Department of Chemistry
NMR Facilities
Director: Dr. Carlos A. Steren

NMR NEWS December 2013

* To find tutorials, links and more, visit our website www.chem.utk.edu/facilities/nmr

* New Student Operators at the NMR Facilities.

Three new Student Operators started this fall. They are,

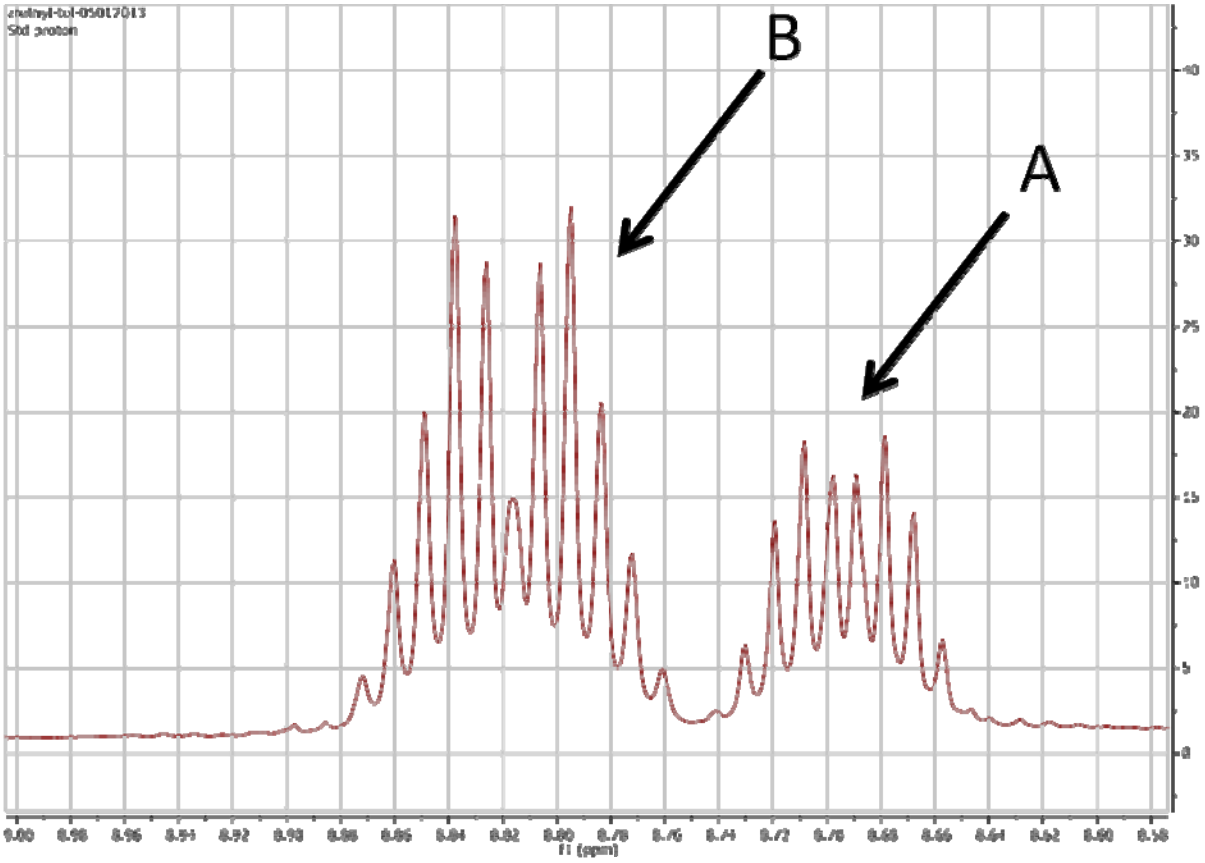
Mr. Wei Lu (wlu14@utk.edu**)** helping with the AC/Tecmag 250 MHz and the Varian 300 MHz.

Mr. Kevin Gmernicki (kgmernic@utk.edu) helping with the Bruker 400 MHz and Varian 400 MHz.

