemenu](#) Study queue file menu commands (M)

xmlockup Move a study queue node up and lock it (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: A macro to move a study queue node up above other completed nodes in the study queue, and lock it so it cannot be moved. This is usually done just prior to acquisition. Usually called from other macros, and not from the command line.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [acquire](#) Acquire data (M)

xmmakenode Make a new study queue node (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: Create a new node in the study queue. Usually only called by other macros.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [locaction](#) Locator action (M)
[xmaddreq](#) Add a required protocol before the main protocol (M)

xmnext Find next prescan or next experiment in study queue (M)

Applicability: *VnmrJ Walkup*

Description: Find the next prescan or next experiment in a study queue. It is used for chaining prescans and experiments. Usually only called by other macros.

See also: *VnmrJ Walkup*

Related:

<code>acquire</code>	Acquire data (M)
<code>startq</code>	Start a chained study queue (M)
<code>xmprescan</code>	Run prescans in study queue (M)
<code>xmwexp</code>	Processing macro for end of acquisition in study queue (M)

xmprescan Run prescans in study queue (M)

Applicability: *VnmrJ Walkup*

Description: Run prescans in a study queue. Usually only called by other macros.

See also: *VnmrJ Walkup*

Related:

<code>cqfindz0</code>	Run an experiment to find the value of z0 (M)
<code>gmapshim</code>	Start gradient autoshimming (M)
<code>prescan</code>	Study queue prescan (P)
<code>xmnext</code>	Find next prescan or next experiment in study queue (M)

xmreact Recover from error conditions during automation study (M)

Applicability: *VnmrJ Walkup*

Description: A macro to recover from error conditions during a study queue automated acquisition. Usually only called by other macros.

See also: *VnmrJ Walkup*

Related:

<code>acquire</code>	Acquire data (M)
<code>react</code>	Recover from error conditions during werr processing (M)

xmreadnode Read attributes from a study queue node (M)

Applicability: *VnmrJ Walkup, Imaging*

Description: Read attributes from a study queue node. Usually only called by other macros

See also: *VnmrJ Walkup, VnmrJ Imaging User's Guide.*

Related:

<code>xmaction</code>	Perform study queue action (M)
<code>xmactionw</code>	Perform study queue action for walkup (M)
<code>react</code>	Recover from error conditions during werr processing (M)

xmrtpar Retrieve parameters from a study queue node (M)

Applicability: *Imaging*

Description: Retrieve parameters from a study queue node after its parameters have been customized. Usually only called by other macros.

See also: *VnmrJ Imaging User's Guide*

Related:

<code>xmmakenode</code>	Make a new study queue node (M)
<code>xmselect</code>	Action when study queue node is selected (M)

xmsample Write enterQ entry for a sample for study queue – liquids (M)

Applicability: *VnmrJ Walkup, systems with automation such as sample changer or LC-NMR.*

Description: Write the information required for a sample in the study queue when the sample is submitted. Usually only called by other macros.

See also: *VnmrJ Walkup*

Related: [loc](#) Location of sample in tray (P)
[xmsubmit](#) Submit sample(s) to the study queue (M)

xmsara Write enterQ entry for a sample for study queue – imaging (M)

Applicability: Imaging

Description: Halt or resume acquisition in the study queue, especially when using multiple viewports. Usually only called from interface panels.

xmsatfrq Processing for Presat experiment (M)

Applicability: *VnmrJ Walkup*

Description: A macro to handle processing steps for the Presat experiment. It is optimized for use with water. Usually only called from other macros.

See also: *VnmrJ Walkup*

Related: [xmHprescan](#) Set up and process Proton prescans (M)

xmselect Action when study queue node is selected (M)

Applicability: *VnmrJ Walkup*

Description: A macro to specify the action taken when a study queue node is selected by double-clicking on it. The action depends on the node status, which is Ready for acquisition, Executing, Completed, etc. The macro also runs the macros associated with selecting a study queue node, and saves the parameters of the current node before retrieving parameters of the selected node.

