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NMR NEWS March 2011

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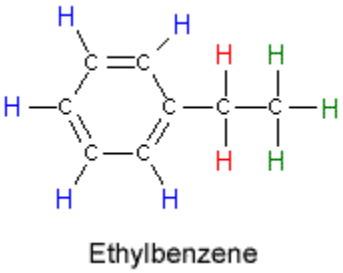
*Integration of ^{1}H NMR lines.

The integration of NMR lines on a ^{1}H spectrum is a powerful tool that helps identifying and verifying the structure of molecules. The area under an NMR line is proportional to the number of protons in the molecule that generate that particular signal. Thus, integrals allow to identify/verify chemical groups of the molecule in the solution.

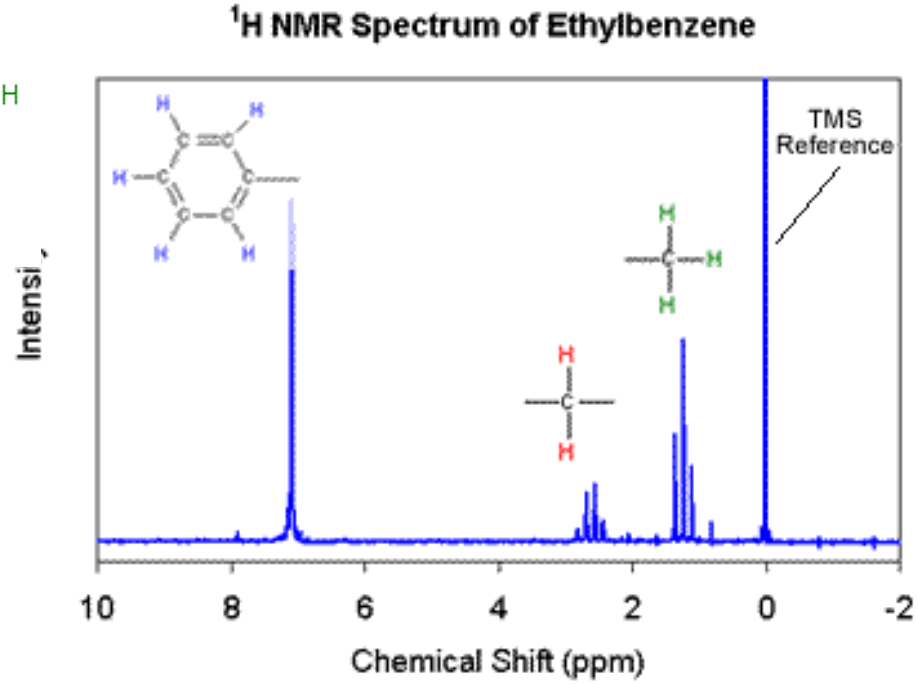
As an example, a 1D-^{1}H spectrum was acquired on an ethylbenzene sample.

