Operation of 60 MHz NMR

Log in to the Student account (password: student).
Open the PNMR program (click the **aii** icon in the taskbar).

**RUNNING A SAMPLE**

**To insert a sample:**
Open the black plastic lid of the NMR instrument. On the control box, press and hold the Eject button. The water sample, which should remain in the instrument in between samples, should be ejected; catch it as it comes up.

**ONLY TOUCH THE SPINNER AND NMR TUBE USING A KIMWIPE!**
Transfer the spinner to the desired sample. Push the tube all the way down in the depth gauge to adjust the spinner to the proper height.
Insert the sample into the instrument. Push the Inject button on the control box to lower the sample into the instrument. Look to make sure the sample begins spinning. Use the flashlight if you need to.
Close the black plastic lid.

**To run acquisitions:**
In the PNMR program, select the Nucleus tab at the top of the page. Select 1H to run proton NMR.
In the command line at the bottom of the page, type `acq` to run the acquisition.
Wait for the acquisition to finish (approximately 2 minutes). Note that the ACQ parameters include shimming, TMS calibration, automatic integration, and automatic peak picking.
(Alternatively, type `shima` if the NMR solvent contains TMS or type `shim` if the NMR solvent does not contain TMS. Then, after the shimming is complete, type `ns` to set the number of scans to one and then type `zg` to run the acquisition. Type `Ctrl+F1` to process the spectrum in the NUTS program.)

The spectrum should open in the NUTS program (the NMR icon in the taskbar).

**Manual Phasing**
If the baseline is not flat (horizontal on both sides of the peaks but slanted), the spectrum is said to be out of phase. To correct this hold down the **ALT** key and type **P, P, A**. The baseline should flatten out.

**Changing Integrals**
To toggle integrals on/off, type `Ctrl+i`
To open the integration mode, type `id`
To change the integration value, click the mouse over the integral region of interest. Type `v`, and then enter the desired integration value (if you think you know what it should be) for that peak in the pop-up window. Type the **ENTER** key. The other peaks will be scaled proportionally. Type the **ENTER** key to exit the integration mode.
To delete an integral region, click the mouse over the integral region of interest. Type **d** to delete this integral region. Type the ENTER key to exit the integration mode.

To manually create a new integral region, click the mouse in the spectrum once, then place the resulting cursor line on the baseline on one side of the desired peak and click to begin the integral region. Then move the cursor line to the baseline on the other side of the peak and click to end the integral region. Type the ENTER key to exit the integration mode.

Alternatively, type **ai** to generate automatic integrals.

**Calibrating the TMS peak**
In the NUTS program, click and move the resulting cursor line over the TMS singlet. Note the position of TMS in ppm. Go back to the acquisition window. Type “**fo**” (field offset). When the window appears asking where the current TMS signal is, type the position you noted in the NUTS program and Enter. For the new position, type 0 and Enter again. Type **acq**. When the new spectrum appears, TMS should be at 0.0 ppm.

**Changing Peak Picking**
To toggle peak-picking on/off, type **Ctrl+p**
To view automatic peak picking, type **pp**
To open manual peak-picking mode, type **dp**
Position the mouse over the desired peak and click to pick.
To delete a peak label, position the mouse over the desired peak and type **k**
Type the ENTER key to exit the manual peak picking mode.

**Print**
Print the spectrum from the NUTS program. (You must click the printer icon once for every copy of the spectrum you wish to obtain. This should be one for every member of your group.)

**FINISHING**
Eject the sample as before and replace the water sample in the instrument.
Sign the logbook.

**Emergency Stop**
Typing **Ctrl+q** halts acquisitions after the current scan and saves the data.
Typing **Ctrl+k** stops the current scan and does not save the data.