See also: *VnmrJ Walkup*

Related: [xmaction](#) Perform study queue action (M)
[xmactionw](#) Perform study queue action for walkup (M)
[xmrtpar](#) Retrieve parameters from a study queue node (M)

xmsetatts Set an attribute for a study queue node (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: Set an attribute for a study queue node.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [xmaction](#) Load colors for graphics window and plotters (M)
[xmactionw](#) Location of sample in tray (P)

xmsetattr Set an attribute for a study queue node (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: Set an attribute for a study queue node.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [xmaction](#) Load colors for graphics window and plotters (M)
[xmactionw](#) Location of sample in tray (P)

xmshowdata Show data from a study queue node (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: A macro that retrieves data from a completed study queue node. In the Walkup liquids interface, data is also processed if *Process data on drag-and-drop* from locator is selected in the *System settings* dialog in the Utilities menu.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: `xmselect` Action when study queue node is selected (M)

xmstartnightq Start the night queue (M)

Applicability: *VnmrJ Walkup*

Description: Start the night queue. It also is used to initialize the night queue settings in the Utilities menu.

Examples: `xmstartnightq` start the night queue
`xmstartnightq('at')` initialize the night queue settings.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: `walkup` Walkup automation (M)

xmsubmit Submit sample(s) to the study queue (M)

Applicability: *VnmrJ Walkup*, systems with automation such as sample changer or LC-NMR.

Description: Submit the sample or samples selected in the study queue tray. If the Submit DayQ button below the study queue area is selected, samples are submitted to the DayQ. If the Submit NightQ button is selected, samples are submitted to the NightQ.

See also: *VnmrJ Walkup*

Related: `xmsample` Write enterQ entry for a sample for study queue – automation (M)

xmtime Update the study queue time (M)

Applicability: *VnmrJ Walkup*, systems with automation such as sample changer or LC-NMR.

Description: Update the study queue time for both DayQ and NightQ. Usually only called from panels or other macros.

See also: *VnmrJ Walkup*

Related: `sqfilemenu` Study queue file menu commands (M)
`startq` Start a chained study queue (M)
`studytime` Study time (P)
`xmsubmit` Submit sample(s) to the study queue (M)

xmtune Check tune parameter during automation (M)

Applicability: Automation

Syntax: `xmtune`

Description: Check tune parameters in the study queue during automation and determine if tuning will occur. Macro is usually called from within automation and not from the command line.

See also: *NMR Spectroscopy User Guide* and *VnmrJ Walkup*

Related: `protune` Macro to start ProTune (M)
`tunemethod` Method to use for tuning (P)
`wtune` Specify when to tune (P)

xmwerr Recover from acquisition error in study queue (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: Recover from an acquisition error in a study queue when not running automation. Usually only called from other macros.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [acquire](#) Acquire data (M)
[xmreact](#) Recover from error conditions during automation study (M)

xmwexp Processing macro for end of acquisition in study queue (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: A processing macro; runs at the end of acquisition in the study queue and keeps track of study queue parameters and settings. Usually only called from other macros.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [acquire](#) Acquire data (M)
[xmreact](#) Recover from error conditions during automation study (M)

xmwritenode Write study queue node attributes (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: Write study queue node attributes. Usually only called from other macros.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [xmaction](#) Load colors for graphics window and plotters (M)
[xmactionw](#) Location of sample in tray (P)
[xmsetattr](#) Set an attribute for a study queue node (M)

xmwritesq Write study queue node order (M)

Applicability: *VnmrJ Walkup*, Imaging

Description: Write the study queue node order. Usually only called from other macros.

See also: *VnmrJ Walkup*, *VnmrJ Imaging User's Guide*

Related: [xmaction](#) Load colors for graphics window and plotters (M)
[xmactionw](#) Location of sample in tray (P)

xpol Cross-polarization (P)

Applicability: Systems with a solids module.

