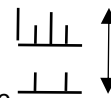
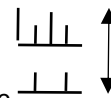


## Running DEPT spectra on the Bruker Avance 400 MHz NMR

- I. Put your sample in the sample holder and note the location.
- II. Enter Automation mode
  - a) Start TopSpin as if you were running a regular NMR spectrum.
  - b) Click on the "Acquire" tab, then the down arrow on the "Options" tab.
  - c) Click on "iconNMR Automation."
  - d) A new (relatively small) window will open. Click on the box that says "Automation."
  - e) An "Identify User" box will open. Pick "CHM 218H" and click on "ok."
- III. Once inside Automation.
  - a) Double click on the line corresponding to your sample location. A table will appear.
  - b) Enter a "Name." The name is not important, but there must be one.
  - c) Click in the box under solvent and choose CDCl<sub>3</sub> from the list that appears.
  - d) Likewise, select "C13DDEPT135" under Experiment from a list that will appear. Two experiments will appear. About 2/3 down the page will be a bar, with an "Add" button. Click on it. A new line (3) will appear. In the experiment column, click and add "C13DEPT90." Finally, repeat this process, but add a normal <sup>13</sup>C NMR spectrum, "C13CPD32."
  - e) Another column header will have a blue box with two parallel yellow lines. Click on that and change the number of scans so that all experiments are set to 32.
  - f) Click on the Submit button (left side of toolbar in middle of the screen), then Scan (left side of toolbar near top of screen).
  - g) Once the experiments have completed, highlight all three experiments in the "Preceding Experiments" frame of the Automation window (bottom half of the screen).
  - h) Type [CTRL+M] and a new window will appear with 3 spectra displayed. They will be colored blue, red, and green. On the bottom right of the screen will be a box with with 3 squares that are also blue, red, and green. The first number next to the screen will indicate which experiment corresponds to which spectrum. That is, "1" will be the spectrum labeled 1 in the "No." column on the acquisition screen in ICON Automation. The blue spectrum should be at the bottom of the 3 and be a normal <sup>13</sup>C NMR spectrum. The middle spectrum should be the DEPT spectrum that shows only CH groups (DEPT90), and the top spectrum that shows CH<sub>2</sub> groups down and CH/CH<sub>3</sub> groups up (DEPT135).



- i) Sometimes the spectra overlap one another. In that case use the  to toggle to the correct view. Also, sometimes the DEPT 90 will appear at the top. In that case, highlight either the DEPT90 or DEPT135 spectrum and use the up or down arrow icon, as appropriate, to move the spectrum into the correct location.

When done, click the "Stop" icon in ICON Automation to be exit the program.