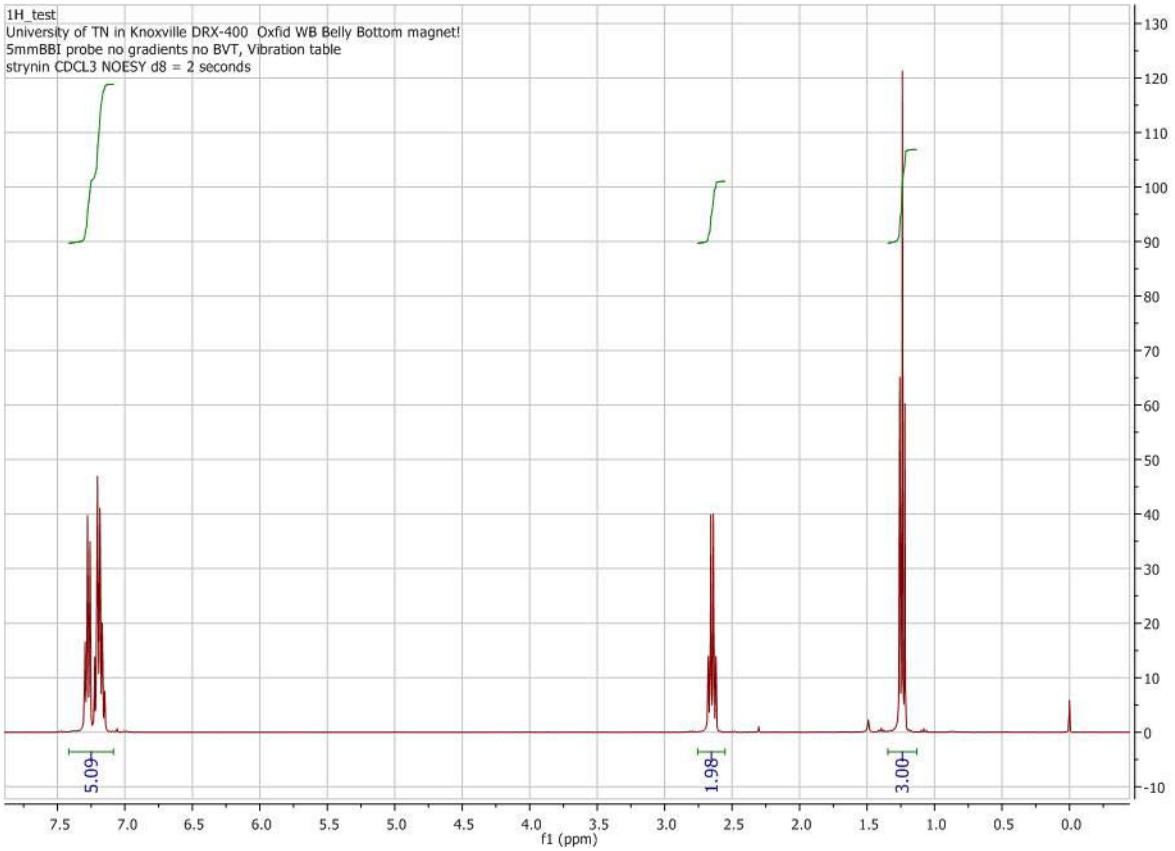
Integrals were calculated on the spectrum. The values of the integrals are presented as ratios, relative to a particular integral chosen as a reference, and typically set to 1.00.

When the number of protons generating one of the peaks is known, that particular integral can be set to the known value. Then, the values of the other integrals will be directly related to the number of protons in those NMR lines.



Ethylbenzene





In our example, the integral of the methyl group was chosen as the reference and set to 3.

As observed in the spectrum shown above, the values of the integrals reflect the number of protons in the methylene and aromatic groups very accurately.

Recently, there has been some concern about the accuracy of the integral values calculated by MestreNova as compared to those calculated by the Bruker and Varian software.

To investigate this, 1D-^{1}H spectra of Ethylbenzene was acquired on the Bruker 400 MHz and on the Varian 300 MHz spectrometers. The spectra were then processed with XWinNMR (Bruker), VNMRJ (Varian) and Mestre Nova. In the table displayed below, the integral values calculated by the different programs are compared. The integral of the methyl group was used as the reference for all cases.

Software	**Aromatic ring**	**CH_2**	**CH_3**
Bruker	**1.71**	**0.67**	**1.0**
MestreNova	**1.70**	**0.66**	**1.0**
Varian	**50.05**	**19.71**	**30.24**
MestreNova	**49.98**	**19.69**	**30.24**

From the results shown in the Table, one can conclude that the integration with MetreNova yields the same values as integration with the Varian or Bruker programs.

Users should be aware that VNMRJ has two ways of normalizing values of the integrals. One method is called “Sum” and the other one is called “Single Peak”. To obtain the same results in VNMRJ as with MestreNova, normalization by “Single Peak” must be selected.