

XVII. Fitting Partially Overlapping Peaks – Deconvolution in VNMR

- prepare baseline region by clearing all reset points: type **cz**
- click on PARTIAL INTEGRALS
- click on DISPLAY NEXT RESET and pick integrals over all sections that are NOT good baseline regions (i.e., this is not to get good integrals, but to define regions of good baseline)
- resave the data to allow simple restarting at this point; use **svf('...')** command
- use **bc(5)** or similar; I recommend you *not* use **bc** which applies a spline fit (this is a very dangerous command that can seriously modify the shapes and integrals of peaks)
- click on DISPLAY INTERACTIVE NEXT TH to change the threshold level; you want to go just below the smallest obvious peak, but not down to where a lot of noise from a large peak will be picked up
- enter **mark('reset')** to ensure that all previous marks are deleted
- move the cursor to each “normal” peak and press MARK (this enters the center frequency and uses a default linewidth)
- move right and left cursor to the approximate half-height points of broad peaks and click MARK (this enters the average of right and left cursors for the center position, and the difference between right and left cursors as the width)
- by opening a shell tool and entering **cd ~/vnmrsys/exp1 more mark1d.out** you can see the file that the MARK command built and will use
- click on MAIN ANALYZE DECONVOLUTE USE MARK FIT to perform the fit
- if you get a “too many points” error message, enter **FN=FN/2 WFT BC(5)** and click through to the FIT command again; keep reducing FN until it will fit
- use the PLOT button to get a quick plot
- use the commands CLRADD SPADD ADDI to compare two spectra