Description: Selects cross-polarization or direct polarization in solid-state NMR experiments such as XPOLAR1.

Values: 'n' sets the experiment for direct polarization.
'y' sets the experiment for cross-polarization.

See also: *User Guide: Solid-State NMR*

Related: [xpolar1](#) Set up parameters for XPOLAR1 pulse sequence (M)

xpolar1 Set up parameters for XPOLAR1 pulse sequence (M)

Applicability: Systems with solids modules.

X

Description: Sets up the solid-state NMR cross-polarization experiment XPOLAR using the parameters. Otherwise, `xpolar1` contains the same functionality as `xpolar`.

See also: *User Guide: Solid-State NMR*

Related: `hsrotor` Display rotor speed for solids operation (P)
`rotorsync` Rotor synchronization (P)

xy XY shim gradient (P)

Description: Holds current setting of the XY radial shim gradient.

Values: If `shimset` is 1, 2, 8, 10: -2048 to +2047, steps of 1, 0 is no current.
If `shimset` is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: `shimset` Type of shim set (P)

xz XZ shim gradient (P)

Description: Holds current setting of the XZ radial shim gradient.

Values: If `shimset` is 1, 2, 8, 10: -2048 to +2047, steps of 1, 0 is no current.
If `shimset` is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: `shimset` Type of shim set (P)

xz2 XZ2 shim gradient (P)

Description: Holds current setting of XZ2 radial shim gradient.

Values: If `shimset` is 2, 8: -2048 to +2047, steps of 1, 0 is no current.
If `shimset` is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: `shimset` Type of shim set (P)

Y

y0	Y-zero position of HP pen plotter or Postscript device (P)
y1	Y1 shim gradient (P)
y3	Y3 shim gradient (P)
y4	Y4 shim gradient (P)
yz	YZ shim gradient (P)
yz2	YZ2 shim gradient (P)

y0 Y-zero position of HP pen plotter or Postscript device (P)

Applicability: Systems with a Hewlett-Packard pen plotter or a Postscript output device.

Description: Adjusts the y-zero position on the chart. Use **hpa** to adjust y0 (and **x0**) to place numbers in a pleasing position when filled in on the blank lines. y0 is part of `vnmr/sys/global`; therefore, it is common to all experiments.

Values: Number, in mm.

See also: *NMR Spectroscopy User Guide*

Related: **hpa** Plot parameters on special preprinted chart paper (C)
x0 X-zero position of HP plotter or Postscript device (P)

y1 Y1 shim gradient (P)

Description: Holds current setting of the Y1 radial shim gradient.

Values: If **shimset** is 1, 2, 8, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

y3 Y3 shim gradient (P)

Description: Holds current setting of the Y3 radial shim gradient.

Values: If **shimset** is 1, 2, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

y4 Y4 shim gradient (P)

Description: Holds current setting of the Y4 radial shim gradient.

Values: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

yz YZ shim gradient (P)

Description: Holds current setting of the YZ radial shim gradient.

Y

Values: If **shimset** is 1, 2, 8, 10: –2048 to +2047, steps of 1, 0 is no current.
If **shimset** is 3 to 7, 9: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

yz2

YZ2 shim gradient (P)

Description: Holds current setting of the YZ2 radial shim gradient.

Values: If **shimset** is 2, 8: –2048 to +2047, steps of 1, 0 is no current.
If **shimset** is 3 to 7, 9: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

