

Current Instructions for Measurement of Self Diffusion Coefficients on I500
Doug Brown, Indiana University 8/30/2006

- 1) Calibrate sample temperature for most accurate results.
- 2) Calibrate the value of gcal (gradient strength in G/cm per DAC unit). One method is in the Varian Acceptance Test Procedures manual using the setgcal macro and doped D2O sample. The I500 has 32767 dac units so the maximum gradient strength = gcal * 32767. For the HCN probe gcal has been measured as 0.00215 (70.5 G/cm max) and for the Nalorac probe 0.00130 (42.6 G/cm max).
- 3) Call in parameters for the the pulse sequence. We currently use DgcsteSL_cc which is a descendant of several other pulse sequences and features self compensating gradients and convection compensation.
- 4) Establish acquisition parameters including 90 degree pulse, appropriate d1 relaxation delay and enough transients (nt) to get useable S/N. Do not spin the sample.
- 5) Set up a linear array of gzlvl1 values. So far I typically use 16 from 2000,3000, 4000 etc. to 17000. The macros can also support exponential arrays.
- 6) When the experiment is finished phase and baseline correct the spectra. Clear any integral set points with "cz" then define one integral area to use for the calculation ("z" on either side of the peak).
- 7) The macro doug_process will do the rest to give a diffusion coefficient and display the fit. 10% H2O in 90% D2O is about 2.0×10^{-9} m²/s for reference.

The macro beeps and gives a "grad_list" error message, it is a bug with the array command and systemglobal variables. This is a hacked (by Doug) version of Brian Antalek's "decra" package in the Varian User Library which in turn uses some modified Varian diffusion measurement macros.