These notes can be obtained at: http://www.ndsu.nodak.edu/instruct/grcook/chem342/notes.shtml

Chapter 13: Nuclear Magnetic Resonance Spectroscopy

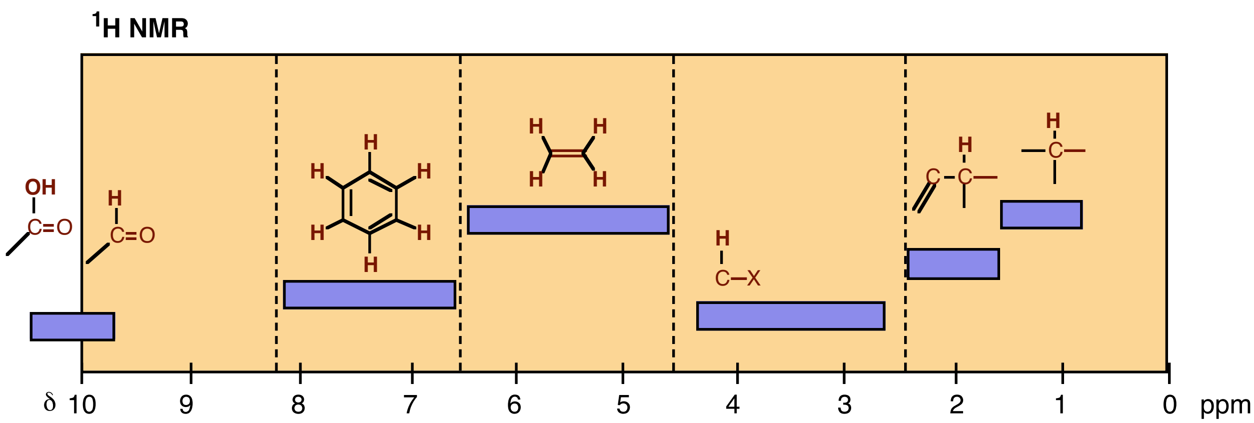
^{1}H NMR Spectroscopy

Provides the number of chemically different protons in the molecule.

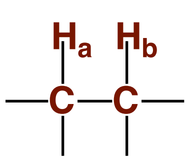
The area under the peaks provides information on the relative number of protons at each resonance.

Spin-Spin splitting (or coupling) provides information about what protons are neighboring what protons.

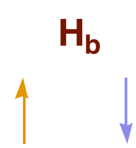
Most protons show resonances in the range of 0 to 10 ppm. There are five regions which one can find different kind of hydrogens.



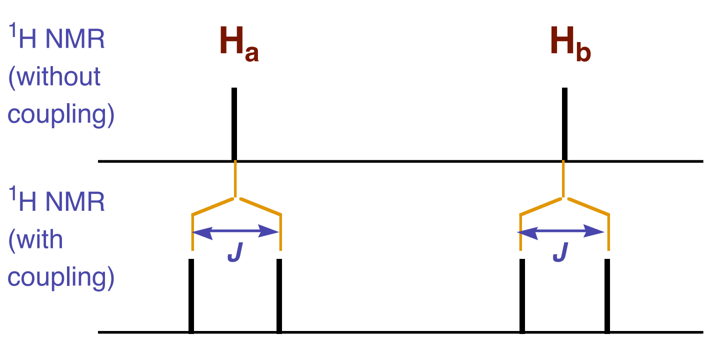
Spin-Spin splitting occurs because each proton feels an influence of the neighboring proton spin states. Peaks will be splint into n+1 peaks, where n is the number of H's.



H_a is split into 2 peaks becuase H_b has two spin states, one aligned with the field and one against.