Mr. Roger Wright (rwrigh23@utk.edu) helping with the Varian 500 MHz and Varian 600 MHz.

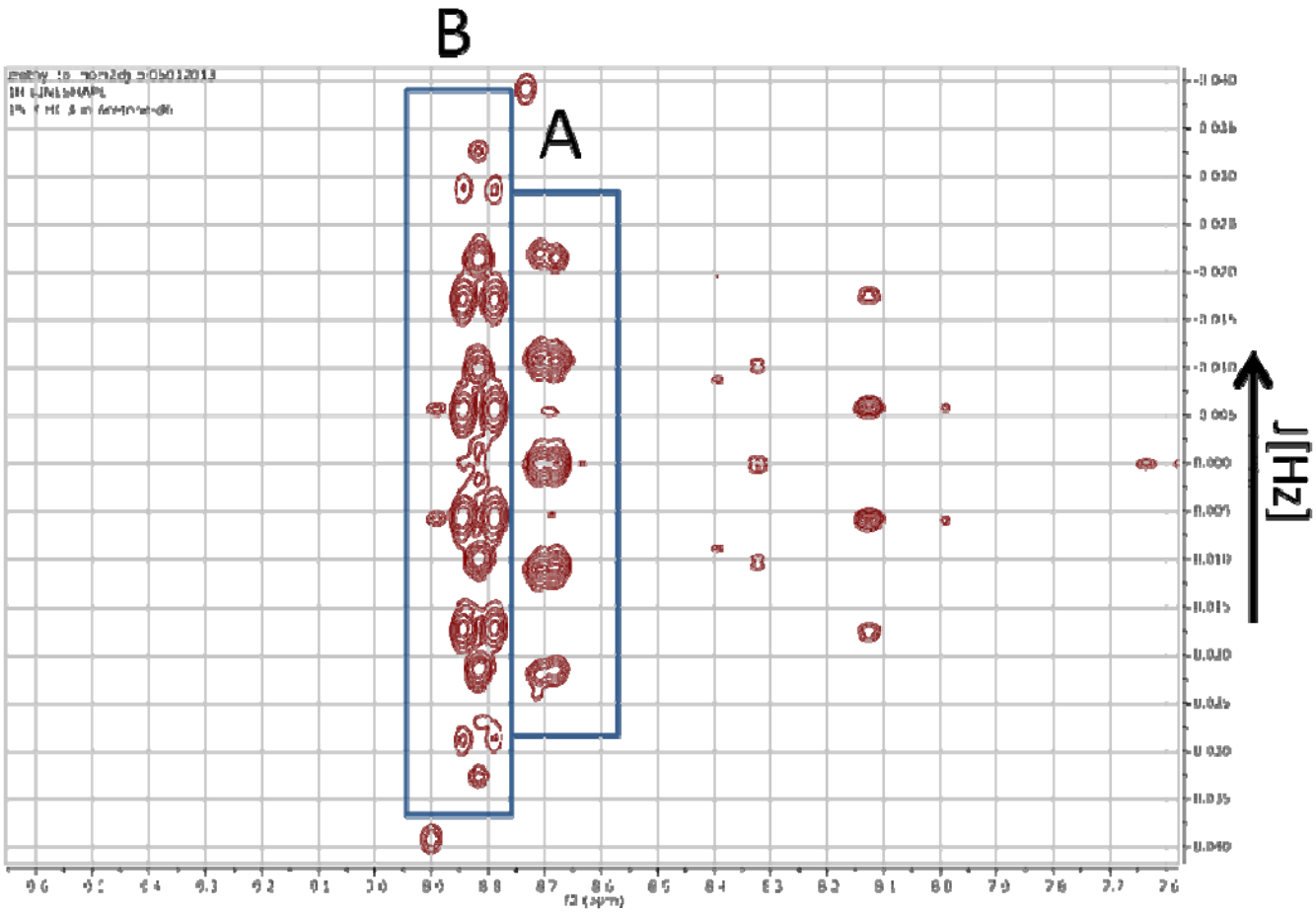
* 2D-J Resolved ^{1}H NMR Spectroscopy

Attempting to model the splitting patterns of ^{1}H NMR resonances is not always an easy task. This is the case for the groups of lines A and B of the ^{1}H spectrum shown below.



