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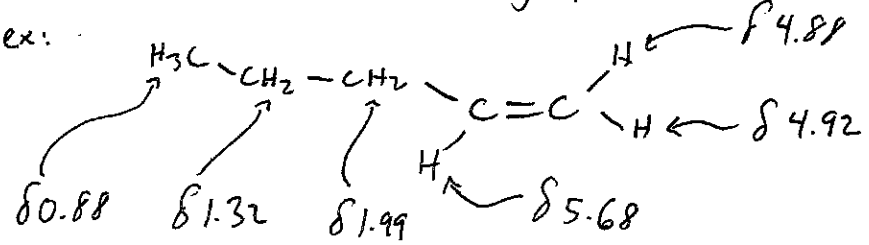
PLEASE COMPLETE NOTES IN INK AND DO NOT STAPLE.

Recall: NMR characteristics of functional groups.

① Alkenes, ex:

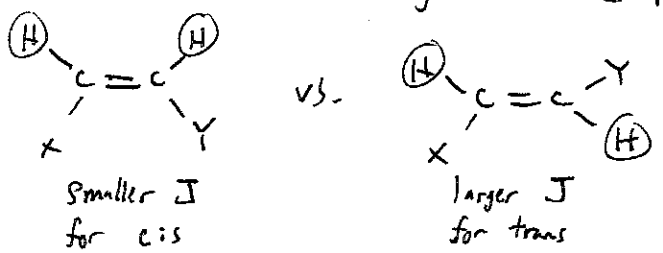


In general: H on alkene C and "allylic" H are downfield (larger δ) relative to an alkane H.

Origin of Effect: Local magnetic field caused by induced circulation of π electrons (augments applied field)

See text on alkene H coupling constants ("splitting") – Table 13.3

Ex:



smaller J for cis

larger J for trans

② Alkynes

$R-C\equiv C-H$ ← δ 1.8–2.2 ppm.

(terminal alkyne)

Note: Smaller than δ for alkene H.

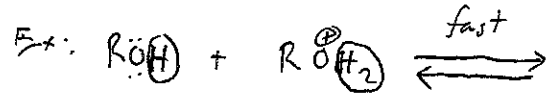
Review: pp. 650–651

③ Alcohols

Ex: CH_3CH_2OH ← δ is quite variable, so is coupling (J)

Complication/uncertainty arises from chemical exchange of ROH protons

equilibrium "blurs" NMR signal

Ex: 

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For these reasons, we use the "D_2O method" to identify hydroxyl protons in an NMR spectrum.

Note: "D" ≡ ^2H (hydrogen isotope)

D is invisible in a ^1H NMR spectrum

Experiment:

$$R-OH \xrightarrow[\text{Shake}]{\text{Add } D_2O} R-OD + HOD$$

(in $CDCl_3$) ← most common NMR solvent

Signal for OH disappears when it is exchanged for OD.

Carbon NMR

Technically more challenging (but getting easier) because:

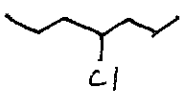
1) Most abundant isotope (^{12}C) is NMR silent (no nuclear spin)
2) ^{13}C is NMR active, but the natural abundance is ~1%
3) ^{13}C is insensitive

Valuable features

1) Broad range for signals (~200 ppm vs. ~10 ppm for ^1H)
2) Direct insight on molecular symmetry

Ex:

7 ^{13}C signals



4 ^{13}C signals

3) Because of low ^{13}C abundance, we never encounter ^{13}C adjacent to another ^{13}C, so we don't observe $^{13}C-^{13}C$ coupling.

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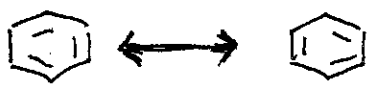
Note: ^{13}C can couple to ^{1}H, but we acquire "^{1}H decoupled" ^{13}C NMR spectra.

4) Because of #3, all ^{13}C NMR signals are single lines
5) See Appendix IV for characteristic ^{13}C δ values
6) Practice using this information by doing problems.

Chapter 16: Reactions of Benzene and Benzene Derivatives
Reactivity With Electrophiles

Rec. Problems: 2, 4-9, 12-34, 36-47, 49-56, 58-64.

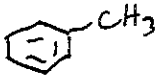
Benzene:



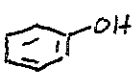
Resonance Structures — used when the localized bonding concept breaks down.

Sometimes drawn this way: "  "

Terminology - "common names"

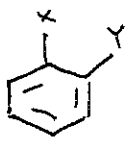


toluene

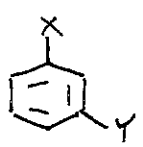


Phenol

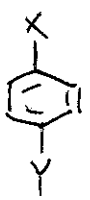
Relative Positions:



"ortho"



"meta"



"para"