

## Glossary of Common Bruker NMR Commands and Terms

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**\*\*WARNING\*\*** *Commands preceded by an asterisk (\*) should not be used in automation mode. These commands are executed automatically by the software.*

<b>.co</b>	display contours (2-D)
<b>.hr</b>	display whole spectrum
<b>.hz</b>	toggle between Hz and ppm axis units
<b>.im</b>	display color map (2-D)
<b>.y</b>	switch y-axis display between abs/rel/off
<b>abs</b>	automatic baseline correction
<b>acqu</b>	switch to acquisition window
<b>apk</b>	automatic phase correction
<b>aq</b>	acquisition time, set by spectral width (swh) and number of data points (td)
<b>* atma</b>	activate automatic tuning and matching
<b>* bsmsdisp</b>	open BSMS display (for manual locking and shimming)
<b>COSY</b>	COrrrelation SpectroscopY, a 2-D experiment, homonuclear one-bond J coupling
<b>cpdprg2</b>	decoupling program (waltz, garp, etc.)
<b>d1</b>	delay time between scans, required to allow for T1 relaxation, in seconds
<b>de</b>	pre-acquisition delay
<b>edc</b>	edit current/create a new data set, same as <b>new</b>
<b>ef</b>	exponential multiply ( <b>em</b> ) + fourier transform ( <b>ft</b> )
<b>efp</b>	exponential multiply ( <b>em</b> ) + fourier transform ( <b>ft</b> ) + apply phase correction from previous experiment ( <b>pk</b> )
<b>em</b>	exponential multiplication
<b>fid</b>	switch to FID display window

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<b>ft</b>	fourier transform the data
<b>gb</b>	gaussian broadening parameter used along with <b>lb</b> for <b>gm</b>
<b>gm</b>	gaussian multiplication
* <b>getprosol</b>	get probehead and solvent dependent parameters
* <b>go</b>	acquires data on top of data already collected, used to resume acquisition stopped with <b>halt</b> or add more transients
* <b>gradshim</b>	start gradient shimming routine. Use primarily on samples in water.
* <b>halt</b>	halt acquisition, this is a soft stop which saves all data acquired to that point
<b>HMBC</b>	Heteronuclear Multiple Bond Coherence, 2-D heteronuclear experiment
<b>HMQC</b>	Heteronuclear Multiple Quantum Coherence, 2-D heteronuclear experiment, one-bond correlations
<b>iexpno</b>	increment experiment number
<b>lb</b>	line broadening parameter used for <b>em</b> and <b>gm</b>
<b>li</b>	list integrals
<b>lipp</b>	list integrals and peaks in displayed region
<b>lippf</b>	list integrals and peaks in full spectrum
<b>LOCK</b>	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 <sub>2</sub> O). The resonance frequency of the nucleus is compared to a reference frequency in the spectrometer and any changes are corrected by adjusting the field.
* <b>lock</b>	starts autolocking routine
<b>Lock gain</b>	The amplification of the deuterium NMR signal, increases the size of the signal, but also increases any other signal or noise that may be present.

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**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 adjustments.

**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.

- \* **lockdisp** Opens window displaying the lock signal
- ns** number of scans or transients
- nuc1** Nucleus for channel 1 (i.e.  $^1\text{H}$ ,  $^{13}\text{C}$ , etc.)
- nuc2** Nucleus for channel 2 (typically the decoupler)
- o1** offset for channel 1 (transmitter offset) in Hz
- o1p** offset for channel 1 in ppm
- o2** offset for channel 2 (decoupler offset) in Hz
- o2p** offset for channel 2 in ppm
- p1** pulse width measured in  $\mu\text{s}$
- \* **paropt** parameter optimization, macro for setting up arrayed experiment
- ph0** zero-order phase correction
- ph1** first-order phase correction
- pl1** transmitter power level attenuation (higher values = lower power, max power = -6 dB)
- pl2** decoupler power level attenuation
- plot** open Plot Editor
- pps** pick peaks and display them on the spectrum
- prosol** table in software that defines probehead and solvent dependent parameters
- \* **pulsecal** au program that performs a single scan  $90^\circ$  pulse calibration based on nutation
- re #** open experiment #

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<b>rg</b>	receiver gain
* <b>rga</b>	automatic receiver gain adjustment
<b>rsc</b>	read column from 2-D data and store as 1-D
<b>rser</b>	read row from 2-D data and store as 1-D
<b>rser2d</b>	read plane from 3-D data and store as 2-D
* <b>rsh</b>	retrieve shim file
<b>setti</b>	opens text editor to edit title
<b>sf</b>	spectrometer reference frequency, in MHz
<b>sfo1</b>	spectrometer frequency at o1, in MHz
<b>sfo2</b>	spectrometer frequency at o2, in MHz
<b>si</b>	number of data points used in processed data
<b>SHIM</b>	The process of “shimming” a sample is performed to minimize or eliminate any field differences across a sample. Eliminating these differences will lead to narrower lines and increased intensity.
<b>sine</b>	sine-bell window function
<b>sinocal</b>	macro to calculate signal-to-noise ratio
<b>slice</b>	interactively extract rows or columns in 2-D data
* <b>stop</b>	stop acquisition, hard stop
<b>sw</b>	spectral width, in ppm, used to sample NMR signals, directly related to the chemical shift range for a given nucleus. Sets the rate at which data is sampled.
<b>swh</b>	spectral width in Hz
<b>sym</b>	symmetrize COSY type spectrum across diagonal
<b>te</b>	temperature in K
* <b>teset</b>	change probe temperature to <b>te</b>
<b>td</b>	time domain, number of data points acquired in the FID

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<b>td (F1)</b>	number of increments (2-D)
<b>TOCSY</b>	TOTal Correlation SpectroscopY, 2-D homonuclear proton experiment, through bond couplings, multiple bonds
* <b>topshim</b>	start topshim gradient shimming routine. Works much better than <b>gradshim</b> on samples with deuterated solvents
* <b>tr</b>	transfer data to disk, saves all data collected to that point in the acquisition
<b>TUNE</b>	Tuning a sample reduces the amount of power reflected back to the transmitter
<b>vconv</b>	convert Varian data into TopSpin format
<b>wm</b>	opens interactive window functions
<b>wpar</b>	save parameter set
<b>wrpa</b>	copy data to another experiment
<b>wsh</b>	save shim file
* <b>zg</b>	zero data and begin acquisition

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