A List of Commonly used Acquisition Parameters in Bruker TOPSPIN

Nearly all of the Acquisition Parameters in TOPSPIN can be modified manually. While many of the preloaded pulse programs for 1D and 2D NMR spectroscopy are optimized for standard experiments, there are times where you may want to modify an existing pulse program in order to meet the needs of your specific experiment.

Parameters in TOPSPIN fall in to four categories by input type:

1. Those that take integer values, such as NS (no. of scans); (**I)**
2. Those that take real values:
    a. either single-precision floating point (**FS**) (i.e. AQ – acquisition time)
    b. or double-precision floating point), (**FD**) (i.e. SW - spectral width)
3. Those that take character array values (**C**) (i.e. DSLIST – dataset list)
4. Those that take values from a predefined list of values (**L**) (i.e. AQ – acquisition mode)

The letters listed above in **bold** are abbreviations created for this reference list to quickly delineate which type of parameter each is.

Those that are of type **L** will be followed by a listing of the options available in *italics*, and a brief explanation of each option will be shown.

While there are very real differences in the way single-precision (32-bit) and double-precision (64-bit) floating point values are handled by computer programs, these differences are, for the most part, transparent to most NMR users. Therefore, types **FS** and **FD** can be treated in the same manner from the standpoint of inputting parameters.

From the TOPSPIN command line, the acquisition parameters page can be accessed by typing the command *eda*. Along the left side of the page are shortcuts to each of the sections listed below. These parameters are in turn read by acquisition commands such as *zg*, *rga,* and *resume.*

Not every acquisition parameter is detailed here. Instead, the purpose here is to list in order of appearance and by tab, the most commonly used acquisition parameters, along with the input category, so that the user can become familiar with these parameters when designing new NMR experiments. Those not listed either cannot be changed, or should not be changed without extensive knowledge of the NMR experiment.

Parameters with a list of numbers after them in brackets (i.e. AMP [0 – 31] have multiple values, each with it's own entry. All entries will be of the same type (i.e. FS)

For 2D experiments, those parameters that can be set independently for each channel will be listed in separately columns labeled F1 and F2.

Experiment Page

Parameters on this page generally relate to overall experiment settings.

Parameter	Input	Units	Description of Parameter

PULPROG **C** **Name of pulse program**

This is the pulse program whose parameters are listed. Clicking the button labeled (…) to the right allows for the selection of preset and user-defined programs; clicking the button labeled (E) allows for the manual editing of the pulse program, either directly into the software, or via a graphical editor that visually displays the pulse program.

FnMODE **L** **Acquisition mode for indirect detections**

Options:	*undefined*	*not defined; no mc statement*
	QF	*successive FID w/o phase program;*
	QSED	*successive FID @ 0, 90°*
	TPPI	*successive FID @ 0, 90, 180, 270°*
	States	*successive FID w/alt. time interval @ 0, 90°*
	States-TPPI	*successive FID w/alt. time interval @ 0, 90, 180, 270°*
	Echo-Antiecho	*special phase handling for gradient controlled experiments*

This option only appears for 2D experiments and is usually specified with the specific experiment used.

AQ_mod **L** **Acquisition mode**

Options:	*qf*	*Single channel detection*
	qseq	*quadrature detection, sequential mode*
	qsim	*quadrature detection, simultaneous mode*
	DQD	*digital quadrature detection*

Sets the acquisition mode of the receiver. Typically, this is set to DQD; however, this setting requires DIGMOD to be set to either *digital* or *homodecoupling digital*, and can only be used up to a certain spectral width (see table 2.6 on page A-44 in the Acquisition Manual). If SW is set above this value, AQ_mod will default to *qsim*, even if the parameter reads *DQD*.

TD **I** **data points** **Time Domain**

This specifies the number data points to be taken with the specified spectrum. A higher value for TD increases resolution, but also increases overall acquisition time. Increasing TD will automatically increase the value for AQ. TD values are typically set to a power of 2 value (i.e. 65536).

NS **I** **scans** **Number of scans**

This is simply the number of scans. Increasing the number of scans increases signal-to-noise ratio, but also increases overall experiment time.

DS **I** **scans** **Number of dummy scans**

This is simply the number of dummy scans. They are used to allow for T_1 relaxation, and to allow for temperature stabilization in experiments with high power settings (i.e. decoupling or TOCSY experiments).

TD0 **I** **counts** **Loop counter**

Used primarily for 2D experiments; does not usually need to be changed.

Width Page

Parameters on this page relate to RF pulse width.

