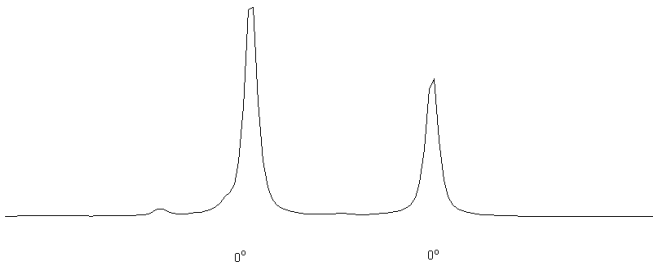
4. Primers for Areas of Common Interest

by *cg fry*: created 2 May 1996 – revised 13-Sep-00

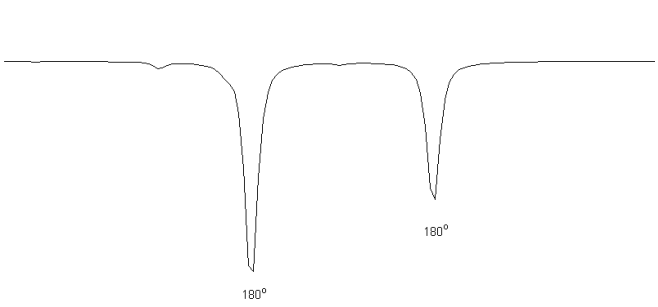
I. Primer on phasing

Phasing involves turning all lines in a spectrum into pure adsorption lines:

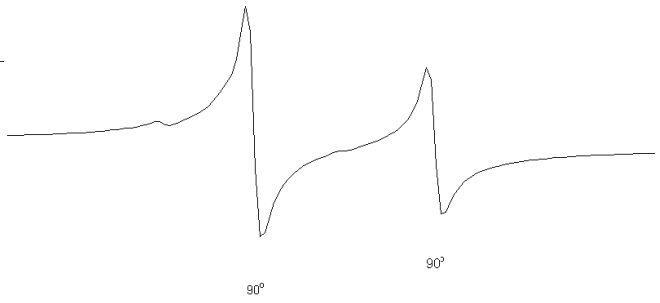


Pure Adsorption

Zero-order phasing rotates all lines in the spectrum identically:

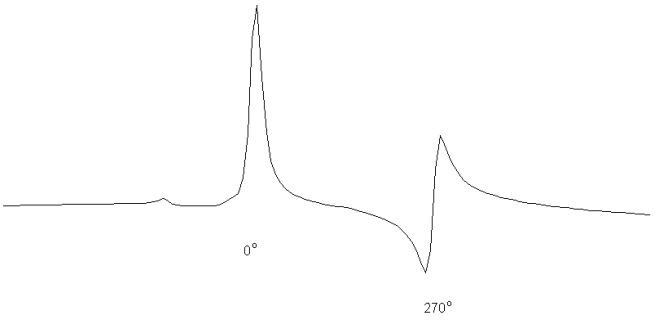


Inverted Adsorptive



Pure Dispersive

First-order phasing rotates lines progressively faster as one moves away from the "pivot" line. The pivot line is assigned in *NUTS* by placing the cursor on a line in the spectrum, and holding the left mouse button down while pressing the P key (*left-hold* P). Since the pivot line does not change angle under 1st order phasing, this is the line that should be correctly phased when performing 0-order phasing:



Mixed Adsorptive and Dispersive

In the other primary method for phasing spectra in *NUTS*, the PS-mode, the tallest peak the zoom region 1 is automatically assigned as the pivot. Chosing between PH or PS modes depends for the most part on the number of points and resolution of the peaks. For most ^1H spectra the PH method works fine. But for very high digital resolution spectra, PE can work better—the data reduction done on entering is less dramatic because of the expansion. See the NUTS help and tutorials at the Acorn website at http://www.acornnmr.com for assistance with both methods. But the primary philosophy stays the same:

- increase the vertical scale of the slope until the baseline is obvious,
- perform 0-order phasing (using the left mouse button) on the peak at the pivot point; the best indicator of reliable phasing is that an extrapolation (by eye) of the baseline would have it connect smoothly under the peak (note in the figure above how the baseline of the 270° dispersive peak runs in essentially opposite directions—curving down the page coming from the left-hand side and up the page coming from the right-hand side—but connects under the absoptive 0° peak,
- perform the 1st-order phasing on a region far from the pivot point,
- ignore the phase of TMS and other solvents peaks (often may be slightly out-of-phase with solute peaks due to saturation effects).

In *PCNMR4Windows* the pivot line is chosen automatically, and colored red. There are a number of ways to phase spectra in *PCNMR4Windows*, but the method I (*cgf*) prefer is:

i) always perform 0th order  phasing on the red peak: start by expanding about the red peak, enough to give clear definition to the peak, but not so much that you cannot see a good amount of baseline on both sides of the peak

ii) scale up by clicking the the  button three or four times (enough to give the baseline better definition)

iii) I like to press and hold the left mouse button while phasing; letting go of the button then fixes the phasing. The other method of click the left button, phasing, and then clicking the left button again to fix the phasing I have problems with; I find that often on the second click, the phase jumps slightly ruining the phasing I had worked to get. *Note that only up-and-down (away-and-towards you) motions of the mouse effect the phasing; sideways motions do nothing.*

iv) use **Display Reset** the expand about the peak *furthest* from the red peak

v) click the  button to get 1st order button (blue)

vi) click and hold the left button: up and down motions of the mouse adjust the phasing; release the button to fix the phasing

vii) use **Display Reset** ; if the phasing looks good—the baseline should appear continuous if followed through all peaks—then press the  button