Paramagnetic Samples XWINNMR

Paramagnetic peaks have a very short T1 (Relaxation time), therefore very rapid pulsing can be done with typical ^{1}H Sweep Widths of 200 ppm. Line-Broadening values of 20hz or larger are used to improve the Signal-to-Noise. When Phasing, set the phase on the paramagnetic peaks & ignore the phase for the diamagnetic peaks. The Spectra will have severe baseline-roll, so "spline automatic baseline" {sab}correction will be utilized for the spectral region of interest. Sometimes the residual HOD peak will need to be Presaturated, refer to the Presaturation Instructional handout.

Set NS = 10,000 or larger

DS = 16

Acquisition Time will be 0.1 to 0.2 sec

D1 = 50ms to 100ms

AQ-Mode will be qsim instead of DQD, so baseline correction will be required.

Use "**tr**" command to monitor progress of Acquisition Signal-to-Noise & "**halt**" if OK

LB = 20

efp

BASELINE Correction:

expand to desired region (i.e. 90ppm to 20ppm)

- **basl**

click on **defpoints** *button*

click Mouse-2 *to define points* (10 to 16 points not on top of a peak)

click return……..return

- **sab**

With the large Dynamic Range difference between the Diamagnetic peaks & the Paramagnetic peaks, for **Peak Labels** on the plots, sometimes "**PC**" needs to be changed from value = 1 to **0.1**

Use layout "H1_Para-js.xwp" for Plots