

# General Usage of the Bruker Avance Spectrometers

## Getting started:

- To eject standard or sample currently in magnet, press LIFT ON/OFF button. The sample in the magnet should rise to the top of the center stack within a minute or so.
- Place your sample in the spinner and center sample using the calibrated tube – centering using lines for a 5 mm probehead. Place sample at the top of the magnet center stack and press the LIFT OFF button again to insert sample into the magnet.
- If you have a starting shim file it can be loaded using the command [ rsh <shimfilename> ]. Shim files can be written using the command [ wsh <shimfilename> ]. For example, to shim on H<sub>2</sub>O sample in the HCN probe you can start by loading in the file hcn\_shigeml.shm or hcn\_wilmad.shm, depending on the tube you are using.
- To adjust sample temperature, type [ edte ] at the command line. A pop-up window will appear. To alter the current temperature, type in the target temperature (in units of Kelvin: 273 Kelvin = 0 degrees Celsius = 32 degrees Fahrenheit), click the apply button, then click the okay button. It will take a few minutes for the temperature to equilibrate.
- Find your lock signal by looking at the sweep. To do this, press the LOCK-SWEEP button. After finding your lock, you can auto lock by typing in [ lock ] at the command line of XWINNMR. You will be asked for the solvent your sample is dissolved in (e.g. D<sub>2</sub>O, H<sub>2</sub>O, Chloroform).
- Shimming in protonated solvents can be done using an automated gradient shimming routine. This routine can be opened by typing [ gradshim ] at the command line of XWINNMR.
- Set PW, pulse width, to 2  $\mu$ s to look at your water peak (or whatever you are shimming on). This is done by typing [ pw 2 ] at the command line (the default unit is microseconds). To look at this peak you will need to collect a 1D:
  - Type [ zg ] (which stands for zero go)
  - Type [ ft ] (which applies a fourier transform to the newly collected FID)
  - Type [ pk ] (which allows you to adjust the phase of your transformed spectra)

- Now you can measure the linewidth using the cursor and if needed shim some more to improve your line shape and width. If you want better resolution you may want to decrease SW.
- Calculating the pulse width: Set PW, pulse width, to a reasonable number representing a 360 degree pulse, for example, 32. Now you can collect a 1D.
- Type [ zg ]
- Type [ fp ] (this applies a fourier transform AND applied the previously used phases)
- Repeat the 360 degree pulse at various values till you get a null signal that is, one with neither a positive or negative component. The latter PW value divided by four will be your 90 degree pulse.