

Course Chem 345

Instructor Gellman

Day Friday

Date 31 January 2014

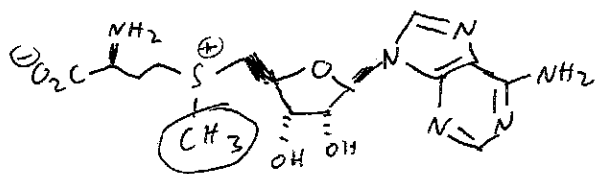
Notes Taken By Kaz Skubi

Total # of Pages 4

Submit notes to the Undergraduate Chemistry Office for posting.
PLEASE COMPLETE NOTES IN INK AND DO NOT STAPLE.

General Interest

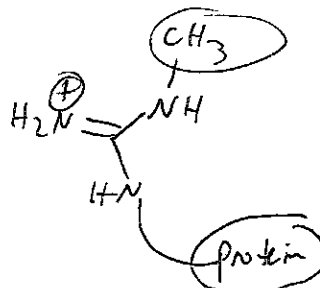
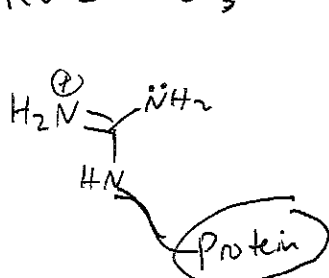
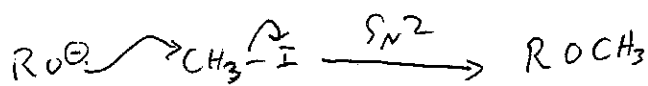
Minkui Luo, Memorial Sloan-Kettering Cancer Center, NYC



S-adenosyl methionine (SAM)

Biology's CH_3I

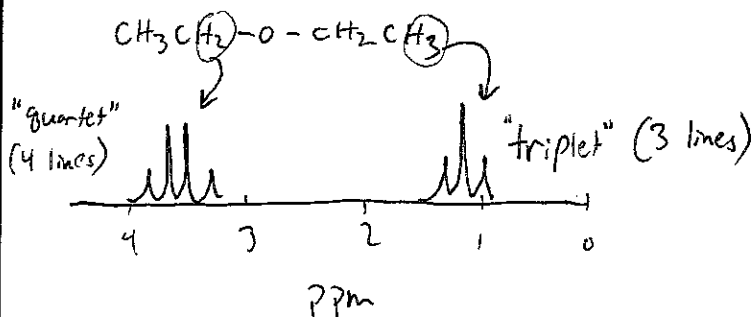
Recall:



"Arginine Methylation"

NMR Spectroscopy

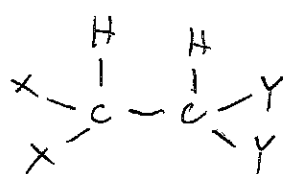
Multiplicity of ^1H NMR Signals



Why are signals "split" by adjacent, non-equivalent H's?

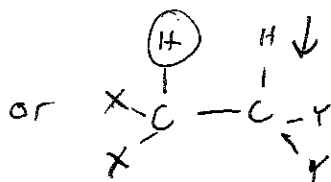
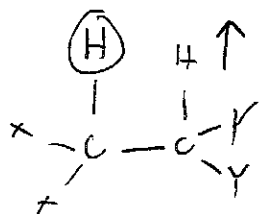
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Each H resonance is a "doublet" (2 lines)
Why?

For a given H, there are two possibilities for the neighboring H spin state.



Ⓜ = observed H

↑ = spin of other H

2 lines: Ⓜ is "coupled" to adjacent H.

Coupling can occur only if the adjacent H is not equivalent.

Typically only observed for 3 band separation.

Increased # of adjacent Hs (equivalent to one another but not equivalent to the neighbor that we're actually observing) increases the number of lines.

