

Geminal
Dihaloalkanes

Vicinal
Tetrahaloalkanes

Alkynes (DFW)

Carboxylic
Acids



Vicinal
Diols

Aldehydes
Ketones

Vicinal or Geminal
Dihaloalkanes (Waco)

Epoxydes

Alkenes (Austin)

Alcohols

Haloalcohols

Allylic
Halides

Haloalkanes (S.M., N.B)

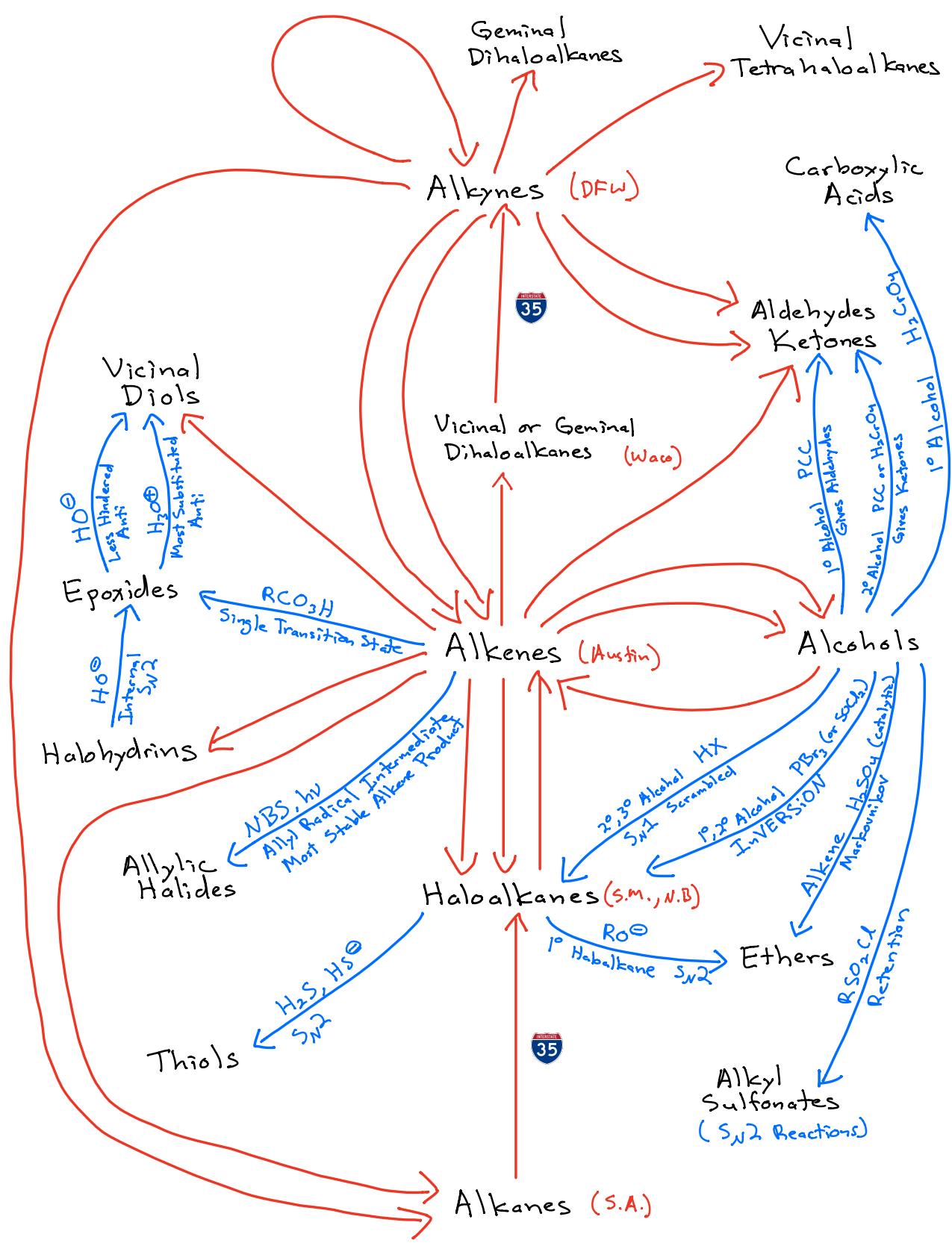
Ethers

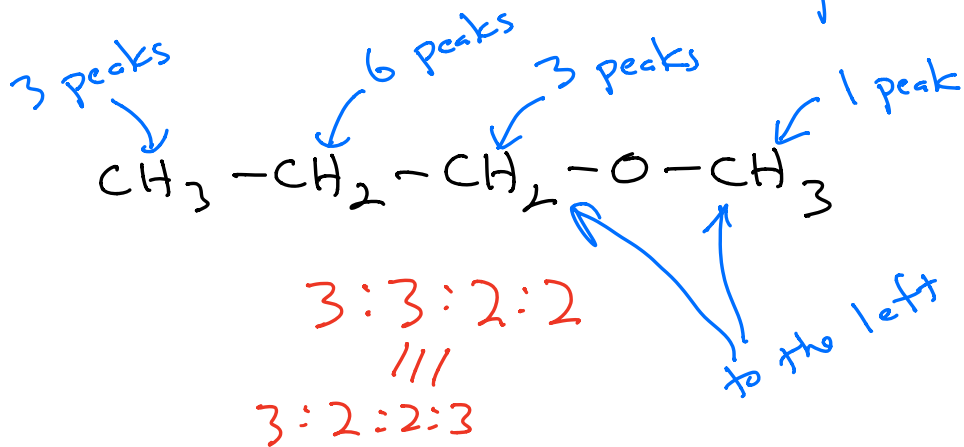
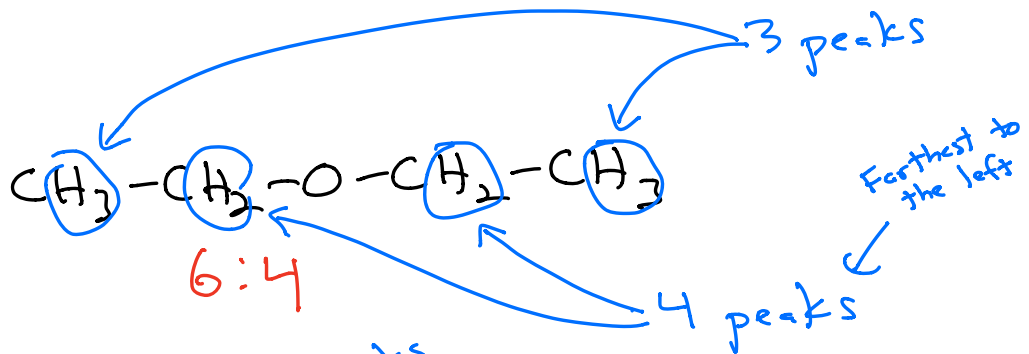
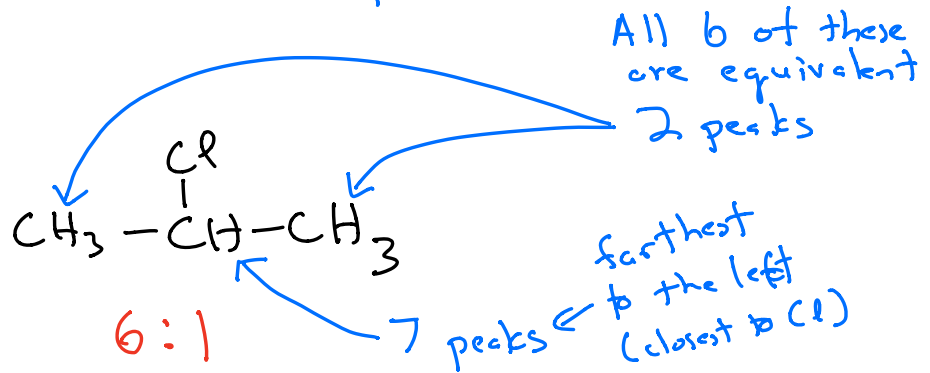
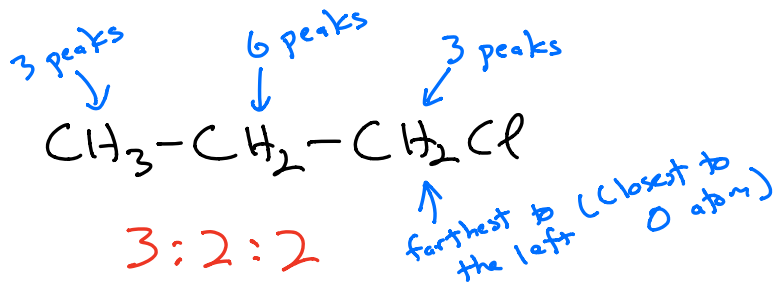
Thiols

