Department of Chemistry NMR Facilities

Varian 500 Tutorial for the acquisition of 1D ^{1}H and ^{13}C spectra

1) log in to the linux account.

2) double click on the VNMRJ icon to start the program.

3) check that the probe file is “OneNMR_W036”.

4) insert the sample tube in the spinner. Use the gauge to measure the depth.

5) click on < eject > in the “start/standard” tab, and take the sample out of the magnet.

6) put your sample on top of the magnet. Be sure that the spiner is floating before dropping it.

7) click <insert> in the “start/standard” tab.

8) the line commands “e” and “i” can also be used to eject and insert samples respectively.

9) wait until the sample is loaded in the magnet. The yellow light, in the switch box on top of the magnet, turns on when a sample is in the probe.

10) **Tune the probe** to ^{1}H: type “protune” on the command line. The tuning window pops up.

11) click on <^{1}H> and wait until the tuning is done. Then, close the tuning window.

12) **Lock to the solvent:** select the solvent on the tab “Start/standard”.

13) on the “Start/Standard” tab, click on <Find z0> to lock the sample.

14) check whether there is a “Mapname:”, then click on <Gradient Autoshim>.

15) while doing gradient shims and Find Z0, the solvent will temporarily switch to D2O and spinning will turn off.

16) on the tab Start/ Spin/Temp, set the spinning rate to 20 Hz and then press the button <Regulate Speed>.

17) temperature can be set in the same tab. Select the temperature and then click on <Regulate Temp.>.

18) choose a 1D-^{1}H experiment, click on the menu “experiment” and then select “proton”.

19) on the tab “Acquire” you can modify the experimental parameters as needed.

20) run the experiment, on the command line type “ga” and then press <enter>. Or just click on <acquire> in the “acquire” tab.

21) to display the spectrum, type “wft” and then press <enter>.

22) usefull commands: wft: to refresh the spectrum, aph: automatic phasing, nt: **number of scans** vsadj : adjust the high of the spectrum, f: brings back the full spectrum after it was zoomed. movesw: adjusts sw automatically, movetof: changes the central frequency.

23) saving files: in the file menu, select “save as”.

Printing spectra

1) select the “process/plot” tab. Select the desire options and then click on <Auto Plot>.

Running a carbon experiment.

1) **Tune ^{13}C:** type “protune” on the command line and then on the window that pops up, click on <^{13}C>.

2) Remember that for a carbon experiment, you also need to tune ^{1}H.

3) change to experiment 2 by typing "jexp2" and then press <enter>.

4) select the experiment "carbon".

5) type on the command line "ga", then press <enter>. Or just click on <acquire>.

Once you are done, put the standard sample back in the magnet and lock it:

1) select the solvent (D_2O), then press <Find Z0>.

2) stop the spinning. On tab "start/ spin/temp" click on <spin off>.

3) set the temperature back to 26 ^{o}C.

4) close VNMRJ; select "File" on the upper left corner and then "Exit Vnmrj".

5) log out from your account.

6) log in the log book.

Retreiving data from the spectrometer computer using SSH

0) Open the WinSCP program.

1) click on <NEW> .

2) Fill in the windows that pops up: host name: juliet.chem.utk.edu, user name: …. , and password:…..

3) click on <save>.

4) click <OK> on next window.

5) when trying to connect for the first time, a windows pops up. Just click on <yes>.

6) the right panel is the host computer, change the directory to vnmrsys/data.

7) download the data.

8) once you are done, diconnect from the host computer.