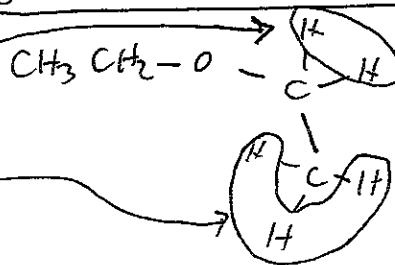
In general, we can use the "n+1 rule"

For ~~n~~ ⁿ H's, we expect splitting into n+1 lines

Return to our earlier example:

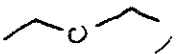
see 3 neighbors = 4 lines (quartet)

see 2 neighbors = 3 lines (triplet)



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Note: split NMR signals ("multiplets") have a characteristic spacing between the lines, "coupling constant" (J)

For , $J = 7.0 \text{ Hz}$

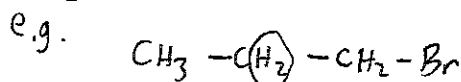
Overall, 3 kinds of information from ^1H NMR data:

① Chemical shift (δ) - information about local environment within a molecule, e.g., presence of electronegative atoms.

② Integration - H proportions (among sets of equivalent H's)

③ Splitting - # of non-equivalent neighboring H's.

(see text for complexity from multiple types of neighbors)



splitting both ways. Can get complicated. See Loudon for more discussion of these complexities.

Students must work problems to master use of NMR data

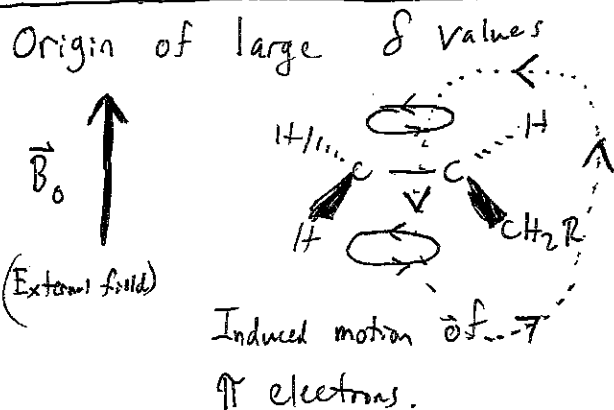
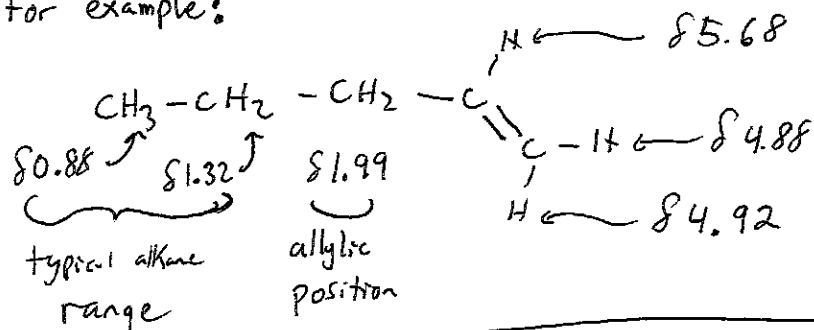
Functional groups often have characteristic signatures in ^1H NMR spectra.

First, let's "fill in" the FG's from Chem 343.

① Alkenes - H's on alkene carbons (sp^2 carbons) or nearby are downfield shifted (i.e., larger δ) relative to alkane H's (on sp^3 carbons).

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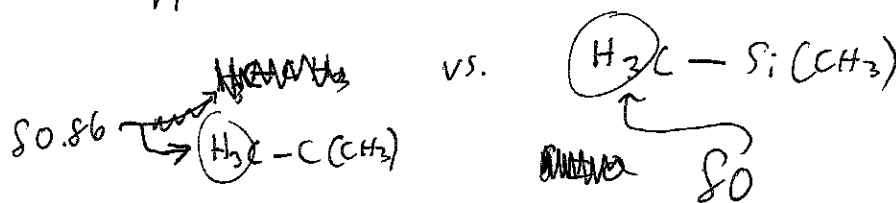
For example:



This motion of the electron induces its own (smaller) magnetic field. Where the alkene H's sit in space, the induced field is in the same direction as (and thus augments) the applied magnetic field, \vec{B}_0 .

This causes a downfield (larger δ) shift.

Recall: Electronegative atom effects seemed to go in the opposite direction



Position of H's relative to electrons is ~~crucial~~ crucial.