For these difficult cases, the “2D Homonuclear J-modulated” experiment can provide additional information and help in the understanding of the splitting patterns of ^{1}H NMR lines.

In the graphic shown below, the 2D ^{1}H homonuclear J-modulated spectrum of the groups A and B is displayed. The homonuclear splitting patterns are resolved in the second (vertical) dimension. J coupling values are directly measured on the vertical axis. The horizontal axis is the chemical shift of the ^{1}Hs.



Now, just at first glance, one can see on the 2D spectrum that group A is actually composed of two ^{1}Hs with different chemical shifts. Each ^{1}H signal is split into a quintet but with a slightly different J coupling.

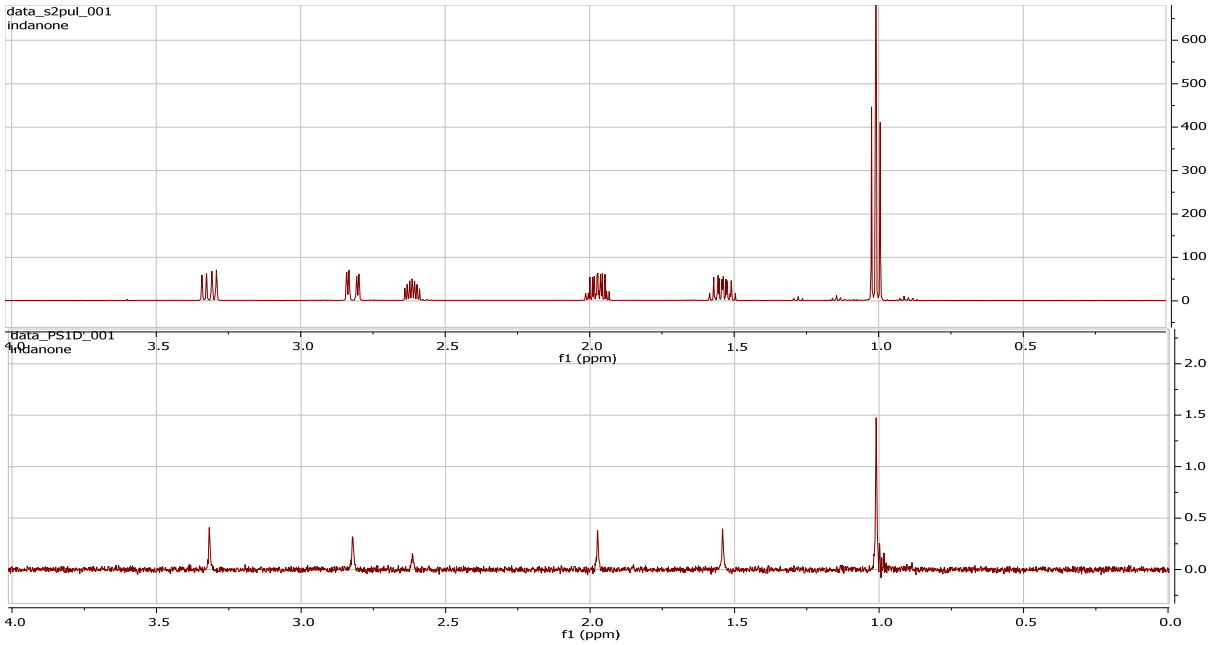
Group B is composed of three protons with different chemical shifts. The proton in the middle is split into two quartets. The other two ^{1}H are split into sextets (or maybe two overlapping quartets).