Z

z	Add integral reset point at cursor position (C)
z0	Z0 field position (P)
z1	Z1 shim gradient (P)
z1c	Z1C shim gradient (P)
z2	Z2 shim gradient (P)
z2c	Z2C shim gradient (P)
z2x2y2	Z2X2Y2 shim gradient (P)
z2x3	Z2X3 shim gradient (P)
z2xy	Z2XY shim gradient (P)
z2y3	Z2Y3 shim gradient (P)
z3	Z3 shim gradient (P)
z3c	Z3C shim gradient (P)
z3x	Z3X shim gradient (P)
z3x2y2	Z3X2Y2 shim gradient (P)
z3x3	Z3X3 shim gradient (P)
z3xy	Z3XY shim gradient (P)
z3y	Z3Y shim gradient (P)
z3y3	Z3Y3 shim gradient (P)
z4	Z4 shim gradient (P)
z4c	Z4C shim gradient (P)
z4x	Z4X shim gradient (P)
z4x2y2	Z4X2Y2 shim gradient (P)
z4xy	Z4XY shim gradient (P)
z4y	Z4Y shim gradient (P)
z5	Z5 shim gradient (P)
z5x	Z5X shim gradient (P)
z5y	Z5Y shim gradient (P)
z6	Z6 shim gradient (P)
z7	Z7 shim gradient (P)
z8	Z8 shim gradient (P)
zeroneg	Set all negative intensities of 2D spectra to zero (C)
zoom	Adjust display to given width (M)
zx2y2	ZX2Y2 shim gradient (P)
zx3	ZX3 shim gradient (P)
zxy	ZXY shim gradient (P)
zy3	ZY3 shim gradient (P)

z Add integral reset point at cursor position (C)

Syntax: `z<(reset1,reset2,...)>`

Description: Resets the integral to zero at the point marked by the displayed cursor. The command **cz** removes all such integral resets and it should generally be used

before starting to enter a series of integral zeros (resets). The resets are stored as frequencies and do not change if **fn** is changed.

Arguments: **reset1**, **reset2**, ... are reset points entered, in either Hz or ppm. The default is the cursor position). Reset points can be entered in any order.

Examples: **z**
z (7.5*sfrq, 5*sfrq, 2.5*sfrq, 0.1*sfrq)

See also: *NMR Spectroscopy User Guide*

Related: **cz** Clear integral reset points (C)
dlni Display list of normalized integrals (C)
ds Display a spectrum (C)
fn Fourier number in directly detected dimension (P)
nli Find integral values (C)

z0 Z0 field position (P)

Description: Holds current setting of the Z0 setting. The value of **z0** can be set by **su**. **lockfreq** can be used to find the lock signal or resonance. To use the lock frequency, deactivate **z0** by typing the statement **z0='n'**. To activate **z0**, enter **z0='y'**.

Values: If **shimset** is 1, 2, 8, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **lockfreq** Lock frequency (P)
su Submit a setup experiment to acquisition (M)

z1 Z1 shim gradient (P)

Description: Holds current setting of the Z1 axial shim gradient.

Values: If **shimset** is 1, 2, 8, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

z1c Z1C shim gradient (P)

Description: Holds current setting of the Z1C axial shim gradient.

Values: If **shimset** is 1, 2, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 5 or 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

z2 Z2 shim gradient (P)

Description: Holds current setting of the Z2 axial shim gradient.

Values: If **shimset** is 1, 2, 8, 10: -2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

z2c Z2C shim gradient (P)

Description: Holds current setting of the Z2C axial shim gradient.

Values: If **shimset** is 1, 2, 10: –2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 5 or 9: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

z2x2y2 Z2X2Y2 shim gradient (P)

Description: Holds current setting of the Z2X2Y2 radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z2x3 Z2X3 shim gradient (P)

Description: Holds current setting of the Z2X3 radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z2xy Z2XY shim gradient (P)

Description: Holds current setting of the Z2XY radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z2y3 Z2Y3 shim gradient (P)

Description: Holds current setting of the Z2Y3 radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z3 Z3 shim gradient (P)

Description: Holds current setting of the Z3 axial shim gradient.

