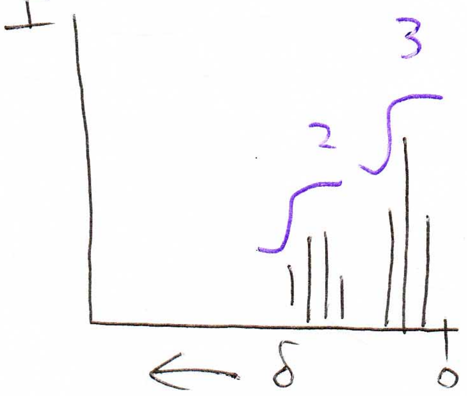
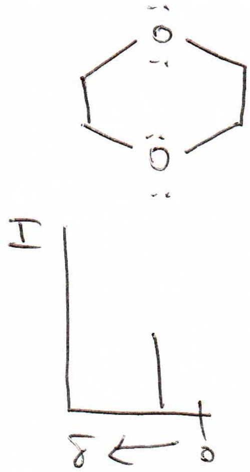
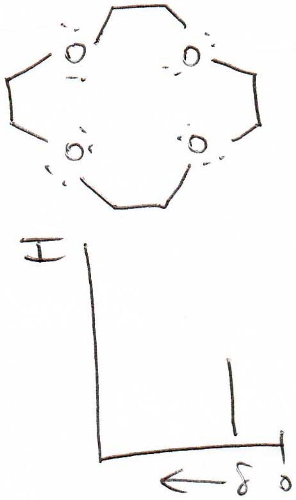
11/29/11 #1

Integration - For ^1H NMR, there is a linear relationship between the strength of an NMR signal and the number of hydrogens that correspond to that signal.





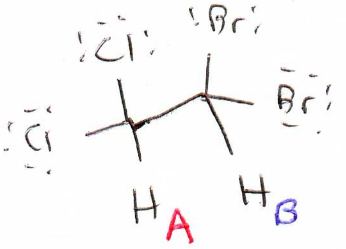


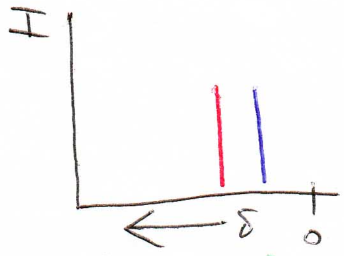
Both of the ethers shown above would generate nearly identical '^1H-NMR spectra', since (ignoring stereochemistry) each compound contains only one type of hydrogen, Although the number of hydrogens is linearly proportional to signal strength, that proportionality constant can only be determined by measurement. Without that constant, the machine would be unable to differentiate between the two compounds.

Splitting -

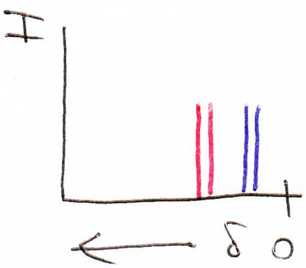
Hydrogens that are chemically <u>in</u>equivalent to each other can perturb each other's magnetic fields, Hydrogens that are chemically equivalent are part of the same magnetic environment so one equivalent proton will not perturb the magnetic field of another.

In all examples below, the effects of stereochemistry are ignored.



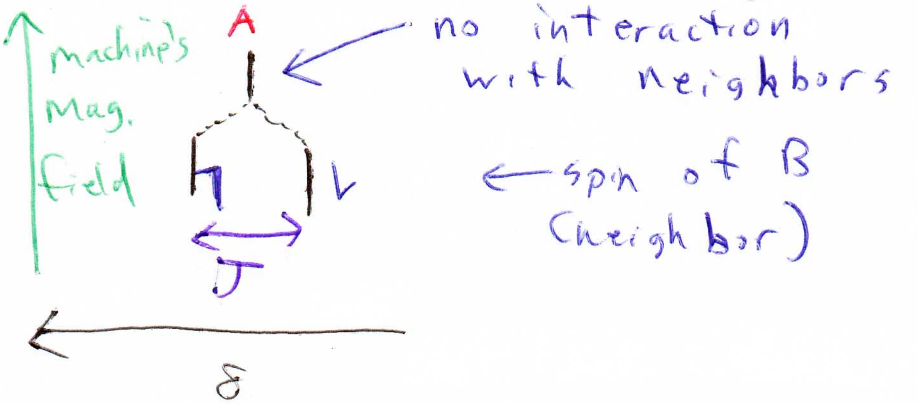


(guess)
(no splitting)

