

NMR NEWS

January 2015

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www.chem.utk.edu/facilities/nmr

* DEPTQ

In the past, there was a difference between a DEPT and an APT experiment; non protonated carbons were not observed on DEPT spectra.

Now, that has changed. The DEPT experiment has evolved. The new experiment, dubbed DEPTQ, allow us to observed non protonated carbons. Below, the different carbon signals observed on DPTQ and DEPT spectra are detailed. Blue and red indicate signal phase up or down respectively.

DEPTQ 45°
C, CH, CH₂, CH₃

DEPT 45°
CH, CH₂, CH₃

DEPTQ 90°
C, CH

DEPT 90°
CH

DEPTQ 135°
C, CH, CH₂, CH₃

DEPT 135°
CH, CH₂, CH₃

DEPTQ is available on the Varian 500 and Varian 600 spectrometers. A tutorial is available on our website.

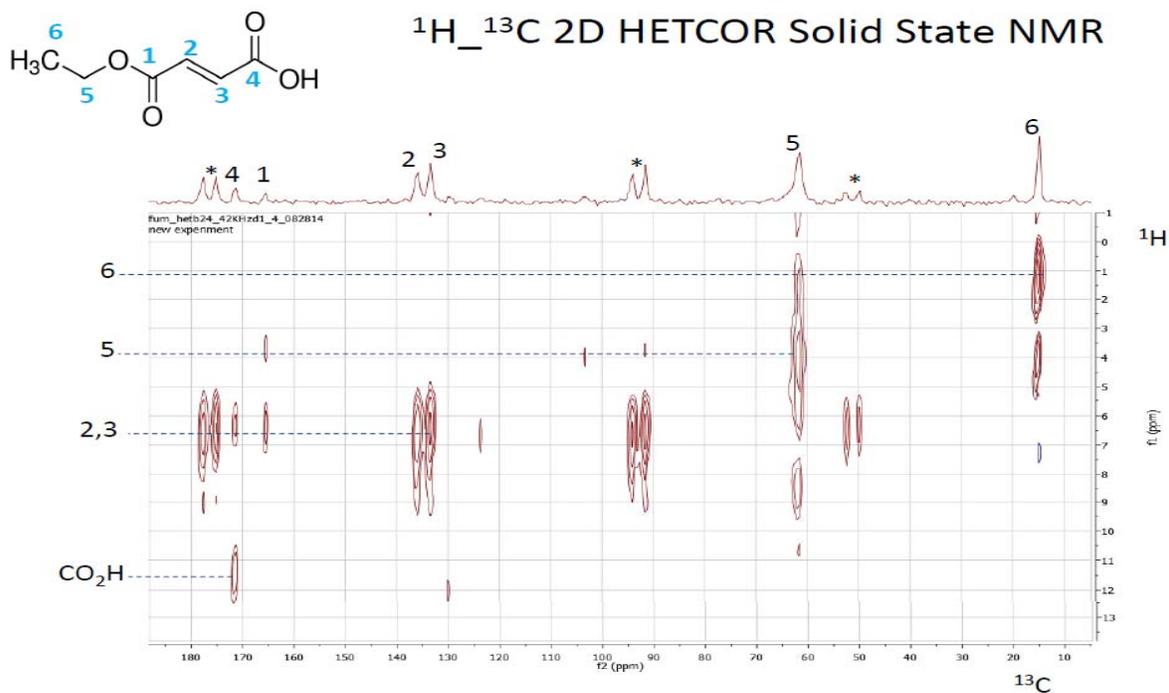
***Solid State HETCOR**

There are 2D HETCOR experiments available for Solid State samples.

The C-H interaction that generates the 2D correlations and cross peaks is the heteronuclear dipole-dipole interaction (through space interaction). In contrast, in the liquid phase, the J coupling interaction (through bond interaction) generates the correlations in the HETCOR and HSQC spectra. Hence, cross peaks in a SSNMR HETCOR spectrum are similar to proton-carbon "NOESY like" (through space) cross peaks.

The HETCOR spectrum resolves the ^1H signals on the vertical axis. The MAS spinning rate is $\sim 4\text{KHz}$. At these spinning rates, the direct ^1H spectrum only shows a single broad signal.

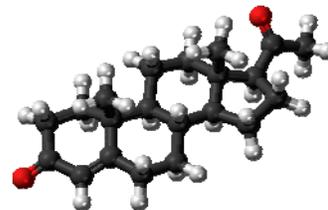
The figure displayed below shows a ^1H - ^{13}C 2D Solid State HETCOR spectrum of monoethyl-fumarate.

