Using the lock channel to get deuterium NMR spectra

E. Alvarado, U of Michigan, 08/13/10

Our Varian spectrometers are capable of detecting deuterium spectra easily by using the lock channel. The probe's lock coil is already tuned to deuterium and no further adjustments are necessary. The cable changes that are needed are done automatically by the software. The user only has to shim the sample (see below) and specify the lock channel as the name of the nucleus to detect: tn=lk. In our old Inova spectrometers, type rtp('/vnmr/stdpar/lk') in the command line to load the appropriate parameters; and in our new Varian consoles, select Deuterium from the list of nuclei on the main menu: Experiments > Other Nucleus. Change the solvent as usual but select an equivalent deuterated solvent when you are using a non-deuterated one. Turn the lock off and shim the sample before you start the acquisition.

Note that sensitivity and resolution won't be as good as they would be if a switchable probe tuned to deuterium were used, but for most common purposes the spectra acquired this way will normally be satisfactory. Deuterium signals are broadened by the quadrupolar relaxation of the nucleus, thus the degraded lineshape obtained with the lock coil may not be noticeable. Referencing can be done by setting the reference on the proton spectrum in another workspace and using the mref macro described in a separate application note. Broadband proton decoupling can be done by typing dm='nny'.

Shimming non deuterated solvents (and deuterated ones too!)

One of the problems with acquiring deuterium spectra is that the solvent should be non deuterated, thus locking and shimming on the solvent's deuterium signal is not possible. However, shimming can be done with proton gradient shimming or by monitoring the FID as described in the writeup "*Gradient shimming non deuterated solvents*" available in our web site. As usual, load the standard set of shims with the command setlock before shimming.