^{2}H NMR Experiments in TopSpin and IconNMR

updated: 20160205 (hh+cgf)

^{2}H (deuterium) NMR experiments require the use of non-deuterated solvents: oddly enough, you will be acquiring a form of no-D NMR spectrum (so the write-up for no-D is similar to that below). On all our spectrometers, we use the simplest method for ^{2}H observation by using the lock channel. Sensitivity is best on cryoprobes (esp. callisto), but will be adequate in most cases on other spectrometers and probes.

A. ***Initial Setup:***

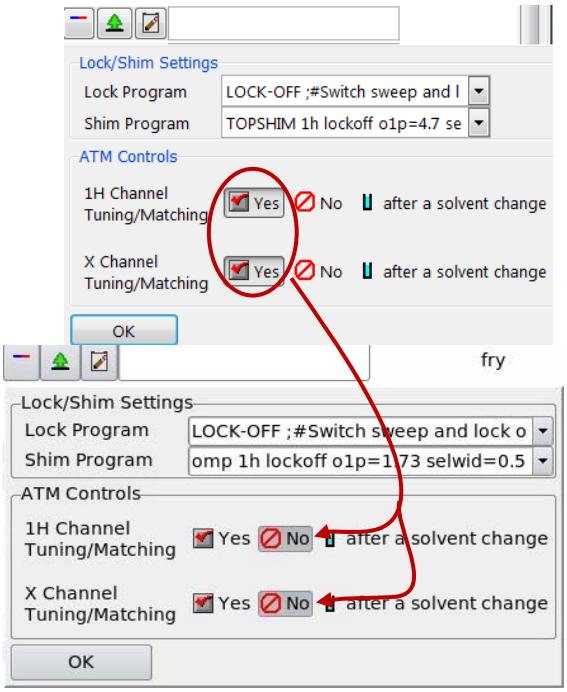
1. Read in parameter set *probename*_H2lk.sUW. The parameter set will be probe specific so make sure to choose the correct one.
2. In the acqu tab set lock to: **LOCK-OFF**
3. ***Do NOT tune and match (atma).*** The instrument will try to tune and match on the X-channel, not the lock channel that is used for acquisition.

B. ***Shimming:***

1. In TopShim, set options: **1h lockoff o1p=<value in ppm> selwid=0.5**
2. If topshim says it's reducing the echo time, add **convcomp** to the line above (always use convcomp with the Prodigy and DCH cryoprobes).
3. Staff prefers **selwid=0.5** in the above, which changes from the default 1 ppm selection width to 0.5 ppm. If that doesn't work, find us….

C. ***^{2}H NMR in IconNMR run on Callisto:***

To perform ^{2}H NMR on callisto, get *cgf* to add the **DCH_2Honlock** experiment to your list. Then change all four setting in the lock panel shown below.



Know your protonated solvent: you must know the value for **o1p** to shim (see section A in the no-D page if you don't).

Click the Change Lock icon and do the following:

a) Lock Program to: **LOCK-OFF**.

b) Shim Program to: **TOPSHIM convcomp 1h lockoff o1p=?? selwid=0.5**

where ?? is the chem. shift of your protonated solvent as found in section A above.

c) **IT IS CRITICAL(!!)** to click both 1H and X Channel Tuning/Matching to **No** (see fig). Failure to do so will interrupt proper locking for other queued samples.