Announcements

1) Revised Schedule (revision #2) is now available on website.

   Important Due Dates:

Experiment #1: Literature	Sept. 13/14
Experiment #10: Molecular Modeling	Sept. 20/21
Experiment #3: NMR	Sept. 27/28

2) Literature Assignment

   Title Page must conform to example in lab manual

3) Molecular Modeling Report (no more than 5 pages total)

   - provide: Title Page, Purpose (objectives listed), Experimental ("see Course Pack"), Results and Discussion, Conclusion (judgment of success)

4) Experiment #2 (Techniques) (note: no documentation for #1, #3, #10):

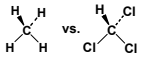
   Prelab: Flowsheet, A-F + G (prelab) for next week (section: Laboratory Notebook)

5) Office hours next week: Wed. 11 am – 1 pm

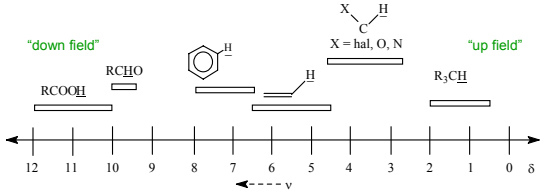
6) Please come to the lab dressed appropriately

NMR Spectroscopy

Question: Will ΔE for the H atom in CH_4 be the same as the H atom in $CHCl_3$?



Answer: No, since they are in different *chemical environments*. Therefore, NMR enables us to distinguish between nuclei.

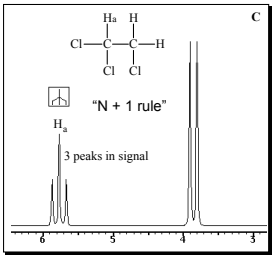


known as "chemical shift" (in ppm)

Other information?

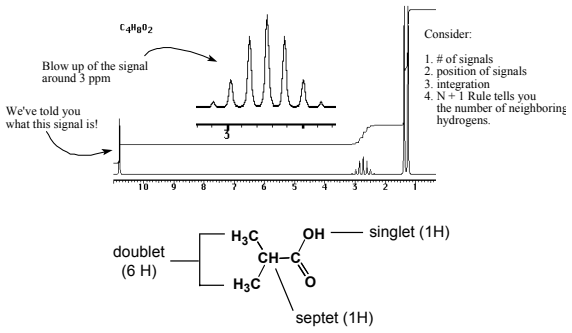
Pascal's Triangle to Predict Multiplicities Involving Vicinal Hydrogen Atoms

1	singlet
1 1	doublet
1 2 1	triplet
1 3 3 1	quartet
1 4 6 4 1	quintet



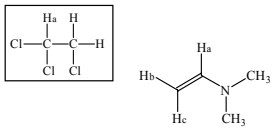
Note: distance between peaks of multiplet (*I.e.* doublet, triplet, etc.) can be measured in Hz and is known as the *coupling constant* (usually < 20 Hz).

Isobutyric Acid

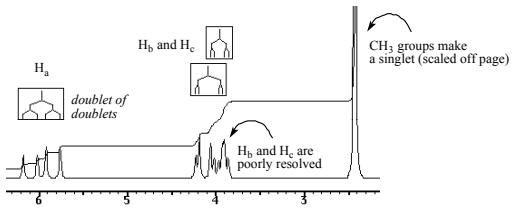


Other effects?

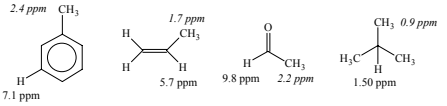
1) Coupling to More Than One Kind of Hydrogen



H_a, H_b, and H_c are not equivalent, coupling constants are therefore different and the spectrum is complex



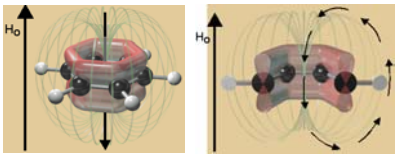
2) Anisotropy



Note: in compounds where hydrogen atoms are attached to carbon atoms of double bonds, protons are shifted downfield (*i.e.* to the left)

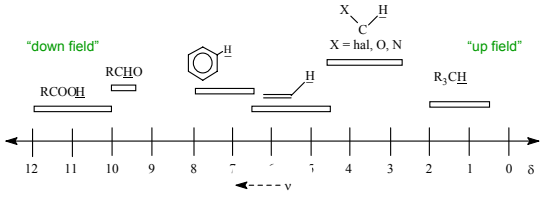
Why? Related to movement of electrons in molecule.

Ring Current



When an aromatic ring is oriented perpendicular to a strong magnetic field, the delocalized π electrons circulate around the ring, producing a small local magnetic field. This induced field *opposes* the applied field in the middle of the ring but *reinforces* the applied field outside the ring. Aromatic protons therefore experience an effective magnetic field greater than the applied field and come into resonance at lower field (*i.e.* 6 to 9 ppm)

Basics of NMR Spectroscopy



NMR Assignment: Complete Problems 1-6 (Exp. 3) + Interpret your spectrum from NUTS

Due Date: Sept. 27/28