

## More on 2-D Data Sets

### Expanding 2-D data

Using the mouse, click the left mouse button on the lower left corner of the box to expand. Click the right mouse button on the upper right corner of the box to expand. Now click [**Expand**]. To see the full spectrum again, click [**Full**] or type **f full dconi**. The **>dconi** command shows the “color map” of the spectrum. To see contours, use **>dpcon**. Viewing 2-D data can also be improved by using the [**Resize**] to have a bigger window or using commands like **>center**, **>left**, or **>right** to move the spectrum around.

### Changing the vertical scale in a 2-D spectrum

The scale color bar on the right side of a 2-D spectrum can be used to coarsely adjust the vertical scale of a 2-D closer and farther away from the noise floor by using the middle mouse button. Alternatively, finer adjustments can be made using [**vs+20%**] or [**vs-20%**] or by typing in different values for the parameter **vs2d** i.e. **vs2d=1000**.

### Displaying and Plotting 2-D spectra with more contours

To show more contours than is automatically displayed, use a command that specifies the number of contours and spacing. To display this, **dpcon(20,1.2)** will display 20 contours at a spacing of 1.2. Other variations of this include **dpcon('pos',20,1.2)**. The modifiers ‘pos’ and ‘neg’ will display only the positive or only the negative peaks in a 2-D spectrum. To make the contour display interactive, use a variation of **dconi** such as **>dconi('dpcon','pos',20,1.2)**.

To plot more contours, **pcon(20,1.2) pltext page**. Adjust the number of contours and spacing for the data. The ‘pos’ and ‘neg’ modifiers can also be used in the plotting.

### Putting Projections on a 2-D plot

1. Projections (1-D) on the edges of 2-D plots can be useful for small molecule interpretations. To display 1-D projections from the 2-D data (lower res.), start with **>center dconi** then use [**Proj**] and then select [**Hproj (max)**] or [**Vproj (max)**]. Sometimes the sum is better so check both.

To plot the spectrum with the projections on it: plot the spectrum (don't send it to the plotter) as in **>pcon(20,1.2) pltext**, then display one of the projections as above. Use the [**Plot**] from the [**Proj**] menu. Display the second projection and use [**Plot**]. Then send the entire plot to the printer **>page**.

2. Projections from 1-D high-resolution spectra

**>fullt dconi** -or- **>center dconi**

**>pcon** (can also add modifiers such as **pcon('pos',20,1.2)**)

**>jexp#** join the experiment containing the 1-D spectrum

**>partop** macro for adding the projection on top of the spectrum

Prompt for exp. # of 2-D experiment

Adjust the vertical scale of the 1-D spectrum.

**>pl('top')**

**>parside** macro for adding the projection to the side of the spectrum

>pl('side')

>page

Note: The partop and parside macros may not be in every /vnmr/maclib but facility personnel can locate them.

### Processing 2-D data sets manually

This routine applies to most phase-sensitive 2-D data sets. COSY requires a slightly different approach and often uses a pure sinebell function.

Start by processing the first increment with >wft(1)

Phase this spectrum as any 1-D.

Then add a weighting function to this data with >wti

Use the interactive weighting screen to add a weighting function. The most commonly used function at this step is a gaussian function [gf].

Then process the data with >wft1da

After the data is processed, the f1 traces will be on the screen. If a display error occurs, use >f full dconi

Select a trace with the cursor. Try to use something other than solvent. Then weight this trace with >wti

This weighting function can also be a gaussian function [gf], but often a shifted sinebell is used. To put in a shifted sinebell, start with [sb] and move the cursor to produce a sinebell curve that is about twice the width of the interferogram. Then select [sbs]. Using the cursor, shift the sinebell back so the maximum starts at the left side of the interferogram.

Process the 2-D data with >wft2da

### Phase correction

Phase errors in phase-sensitive 2-D data sets can often be seen near the diagonal where the peaks may be streaked positive and negative.

Display the entire 2-D spectrum. Choose 3 traces containing cross peaks near the top, middle and bottom of the spectrum and note the index #'s of each trace. The index # of the trace can be seen in the top window of VNMR next to the seq. and exp #. Set

>r1=index# r2=index# r3=index#

The values r1-r3 are place holders in VNMR. Then display the first trace:

>ds(r1)

Phase the 1-D trace. Display the 3<sup>rd</sup> trace.