Values: If **shimset** is 1, 2, 8, 10: –2048 to +2047, steps of 1, 0 is no current.
 If **shimset** is 3 to 7, 9: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

z3c Z3C shim gradient (P)

Description: Holds current setting of the Z3C radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z3x Z3X shim gradient (P)

Description: Holds current setting of the Z3X radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

Z

See also: *NMR Spectroscopy User Guide*

z3x2y2 Z3X2Y2 shim gradient (P)

Description: Holds current setting of the Z3X2Y2 radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z3x3 Z3X3 shim gradient (P)

Description: Holds current setting of the Z2X3 radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z3xy Z3XY shim gradient (P)

Description: Holds current setting of the Z3XY radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z3y Z3Y shim gradient (P)

Description: Holds current setting of the Z3Y radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z3y3 Z3Y3 shim gradient (P)

Description: Holds current setting of the Z3Y3 radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z4 Z4 shim gradient (P)

Description: Holds current setting of the Z4 shim gradient.

Values: If **shimset** is 1, 2, 8, 10: –2048 to +2047, steps of 1, 0 is no current.
If **shimset** is 3 to 7, 9: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

z4c Z4C shim gradient (P)

Description: Holds current setting of the Z4C shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z4x Z4X shim gradient (P)

Description: Holds current setting of the Z4X shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z4x2y2 Z4X2Y2 shim gradient (P)

Description: Holds current setting of the Z4X2Y2 radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z4xy Z4XY shim gradient (P)

Description: Holds current setting of the Z4XY radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z4y Z4Y shim gradient (P)

Description: Holds current setting of the Z4Y shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z5 Z5 shim gradient (P)

Description: Holds current setting of the Z5 axial shim gradient.

Values: If **shimset** is 2, 10: –2048 to +2047, steps of 1, 0 is no current.
If **shimset** is 3 to 7, 9: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

z5x Z5X shim gradient (P)

Description: Holds current setting of the Z5X radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z5y Z5Y shim gradient (P)

Description: Holds current setting of the Z5Y radial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z6 Z6 shim gradient (P)

Description: Holds current setting of the Z6 axial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

z7 Z7 shim gradient (P)

Description: Holds current setting of the Z7 axial shim gradient.

Values: –32768 to +32767, steps of 1, 0 is no current.

Z

See also: *NMR Spectroscopy User Guide*

z8 **Z8 shim gradient (P)**

Description: Holds current setting of the Z8 shim gradient.

Values: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

zeroneg **Set all negative intensities of 2D spectra to zero (C)**

Description: Sets to zero all negative intensities of 2D-J spectra.

See also: *NMR Spectroscopy User Guide*

Related: **foldj** Fold J-resolved 2D spectrum about $f_1=0$ axis (C)
rotate Rotate 2D data (C)

zoom **Adjust display to given width (M)**

Syntax: `zoom (width)`

Description: Adjusts the display limits. It is useful in the display of powder patterns after **split** has been used. **zoom** both zooms in and out from the current display.

Arguments: `width` is the total display width, in Hz. Display limits are set to $\pm \text{width}/2$.

See also: *NMR Spectroscopy User Guide*

Related: **split** Split the difference between two cursors (M)

zx2y2 **ZX2Y2 shim gradient (P)**

Description: Holds current setting of the ZX2Y2 shim gradient.

Values: If **shimset** is 2, 8: -2048 to +2047, steps of 1, 0 is no current.
If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

zx3 **ZX3 shim gradient (P)**

Description: Holds current setting of the ZX3 shim gradient.

Values: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

zxy **ZXY shim gradient (P)**

Description: Holds current setting of the ZXY shim gradient.

Values: If **shimset** is 2, 8: -2048 to +2047, steps of 1, 0 is no current.
If **shimset** is 3 to 7, 9: -32768 to +32767, steps of 1, 0 is no current.

See also: *NMR Spectroscopy User Guide*

Related: **shimset** Type of shim set (P)

zy3 **ZY3 shim gradient (P)**

Description: Holds current setting of the ZY3 shim gradient.

Values: -32768 to +32767, steps of 1, 0 as no current.

See also: *NMR Spectroscopy User Guide*

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