

## Bruker WinNMR Notes by Dave D. (Jul 2002)

### Probe Positioning:

- Vertical (Z1 values + / - 128K, use 13K for 10% change)
  - collect spectrum on CHCl<sub>3</sub> and reference to 0 Hz
  - change Z1 by 13K
  - set spectrometer for continuous acquisition and position screen so you can view it while moving probe at magnet
  - move probe up / down until peak near 1 Hz
- Horizontal
  - shim stack ribbon cable is y axis

### Tuning:

- wobb start tuning process
- acqu displays tuning window / fid window
- gs to start acquisition
- stop halts tuning process
- Notes:
  - adjust tune first move tuning dip on console display to center of screen
  - adjust match to maximize the depth of the tuning dip
  - adjust tune & match alternately to max and center dip
  - can read out tuning progress on preamp by magnet

### Shimming:

- type solvent, enter acetone and then type lopo to reset referencing
  - alternatively, type lock and choose solvent from a list
- type lockdisp to show lock window if not showing
- make sure lock and sweep buttons are of on BSMS
- adjust gain & power to avoid saturation
- adjust field and phase
- ased shows pulse sequence parameters
- rga auto adjust receiver gain **Caution** Don't do this 'till power and pulses set!
- efp apply exponential function (lb), fourier transform and phase spectrum
- fp fourier transform and phase spectrum
- Notes:
  - rsh to view list and load shim file from disk
  - vish to view list and print a shim file on disk
  - wsh to save current shims to disk

### Lineshape Measurement:

- automatic
  - display region of spectrum and hit the DP1 button to set display region
  - type humpcal and lineshape results will show in dialog box
- manual

- type cy 1000 (sets vertical scale to 10000)
- click on YU button until absolute scale show (1000 scale on left side)
- use cursor to mark peak and measure width at 5.5 and 1.1

### Array optimization:

- adjust spectrum display and select DP1 from toolbar to set display area for array optimization
- paropt is like array on Varian system, starts interactive optimization
- enter name of arrayed parameter (e.g., p1)
- answer questions that pop up in window
- zg once you are ready
- Notes:
  - cannot be used for time-based NMR experiments
  - use a dummy variable to array a sequence without variation (stability test)
  - paropt dumps you in to proc 999, re x y to jump to your original experiment x process y
  - type kill and select paropt process from list to stop

### Miscellaneous Commands:

- Major Editing Screens
  - edasp displays router window where you can turn decouplers off/on
  - ased display autoseup editor window for acquisition parameters
  - type edc to create a new dataset on disk where
    - you can enter a name for the directory to hold the data (eg CapNMR\_installation)
    - you can enter an experiment number (eg 1)
    - you can enter a process number (eg 1)
  - setsh displays shimming screen where values can be typed
  - ased displays portion of acquisition parameters (1D params?) of current pulse sequence
  - eda displays portion of acquisition parameters (2D params?) of current pulse sequence
- type o1p to enter 1H transmitter frequency in ppm (o2p for decoupler)
- type ii if hardware doesn't seem to be responding (initialize interface)
- setTi sets the text title for an experiment
- expt reports estimate of experiment length
- rga (auto adjust receiver gain) **Caution** Don't do this 'till power and pulses set!
- pulprog display which pulse program you are using
- efp apply exponential function (lb), fourier transform and phase spectrum
- fp transform and phase spectrum
- xf2 transform f2 in 2D experiment
- xfb transform f2 and f1 in 2D experiment
- edcpul display pulse program for printing
- edlist displays lists associated with current pulse sequence for editing
- rpar presents list of parameter sets where you can load in default settings (usually pick all which includes pulse parameters, default plotting displays, etc)

- type acqu to display fid

### Installation Task Tips:

- **Time based experiments for HTSL Installation:**
  - cannot use paropt or multizg for precisely controlled collection of a series of 1D spectra
  - must use above Time base sequence or similar since 2D is only time precise data acquisition mode
  - load flowtime pulse sequence
  - edpar to ensure parameters (e.g., power levels, d1 and aq should add to 6 seconds) are set
  - click on PARMODE and set to 2D MODE
  - eda and set TD value in F1 to appropriate number of increments (60 = 10 minutes)
  - type zg to start and xf2 to process
  - use display tools to view rows and columns (go in to utilites menu)
- **pw90 Calibration for 13 C**
  - edasp and turn on decoupler channel
  - pulprog and select decp90 pulse sequence
  - set 90 pulse and power levels for transmitter (proton)
  - set d1 (relaxation delay) to around 15
  - set power level for carbon (decp90 to similar value as proton 19)
  - array carbon pulse (P3) around expected 90 (simliar to proton)
  - 13 C satellites are antiphase away from 90, null at 90 and change phase on either side of 90
- **gradient test**
  - edpul to cosygpqf (magnitude cosy)
  - rpar and load all parameters
  - set P1 & P0 to 90 degree 1H pulse and PL1 to 1H power
  - zg
  - xfb to process both dimensions