

How to print several different spectra onto one page

Outline:

The following steps are involved:

1. Data is “worked up” different experiments.
2. Determine the spectral regions you wish to plot for each spectrum.
3. Set the spectral heights (vertical scale).
4. Repeat steps 1 through 3 for the next spectrum.
5. Send the completed plot to the printer.

1. It is important to work up the spectra in different experimental buffers i.e. (exp1, 2, 3, etc.). Therefore, join experiment #1 (**jexp1**), and load your first spectrum (let's assume this is the spectra you want at the bottom of the plot) and work it up in your usual way (i.e. **wft**, **phase**, **bc** (baseline correct) if you wish).

2. Determine the region you wish to plot:

Set the cursor brackets around the areas you want to print if you wish to expand on the spectra. You can do this several ways:

- ❑ You may decide you want a well-defined ppm region, for example from 7.0 ppm to 2.0 ppm. This can easily be accomplished by typing **sp=2p wp=5p <return>**. **sp** and **wp** are start and width of plot, respectively. This is the recommended method.
- ❑ Another method is to type **cr=7.0p** (left ppm value) and **delta=5.0p** (difference between right and left edge in ppm). Then click on ‘expand’.
- ❑ You may also manually select a region with the left and right mouse buttons, although this method may seem less cumbersome. Since it is important to get all of the spectra from top to bottom onto the same scale, you will need to type **cr?** and **delta?**. These values will be displayed in Hz. Record these values for the other spectrum. Finally click on expand.

3. Set the spectral heights:

You can manually set the vertical scale by using the middle mouse button, so that the spectrum fills half the window. If you want all peaks contained in half of the window, you can type **vsadj vs=vs/2**. Note that the default vertical position (**vp**) is 12 in order to shift the spectra up from the bottom of the page to allow enough room for integral values.

4. Repeat steps 1 through 3 for the next spectrum:

Join the next experimental buffer by typing **jexp2**. Read in the spectrum (**rt ('/pathname/mydatafile.fid')**) and work it up in the usual way. Now expand the spectral region using the parameters you determined in step 2. Type **cr=X** and **delta=Y** (*X* and *Y* are the recorded values from step 2), and adjust the vertical scale in the same way as above, for example with **vsadj vs=vs/2**. Now set the vertical offset by adjusting **vp**. A reasonable starting value is **vp=80**.

5. Send the plot to the printer

Type **pl pscale ppf** (or whatever you want on the plot) **<enter>**. Do not type **page!** This will send the most recent plot, scale, and peak frequencies to the plot buffer. Type **jexp1** to join the first experiment (experiment #1). Type **ds** (display spectrum) and **dscale** (display scale) to make sure everything is still OK. Then send this to the printer by typing **pl pscale** (or whatever else you would like on the plot) **page**. Your spectrum should appear in the selected plotter (printer).

Comments:

- ❑ You can plot several spectra on the same scale. Simply perform steps 1-3 on the third (or fourth or more) spectrum and change **vs** and **vp** correspondingly.
- ❑ An alternate method to plot spectra above each other is to create a whitewash plot (see "How to make a whitewashed stacked plot".)
- ❑ This method may also be used to plot both a ¹³C and a ¹H on the same page.
- ❑ When quantitatively comparing spectra of the same type (i.e. proton), it is imperative that you compare apples to apples. Therefore, you can only truly compare spectra where the *gain, number of transients*

(**nt**), and the *pulse width* (**pw**) are the same. Additionally, they must be displayed in absolute-intensity display mode (**ai**) in which the vertical scale is kept constant. The alternative is normalized-intensity display mode (**nm**) in which spectra are scaled to the largest peak. To query the current display mode type **aig?**.

- Spectra may also be printed in multiple columns, such as 2 columns of 3 spectra (see example below). The pertinent parameters to modify are **wc** (width of chart, in mm), **sc** (start of chart, in mm from right edge of plotter), **wcmax** (maximum width of chart, in mm), and **wc2max** (maximum width of chart in 2nd dimension, in mm). These numbers will vary from printer to printer, but the HP Laser Jets in this lab have **wcmax=250** and **wc2max=180**.