Bruker DPX 400MHz Nuclear Magnetic Resonance (NMR) Spectrometer

Instrument instructions can be found at:
http://academic.bowdoin.edu/chemistry/resources/instructions.shtml

If you have any problems with the instrument or would like training, please contact
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1. Startup Procedure

a. **Login to computer.**
   i. At the login screen, select your username and hit Enter.
   ii. Type your password and hit Enter.
b. **Open TopSpin 1.3.**
   i. Double click on the Top Spin 1.3 icon on the desktop.

2. File Browser Overview ñ Review Before Creating New File

a. **A standard Bruker dataset is a directory tree, not a single file.**
   i. <*dir*>/data/<*user*>/nmr/<*dataset name*>/<*expno*>/pdata/<*procno*>
   ii. The information in ñ< >ò is what you enter in the ñNewé ò window that appears when you type ñedcò
   iii. Example:
      1. Name (<*dataset name*>): proton
      2. Expno (<*expno*>): 1
      3. Procno (<*procno*>): 1
      4. Dir (<*dir*>): /opt/topspin/chem226
      5. User (<*user*>): Orgolab
      6.

6. Insert your Sample

Note

b. **To shim the magnet, you will adjust Z^1 and Z^2.**

   i. Press the ñZ^1ò button (ñZ^1ò light will turn on) and rotate the wheel, in either direction necessary, until the signal improves (lock signal in ñlockò window

ii. Click on the second icon from the left (ñDefine new region using cursor (toggle)ò). To integrate a peak, move the red cursor line to where you want the integration to start and click and hold the left mouse button. While holding the left mouse button, move the second red cursor line that appears to where you want the integral to end. Release the left mouse button when finished.

iii. To phase an integral, you must first select it. Move the red line cursor over the integral and click the right mouse button. A shortcut menu will appear. Select ñSelect/Deselectò. Near the bottom of the sc

b. **A “Print [Ctrl+P] – prnt” window will pop up with two sections.**
   i. Options
      1. **Select “Print active window” and click OK to print the spectrum as is in the window. (Skip to step c. if using this option)**
      2. Select ñPrint with layout ï plot directly [autoplot]ò, using a specified template. (see required parameters below)
   ii. Required parameters
      1. To use a saved template, set ñLayout=ò to the template name.
      2. For a generic 11 x 17 layout, set ñLayout =ò to ñ+/Bowdoin.xwpò.
      3. For a generic 8 İ x 11p u[m] l א ɔ ˛ p [m] wpò.

selected window). Near the top of the screen, click on the 1D/2D-Edit button. At the very top choose the scope. Adjustments will only affect what is selected (dark gray color). The top row of icon will move and zoom the spectrum. The second row will increase/decrease the height of the spectrum. The third row of icons is used to return the spectrum to its original scale. Below the icons are more check boxes that shows what will appear on the spectrum. If a feature is selected, it will be shown on the graph. Options here include X-Grid, Y-Grid, Show Peaks, and Show Integrals.

v. To remove an object, click on the ñMark Objectsò icon and select a window. Near the top of the screen, click on the Delete button. The window will be removed.

vi. Mark Objects ï used to resize and move objects on the screen.

1. To move, click and hold the center wheel on the mouse. This will grab the object. Move to the new location and release the center wheel.
2. To resize an object, left click once on the object and eight green boxes will appear around the object. Move cursor over a green box until it changes into an arrow cursor. Click and hold the left mouse button and move the mouse to resize.

d. **Save template**.

i. In the ñSelectionò box, navigate to ñ\opt\topspin\plot\layouts\ò. You do this by double clicking the folders listed vertically in the left column.

ii. Type the name you want for the template after this directory.

1. Example: ñ\BT/F8 12 Tf1 0 0 1 180 422.23 Tm0 g0 G[<002800 5B>-8 <0044>4<00To res