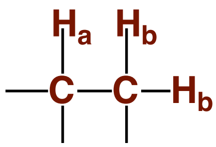


likewise, the H_b proton will be split because of the two spin states of H_a

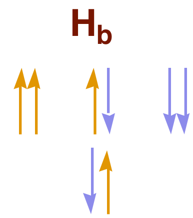


Protons which are coupled to each other will each be split the same distance. This is referred to as the **Coupling Constant (*J*)**

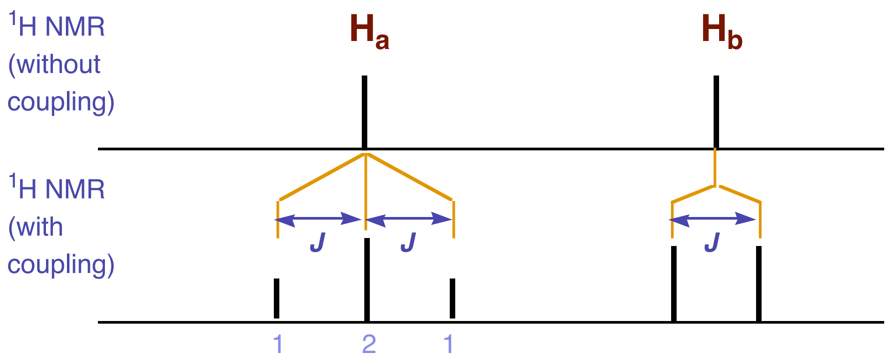
An example of splitting with two neighboring H's.



If there are 2 neighboring H's, there are three statistical arrangements of the spin states. In this example, **H_a** will be split into a triplet.

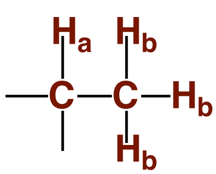


Note that there are two ways to have one spin up and one down. Thus, the middle peak of a triplet will be twice as large as the two outer peaks.

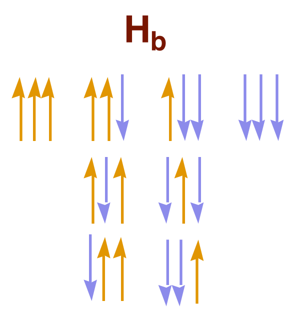


H_a will be a triplet (it sees 2 neighbors) while **H_b** will remain a doublet (it sees one neighbor)

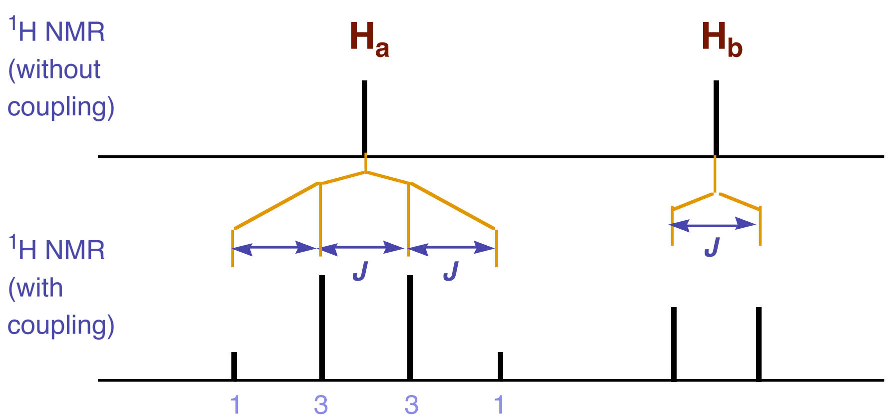
An example of splitting with three neighboring H's.



If there are 3 neighboring H's, there are four statistical arrangements of the spin states. In this example, **H_a** will be split into a quartet.



Note the number of statistical arrangements of the various spin states will give rise to a 1:3:3:1 ratio of peaks.



H_a will be a quartet (it sees 3 neighbors) while **H_b** will remain a doublet (it sees one neighbor)

The relative size of the peaks in a split resonance follows Pascal's triangle.

singlet	1
doublet	1 1
triplet	1 2 1
quartet	1 3 3 1
quintet	1 4 6 4 1
sextet	1 5 10 10 5 1
septet	1 6 15 20 15 6 1

Notes about coupling

Protons will split into n+1 peaks where n = number of neighboring H's.

The relative ratio of the split peaks correlates with the statistical combination of the neighboring spin states.

Chemically equivalent protons do not show coupling even if the are on adjacent carbons (eg. $Cl\text{-}CH_2\text{-}CH_2\text{-}Cl$ would just show one single peak in the ^{1}H NMR).

Protons farther away than one carbon do not usually couple.

Protons coupled to each other will have the same coupling constant.