^{1}H-NMR SPECTRA DETERMINATION

Chemistry 118B Workshop
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1. <u>Determine the degrees of unsaturation.</u>

   Step a) $H_{sat'd} = 2(C)+2-X+N$

   Step b) $\dfrac{Hsat'd - Hactual}{2}$ = degrees of unsaturation

2. <u>Determine the number of signals.</u> Each signal represents a group of chemically equivalent protons, H's (or a single H).

3. <u>Relative intensity of signal.</u> The area under a signal is proportional to the number of equivalent protons for that signal. (If the spectrum does not provide an integration line, measure the height of each integration line from shoulder to shoulder; use the smallest value as a divisor of the other integration values. The answers should give an idea of the ratio of protons for each signal.) Professors usually give the integration of the signal.

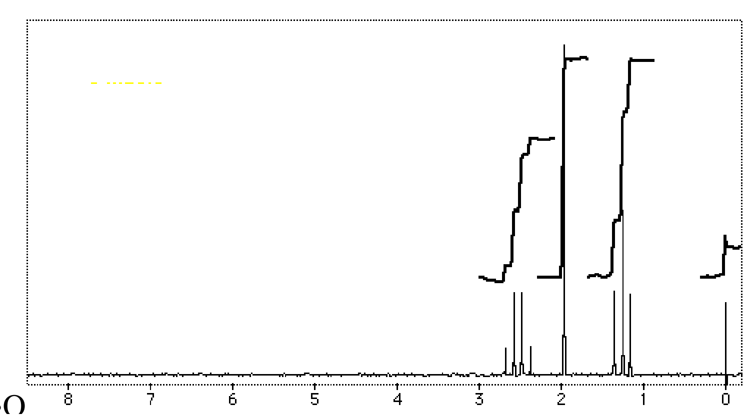
4. <u>Chemical shift.</u> This value gives information about the electron environment around the protons. For example, the more an element attracts electrons, the more the proton is deshielded.

   Memorize the chemical shift ranges for the various electron environments.

5. <u>Spin-spin splitting (coupling): the (**n + 1**) rule.</u> Chemically non-equivalent proton nucleii mutually split each other's signals. The result is the N + 1 rule: That is, if some proton designated H_a has **n** magnetically **non-equivalent neighboring H's** to itself, the signal for H_a will be split into n + 1 peaks. Equivalent nucleii, protons which have the same chemical shift, do not split each other. [For Chem.118B: The coupling constant, J , (or]), is the distance in Hz between two of the peaks in a split signal. The distance J is the same for non-equivalent proton nucleii signals which split each other.]

   example: A single signal, a singlet, has no neighboring non-equivalent protons. A triplet signal must have a total of two neighboring protons which are non-equivalent to the protons which generate that triplet signal. A quartet signal must have a total of three neighboring protons which are non-equivalent to the protons which generate that quartet signal.

   Show the structure that produced the following ^{1}H-NMR spectrum:



Ex. 1: C_4H_8O