Parameter	Input	Units	Description of Parameter

SW **FD** **ppm** **spectral width (in ppm)**

Sets the spectral width of the pulse. Should be set so that all relevant peaks will be captured; for unknown samples, this should be a large (50 ppm or greater) value. The instrument hardware can only handle discrete values of SW; therefore, you may notice that the value is adjusted slightly after entry. Changes to SW will also result in changes to DW (dwell time) and SWH, since both are calculated based on SW and SFO1.

SWH **FD** **Hz** **spectral width in Hz**

Performs the same function as SW, but entry is in Hz instead of ppm. Changes to SWH result in changes to SW and DW (see explanation in SW).

IN_F **FS** **µs** **delay interval**

Sets the delay interval from F1 to F2; used only in 2D experiments. Shown under the F1 column only.

AQ **FS** **seconds** **Acquisition time**

Acquisition time is automatically calculated based on TD, SW, and SFO1; therefore, this value generally is informational only. If AQ is changed, TD will be adjusted accordingly to match.

FIDRES **FS** **Hz** **FID resolution**

Sets FID resolution in Hz. FIDRES is calculated based on SW, SFO1, and TD; however, if FIDRES is adjusted, TD alone will be recalculated then adjusted to the nearest power of 2. As a result, values entered for FIDRES may change slightly after entry.

FW **FS** **Hz** **Analog filter width**

Defines the width of the analog filter. Not usually adjusted, since when DIGIMOD is set to digital (used in most cases), FW is automatically set for maximum oversampling (typically 125000 Hz)

Receiver Page

Parameters on this page relate to settings for the receiver.

Parameter	Input	Units	Description of Parameter

RG **I** **0 - 200** **Receiver gain**

Controls the amplitude of the FID signal before it enters the digitizer. It is usually determined automatically through the use of the *rga* command, but may be set manually here. 200 is the maximum gain value that can be entered.

DW **FS** **µs** **Dwell Time**

Dwell time is the time between acquisition of two successive data points. While DW is normally calculated automatically based on SW, it may be adjusted manually. This will result in a corresponding change to SW. Additionally, setting DW manually may result in a slight value adjustment after entry, since DW is based on DECIM during oversampling, and DECIM only uses integer values.

DSPFIRM **L** **Firmware used for digital filtering**

sharp, smooth, medium, rectangle, user-defined

Defines the filter function used for digital filtering. Normally set to *sharp*; *smooth* cannot be used with AQ_mod set to *DQD*. Some applications may be helped by the use of *rectangle*, which corrects the initial points in the FID.

DIGMOD **L** **Digitizer mode**

analog, digital, homodecoupling-digital, base-opt

For nearly all cases, this is set to *digital.* Howver, when DSPFIRM is set to *rectangle*, this will be automatically set to *base-opt.*

DR **I** **Digitizer resolution**

Digitizer resolution is automatically set to the maximum for the current digitizer. Not to be set by user.

DE **FS** **µs** **Pre-scan delay**

This is the delay prior to sampling of data points. Four subdelays are part of this parameter: DEPA, DERX, DE1, and DEADC. These can be individually adjusted via the *edscon* command; however, they are typically left at default values of 1, 2, 3, and 4 µs, respectively. However, if DIGMOD is set to *analog*, the four subdelays are not included and DE is automatically adjusted whenever SW or DW are changed.

NBL **I** **blocks** **Number of blocks of acquisition memory**

Specifies the number of blocks of acquisition memory; typically only used for NOE difference experiments.

PRGAIN **L** **High power preamplifier gain**

low, high

Typically set to high; only set to low for experiments with a very strong NMR signal.

DQDMODE **L** **Sign of freq. shift for digital quadrature detection**

add, subtract

Defines the frequency shift applied in DQD mode as positive (*add*) or negative (*subtract*)

PH_ref **FS** **degrees** **Receiver phase correction**

Adds a phase value to the receiver phase. Can be automatically calculated for 2D dataset using the command *phtran.*

Nucleus Pages

Parameters on these pages relate to settings for the individual nuclei being observed.

Parameter	Input	Units	Description of Parameter

NUC1 – NUC8 **L** **Nucleus observed**

1H, 13C, 15N, 19F, etc., off

Defines the nucleus observed for up to 8 channels. 1D experiments without decoupling will have only NUC1; 1D experiments with decoupling will have NUC1 and additional channels for decoupling specified; 2D experiments will have NUC1 and NUC2 specified, plus additional channels for any decoupling. All others should be set to *off*. To change a nuclei, it is necessary to click the (Edit) button, and insure that the appropriate receivers and other hardware necessary to process the signal are properly selected on the graphic interface.