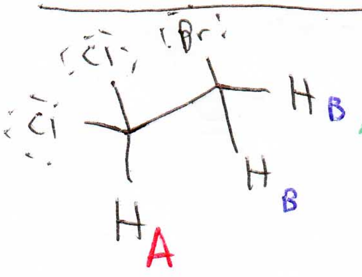


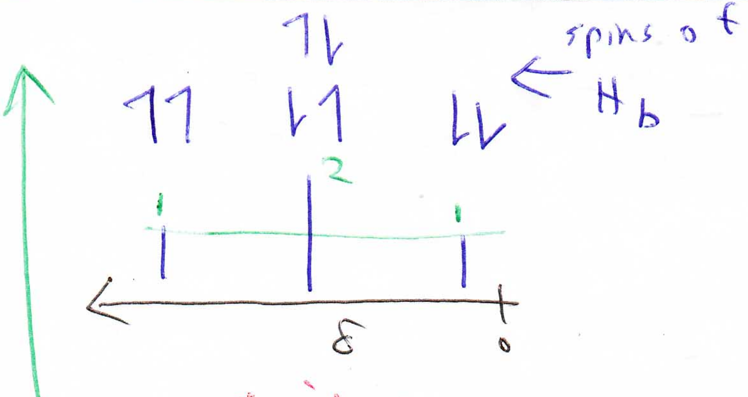
(actual)

A neighboring proton (B) that is non-equivalent to a proton being observed (A) can effectively add to or subtract from the magnetic field (as experienced by A). The neighbor (B) can therefore cause an increase or a decrease in the chemical shift observed for A. Since both possibilities occur with equal likelihood, the signal for A will appear to be split into. → doublet



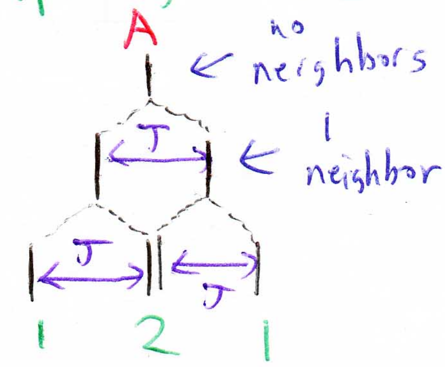
J-coupling constant
- indicates the extent of interaction between two neighbors

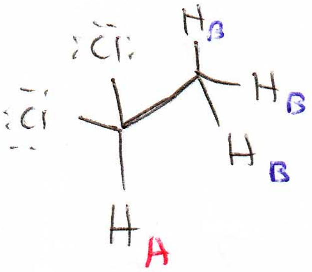




triplet

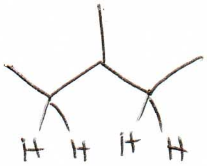
splitting tree

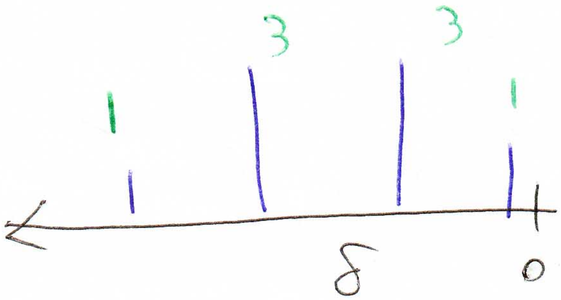


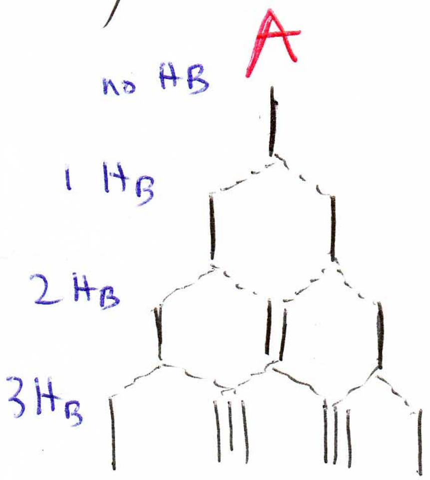


degenerate - equal in energy

↑↑↑   ↑↑↓   ↑↓↓   ↓↓↓
      ↑↓↑   ↓↑↓
      ↓↑↑   ↓↓↑







quartet

$(x+y)^1 = 1x + 1y$ $(x+y)^2 = 1x^2 + 2xy + 1y^2$

$(x+y)^3 = 1x^3 + 3x^2y + 3xy^2 + 1y^3$ let x = ↑ y = ↓

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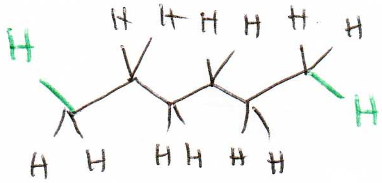
n+1 rule - when observing a proton with 'n' equivalent neighbors, a multiplet with n+1 peaks will be generated.

Degree of unsaturation

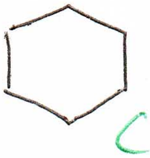
Saturated - a compound that contains the maximum number of hydrogens possible, given the number of carbons present.