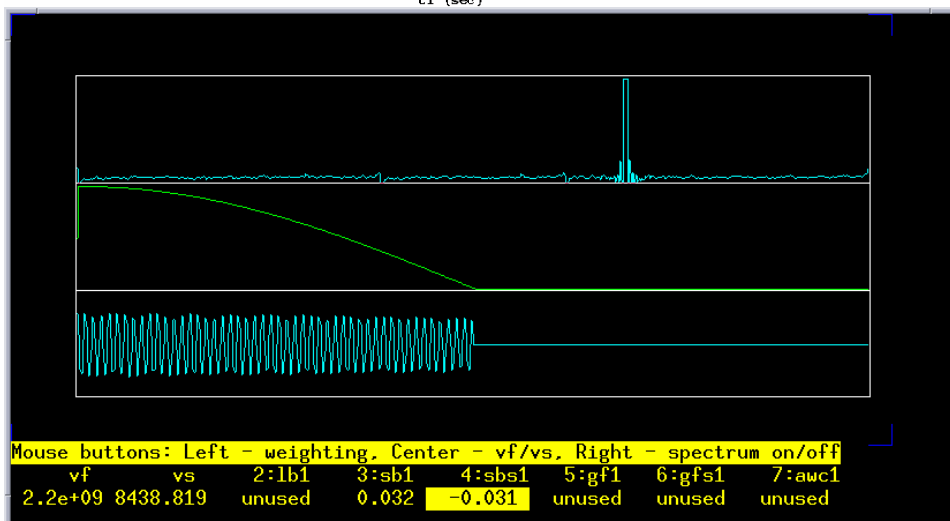
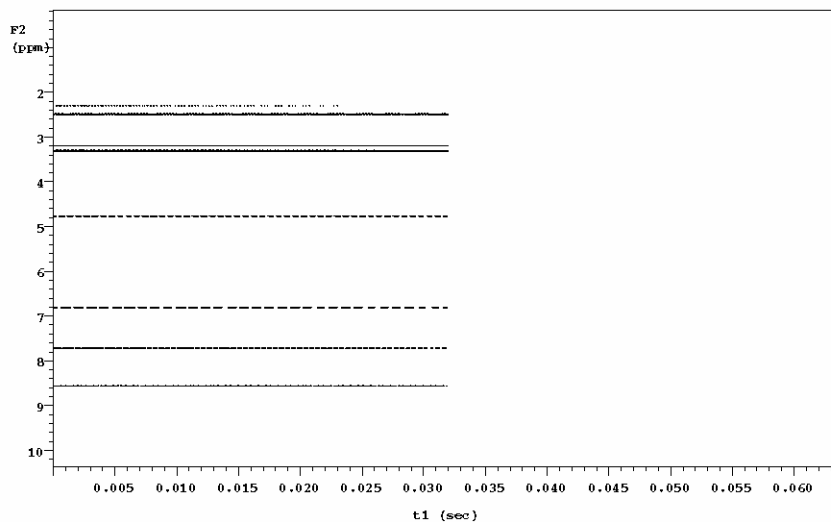
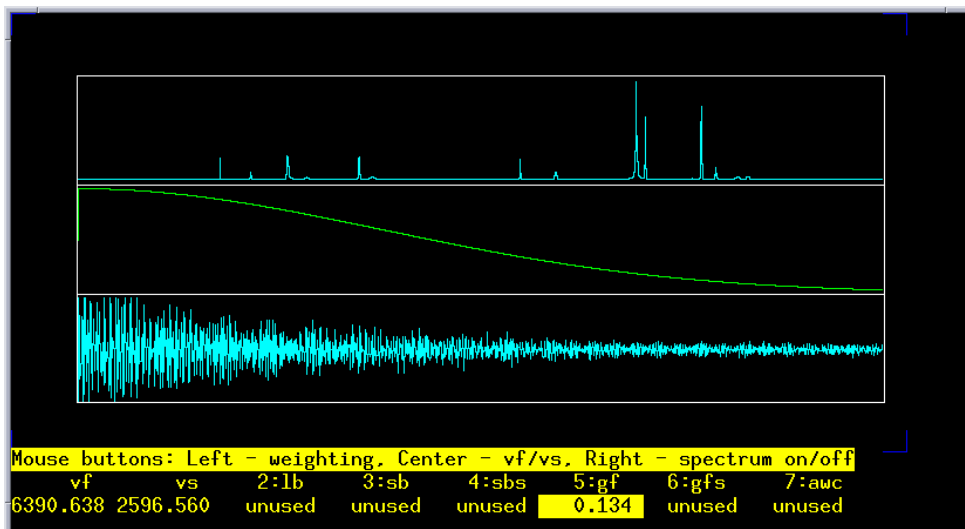
>ds(r3)

Click [Phase]. Click the left mouse button on both sides of the spectrum to accept the previous phase changes. Then phase this trace.

Go back to the first trace >ds(r1)

Continue phasing r1 and r3, clicking to accept phase changes in-between until they are both phased. Look at the middle trace to check >ds(r2)

Then go back to the 2-D spectrum: >dconi



**Figure 29:** Manual 2-D processing includes weighting of f2 (top), selecting a trace from the transformed f2 (middle) and weighting the f1 (bottom).