

A4. Glossary of Common NMR Commands and Terms

aa	abort acquisition, hard stop
acqi	Open acqi window if the button has been lost
ai	absolute intensity mode
alock	autolocking routine, alock='y' for autolocking, alock='n' for typical manual locking
aph	autophasing, not recommended for most spectra
array	macro for setting up an arrayed experiment
at	acquisition time, set by spectral width (sw) and number of data points (np)
axis='p'	specify ppm or hertz for the axis, i.e. axis='p' or axis='h' , use axis='pd' referencing in an indirect detect experiment with >decref
bc	baseline correct
bs	block size, data is stored to the disk every time an increment of bs is reached, i.e. bs=16 , every 16 scans data is saved and can be transformed
cd	change directory, changes the directory back to home default directory
cexp(#)	create the experiment #
COSY	correlation spectroscopy, a 2-D experiment, homonuclear one-bond J coupling
center	re-size a 2-D spectrum to a centered square, same as [DispMenu][Size][Center]
ct	completed transients
cz	clear all integral reset points
d1	delay time between scans, required to allow for T1 relaxation, in seconds
da	display arrays
dc	drift correct
dconi	display interactive color map (2-D)

df	display FID
dfrq	decoupler frequency (2 nd channel)
dg	display first text screen of parameters
dli	display list of integrals
dm	decoupler mode
dmf	decoupler modulation frequency
dmm	decoupler modulation mode (c, g or w)
dn	decoupler nucleus (2 nd channel)
dof	decoupler offset (Channel 2 transmitter offset) in Hertz
dp	double precision, set to 'y'
dpcon	display contours in 2-D spectra
dpf	display peak frequencies
dpir	display integrals on screen (requires vp=12)
dps	display pulse sequence
dpwr	decoupler power
dres	display digital resolution
ds	display spectrum
dscale	display the scale (in ppm or Hertz)
dsn	display signal to noise
dss	display stacked spectra
dssa	display stacked spectra automatically
dssh	display a series of spectra in an arrayed experiment
dssl	display corresponding numbers in arrayed experiment

explib	display experiment library (or list of current exps.)
f	display the whole spectrum
fb	filter bandwidth
fn/fn1	Fourier number for direct (fn) detected dimension, indirect (fn1)
foldt	fold COSY type spectrum along diagonal
ft	fourier transform the data (no weighting functions)
full	display over the whole screen
fullt	re-size a 2-D spectrum for full with traces, same as [DispMenu][Size][Full with Traces]
ga	get acquisition (start acquisition and transform data)
gain	the receiver gain, to see the value of >gain? to set the value >gain=40
gCOSY	gradient COSY, same as a COSY, fewer scans required
gettext	will bring up a very simple editing window to type text into
gf	gaussian weighting function
gmapsys	start gradient shimming routine and open menu
go	acquire the spectrum, don't transform
gzsize	number of Z shims to use in gradient shimming
HMBC	heteronuclear multiple bond coherence, 2-D heteronuclear experiment
HMQC	heteronuclear multiple quantum coherence, 2-D heteronuclear experiment, One-bond correlations
jexp#	join a particular experiment, jexp2
lb	line broadening weighting function (exponential)
left	set display to left side of screen

LOCK	The deuterium nuclei in the sample are used to maintain a "lock" on the sample. The nuclei are used to monitor and correct for any drift in the magnetic field. If the field "drifts" or changes in strength, the precessional frequency of a nucleus will change accordingly. In a pulsed lock system, the field is monitored by observing the resonance frequency of the deuterium nucleus of the solvent (i.e. D ₂ O). The resonance frequency of the nucleus is compared to a reference frequency in the spectrometer and any changes are corrected by adjusting Z ₀ .
Lock gain	the amplification of the deuterium NMR signal, increases the size of the signal, but also increases any other signals or noise that may be present.
Lock phase	the phase angle used to control the phase of the deuterium NMR signal and the phase of the reference signal for the deuterium lock, normally needs very little if any adjustment.
Lock power	The quantity of rf energy used to irradiate the deuterium nucleus, controls the amplitude of the rf pulse at deuterium frequencies. Must be large enough to produce a signal for the deuterium but still below the saturation limit. If the power is too high, the lock signal may decrease in intensity.
lp	left phase, first – order phase correction
man	a very useful command to access the manual on an experiment i.e.>man('noesy')
movesw	move sweep width, first enclose the region for the sweep width with the cursors, then type movesw , this will move the tof
movetof	move transmitter offset, place cursor on peak or position to the center point of the spectrum, type movetof , does not change sw value.
ni	number of increments
nl	nearest line
np	number of data points acquired in the FID
nt	number of transients or scans
p1	another pulse that can be used in certain experiments
pad	pre-acquisition delay
page	sends plotting commands to the printer

pap	print parameters on plot, long version
phase	used to set phase selection in multi-dimensional experiments
phase(180)	phase the spectrum - 180 degree flip
pl	plot the spectrum
plfid	plot the FID
pll	plot line list
pltext	plot the text
plww	plot arrayed spectra in whitewash mode
ppa	print parameters, written out on plot
ppf	print peak frequencies
printon/ printoff	starts the printer job and ends the job
pw	pulse width measured in microseconds
pw90	the 90-degree pulse width, corresponds to the amount of time the transmitter is on in order to achieve a 90 degree tip angle
ra	resume acquisition stopped with sa
rl(4.6p)	reference a line to 4.6 ppm
rl1(4.6p)	reference a peak in a 2-D homonuclear experiment in f1 to 4.6 ppm
rl1(77d)	reference a peak in 2-D indirect detection in f1 to 77 ppm
rp	right phase, zero-order phase correction
rts	retrieve shims
sa	stop acquisition, this is a soft stop which means it will stop after the next FID
sb	sinebell weighting function

sd	set decoupler
sfrq	spectrometer frequency in MHz
SHIM	The process of "shimming" a sample is to minimize or eliminate any field differences across a sample. Eliminating these differences will lead to narrower lines and increased intensity.
ss	steady state scans, scans put in before acquisition really begins to create a steady state
su	set up the experiment, must be used when retrieving shims, setting nucleus for tuning, changing the temperature, etc.
svf	save file
svp	save parameters
svs	save shims
sw	the spectral width used to sample NMR signals, directly related to the chemical shift range for a given nucleus, given in hertz, sets the rate at which data is sampled.
tn	transmitter nucleus (i.e. H1, channel 1 on tune box)
TOCSY	total correlation spectroscopy, 2-D homonuclear proton experiment, through bond couplings, multiple bonds
tof	transmitter offset (Channel 1) in Hertz
tpwr	transmitter power in dB
trace	mode for 2-D or greater display (trace='f1' or trace='f2')
TUNE	Tuning a sample reduces the amount of power reflected back to the transmitter
vp	vertical position
vs	vertical scale
vs2d	vertical scale for a 2-D spectrum
vsadj	vertical scale adjust, adjusts to tallest peak in display

vtttype setting for temperature control, **vtttype=2** allows temperature changes, **vtttype=0** does not allow temperature changes

wbs('wft') with the next block store, transform the data

wft weighted Fourier transform

wti open interactive weighting

Z0 The Z0 allows the operator to match the resonance frequency of the deuterium to the reference frequency for the deuterium lock.