$\# H = 2C + 2$

$3 \times 3 + 1 + 2 = 12$

$C = 5$ $2C + 2 = 12$



C_6H_{12}

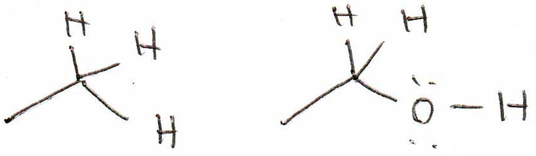
(2H "missing") ← A ring and a double bond each count as one degree of unsaturation

C_5H_8

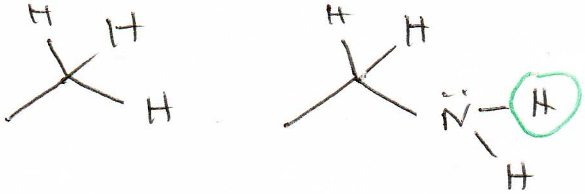
(4H "missing")

A triple bond counts as two degrees of unsaturation

$$D.O.U = \frac{(\#\text{ of H based on }\#\text{ of C}) - (\#\text{ of H present})}{2}$$



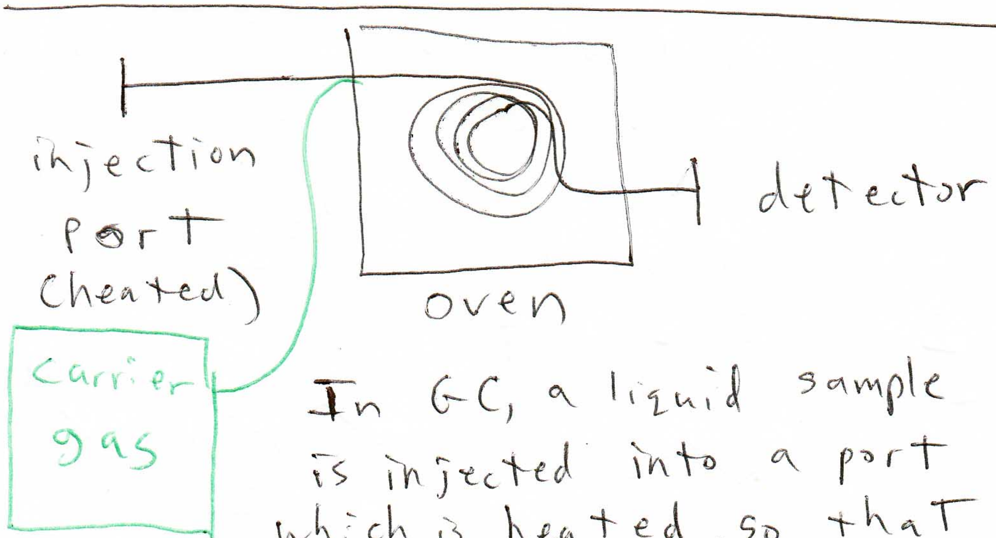
oxygen (and sulfur) doesnot affect the hydrogen count as it is divalent

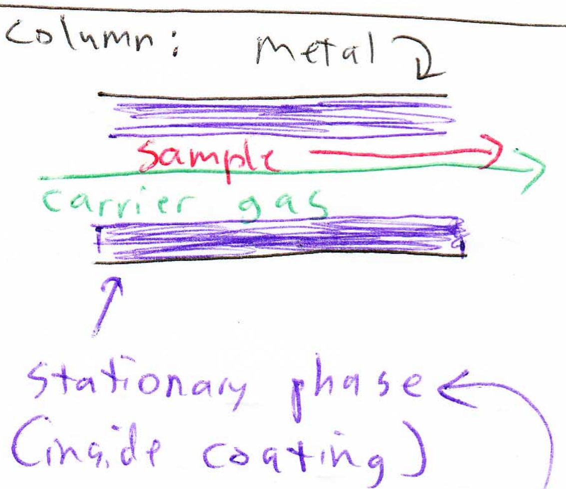


nitrogen (and phosphorus) adds to the hydrogen count because it is trivalent

halogens subtract from the hydrogen count since they are (normally) monovalent.

$$D.O.U = \frac{[2C+2]+N-X-H}{2}$$

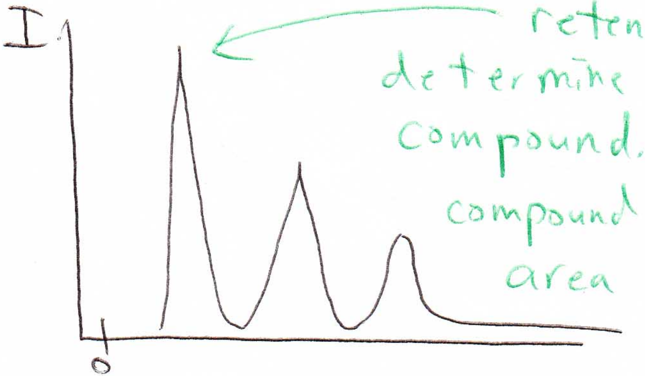




In GC, a liquid sample is injected into a port which is heated, so that the sample can be vaporized upon injection. The sample is then passed through a column* that is also heated so as to maintain the samples in the gas phase. A carrier gas (mobile phase) (an inert gas, usually N_2, He, or Ar) is used to help push the sample through the column.

#5

As the sample passes through the column, the components of the sample are separated based mainly on the basis of polarity and boiling point. As the compounds successfully transit through the column, the quantity of the compound exiting the machine is registered by a detector.



retention time is used to determine the identity of a compound. the quantity of a compound is determined by the area of the peak observed.

retention time → the time it takes for a compound to pass from the injection port to the detector