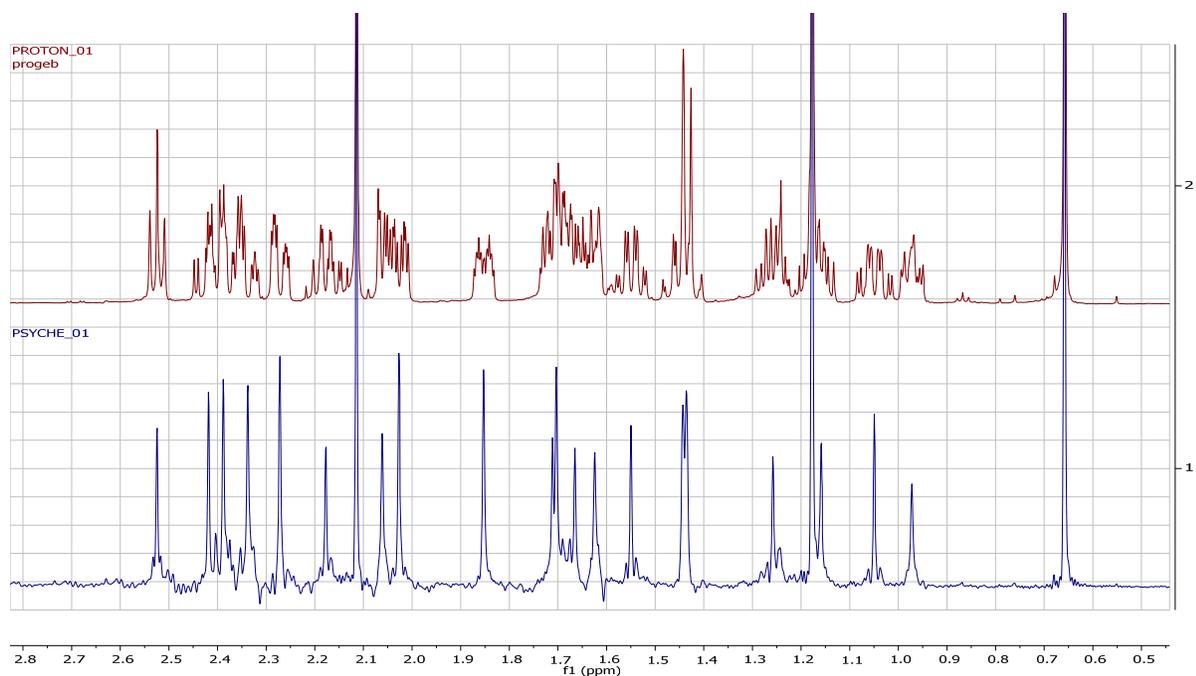


* More on Pure shift ^1H NMR: PSYCHE.

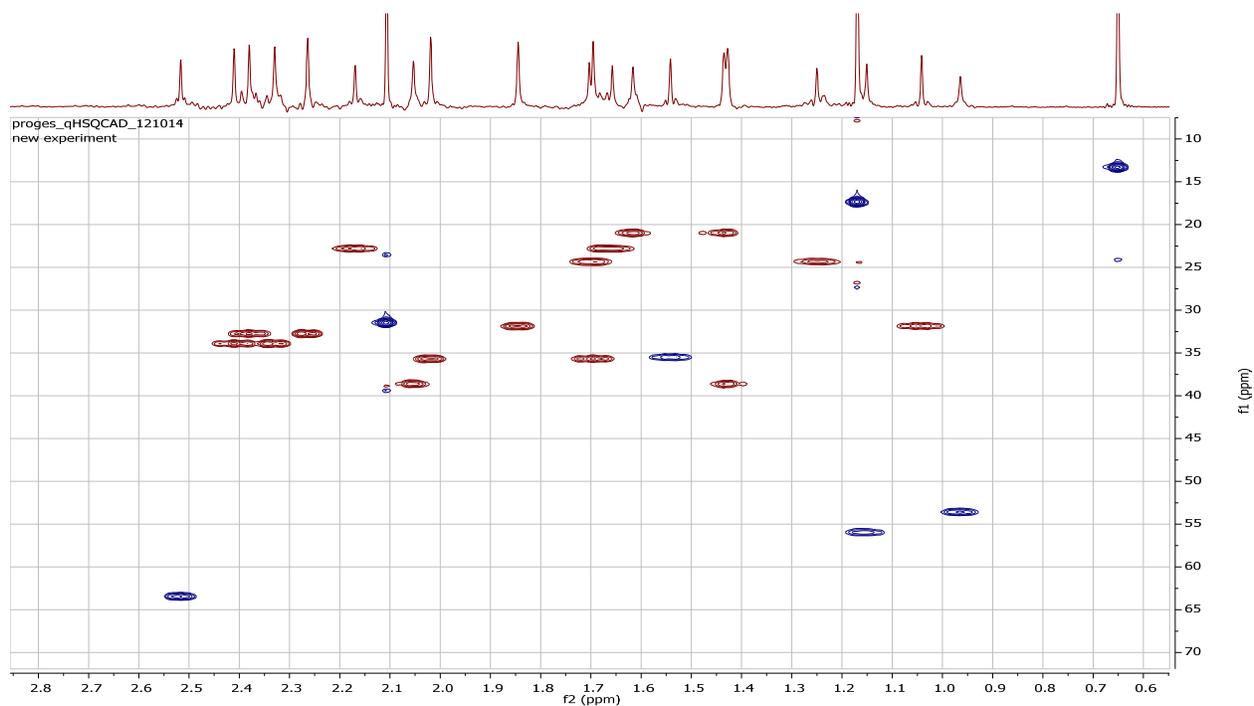
A new pulse sequence, Psyche, for “pure shift” ^1H NMR experiments is available on the Varian 500 and Varian 600. A “pure shift” ^1H spectrum displays a single peak for each proton in the sample. This is similar to a standard ^{13}C spectrum, where a single peak without splitting is observed for each carbon in the sample.

In the Figures shown below, the ^1H spectrum of a sample of progesterone is compared with its pure shift ^1H spectrum.





In the next figure, by comparing with the HSQC spectrum, it can be observed that most of the proton peaks are resolved on the pure shift ^1H spectrum.



A tutorial on PSYCHE, pure shift ^1H NMR, is available on our Facilities website.