* Pure shift ^{1}H NMR

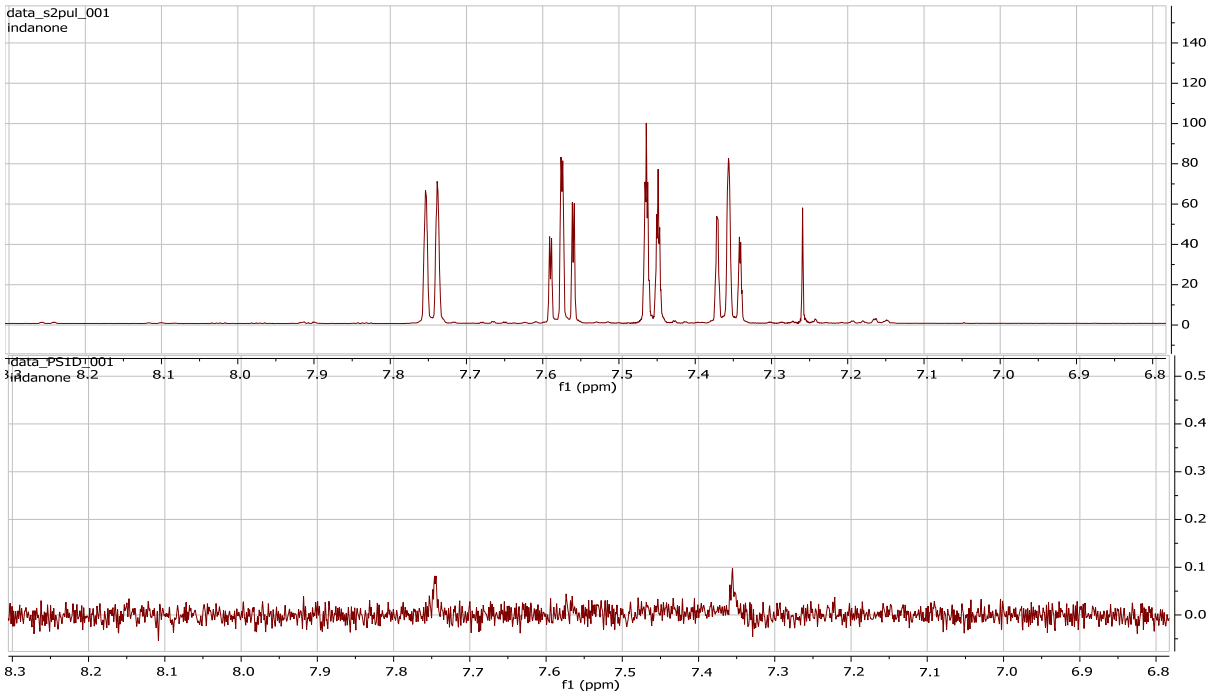
Until recently, a homonuclear decoupled ^{1}H spectrum was only attainable in an indirect way. It had to be done first recording a 2D J modulated Homonuclear spectrum like the one discussed above, then projecting that spectrum onto the horizontal axis.

Now that is not the only way anymore. A new pulse sequence, "pure shift ^{1}H NMR" has been developed that allows homonuclear decoupling on a 1D ^{1}H spectrum.

In the Figure below, the aliphatic region of the ^{1}H spectrum of a sample of 2-ethyl-1-indanone is displayed. The ^{1}H pure shift spectrum is shown below the ^{1}H spectrum.



The aromatic region of the ^{1}H and ^{1}H pure shift spectra of 2-ethyl-1-indanone are displayed in the Figure shown below. The homonuclear decoupling does not work well for the two middle proton lines, where there are strong second order J couplings.



* HMQC in 1 minute!!

A new HMQC pulse sequence available on the Varian 500 allows for the acquisition of a 2D HMQC spectrum in just 1minute! The only disadvantage as compared to a standard gHSQC (that takes 10 minutes) is that the carbon signals are not edited. All the CHn cross peaks have the same phase.

For more information on the experiments discussed in this Newsletter, contact me at steren@utk.edu.