O1 – O8 **FD** **Hz** **Irradiation frequency offset for channel 1 – 8**

This value sets the center of the spectral region to be acquired. It is related to SFO1 and BF1, but can be manually adjusted, either by direct entry or from a related spectra.

O1P – O8P **FD** **ppm** **Irradiation freq. offset for channels 1 – 8 in ppm**

This serves the same purpose as O1 to O8, but allows the user to manually enter the value in ppm, which is often more convenient when choosing a region from an existing spectrum.

SFO1 – SFO8 **FD** **MHz** **Irradiation freq. for channels 1 – 8**

Typically automatically set automatically based on O1 – O8 and BF1 – BF8; usually should not be adjusted manually.

BF1 – BF8 **FD** **MHz** **Basic frequency for channels 1 – 8**

Set automatically based on nucleus selection. Should not be changed by most users.

Power Page

Parameters on these pages relate to power levels of RF pulses.

Parameter	Input	Units	Description of Parameter

P[0-63] **FS** **µs** **Pulse lengths**
This is the array of lengths, in µs, for pulses 0 through 63. Note that the first pulse is numbered 0, not 1.

D[0-63] **FS** **s** **Delay lengths**
This is the array of lengths, in seconds, for delays 1 through 63. Like other arrays, the first is numbered at 0, not 1.

IN[0-63] **FD** **s** **Delay increment values**
This is the array of lengths, in seconds, for delay increments 0 through 63. These increments can be used in 1D experiments to increase or decrease the relevant delay. However, in 2D and 3D experiments, SW is directly affected by these values for the F1 direction only.

INP[0-63] **FD** **µs** **Pulse increment values**
This is the array of lengths, in seconds, for pulse increments 0 through 63. These increments can be used to increase or decrease the relevant delay.

HDDUTY **FS** **%** **Homodecoupling duty cycle**
This sets the ratio between the time used for homodecoupling, and the time used for signal detection.

PCPD[0-9] **FS** **µs** **Composite pulse decoupling pulse lengths**
This array of values is used by the composite pulse decoupling (CPD) programs to set pulse lengths for those types of experiments.

V9 **FS** **%** **Maximum variation of delay**
This values sets the maximum amount of variation in a delay when a random variation in a delay by the command dX:r.

Power Page

Parameters on these pages relate to power levels of RF.

Parameter	Input	Units	Description of Parameter

PL[0-63] **FS** **dB** **Power level**
This is the array of power levels, in dB, for pulses 0 through 63. These values can also be called up to assign power levels to individual channels (i.e. F1, F2)

PLSTRT **I** **dB** **Starting Power level**
This is the initial power level in dB for the pulse transmitter. It should not be modified.

PLSTEP **FS** **dB** **Power Level Step**
This is the minimum value that the power level can be incremented. Can not be modified by the user.

Shape Page

Parameters on these pages relate to shaped pulses.

Parameter	Input	Units	Description of Parameter

SP[0-31] **FS** **dB** **Shaped pulse power level**
This is the array of power levels, in dB, for shaped pulses 0 through 31.

SPOFFS[0-31] **FS** **Hz** **Shaped pulse frequency offset**
This is the array of values, in Hz, for the frequency offset for shaped pulses 0 through 31.

SPOAL[0-31] **FS** **degrees** **Shaped pulse phase alignment**
This is the array of values, in degrees, for the phase alignment for shaped pulses 0 through 31.

SPNAM[0-31] **C** **name** **Shaped pulse file name**
This is the array of values for the file names of each of the shaped pulses 0 through 31.

Gradient Page

Parameters on these pages relate to magnetic field gradients.

Parameter	Input	Units	Description of Parameter

GPX[0-31] **I** **%** **Gradient in x-axis**
This array of values, in % of max, gives the gradient level for x-axis gradients 0 to 31.

GPY[0-31] **I** **%** **Gradient in y-axis**
This array of values, in % of max, gives the gradient level for y-axis gradients 0 to 31.

GPZ[0-31] **I** **%** **Gradient in z-axis**
This array of values, in % of max, gives the gradient level for z-axis gradients 0 to 31.

GPNAM[0-31] **C** **name** **Gradient file name**
This is the list of file names for each of the gradients. GPNAM0 encompases gradients in all 3 axes (GPX0, GPY0, GPZ0).

AMP[0-31] **FS** **%** **Gradient maximum amplitude**
This array of values, in % of maximum, gives the maximum amplitude for each of the gradients 0 to 31.

PWMOD **L** **Power mode**
low, high, linear
This parameter sets the power mode. Only used on spectrometers with a high power accessory; leave set at *low.*