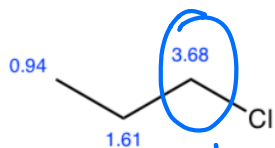


Alkyl
Sulfonates

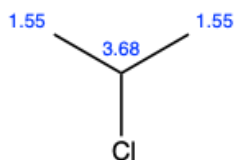
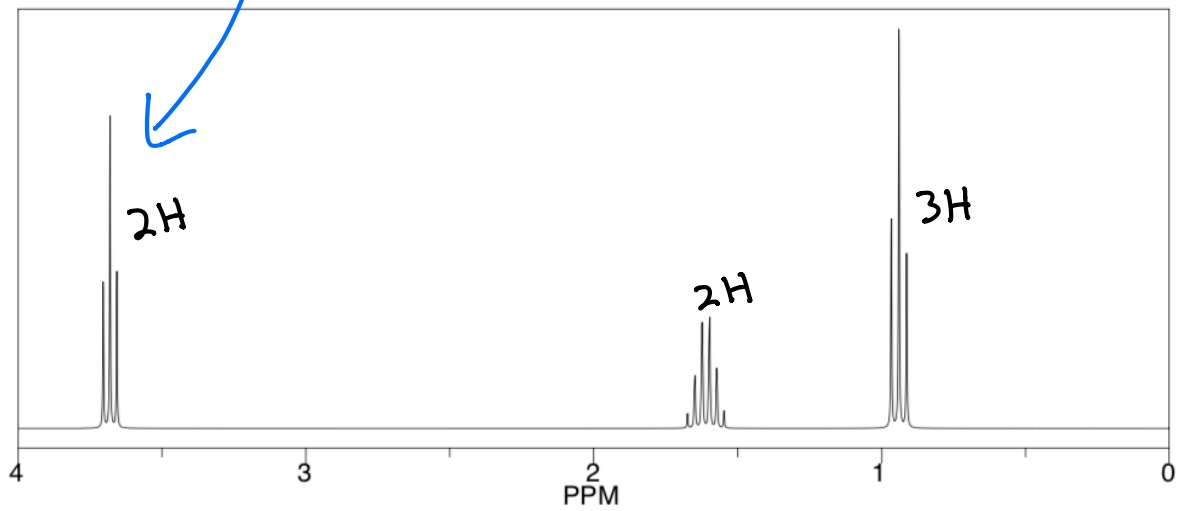
Alkanes (S.A.)



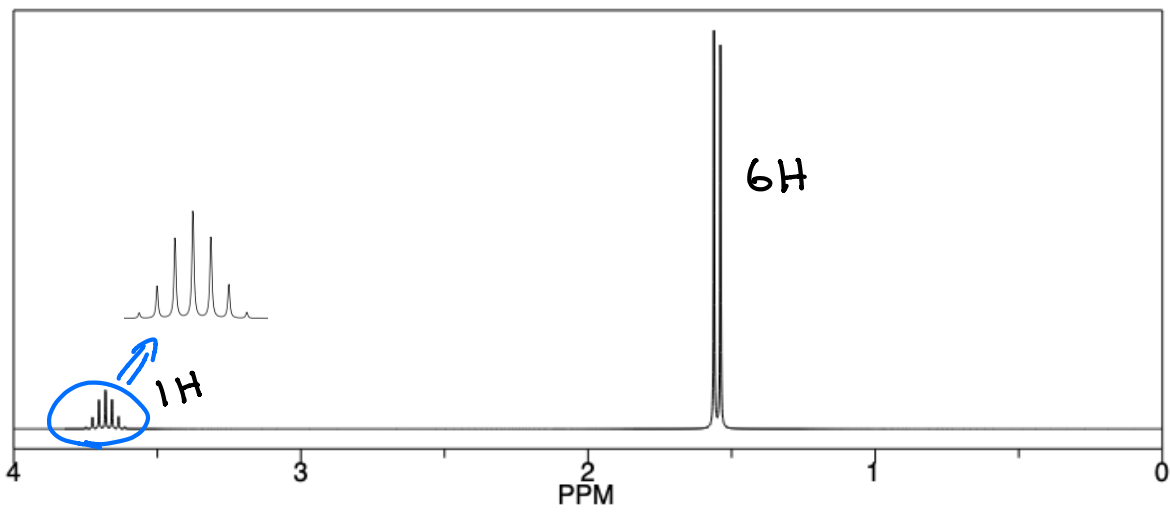


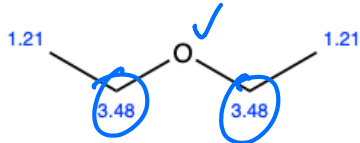
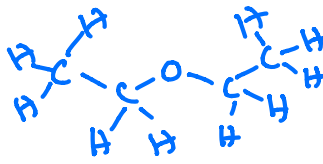


Estimation quality is indicated by color: **good**, **medium**, **rough**

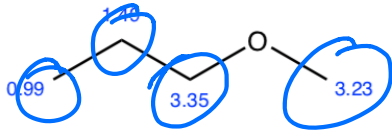
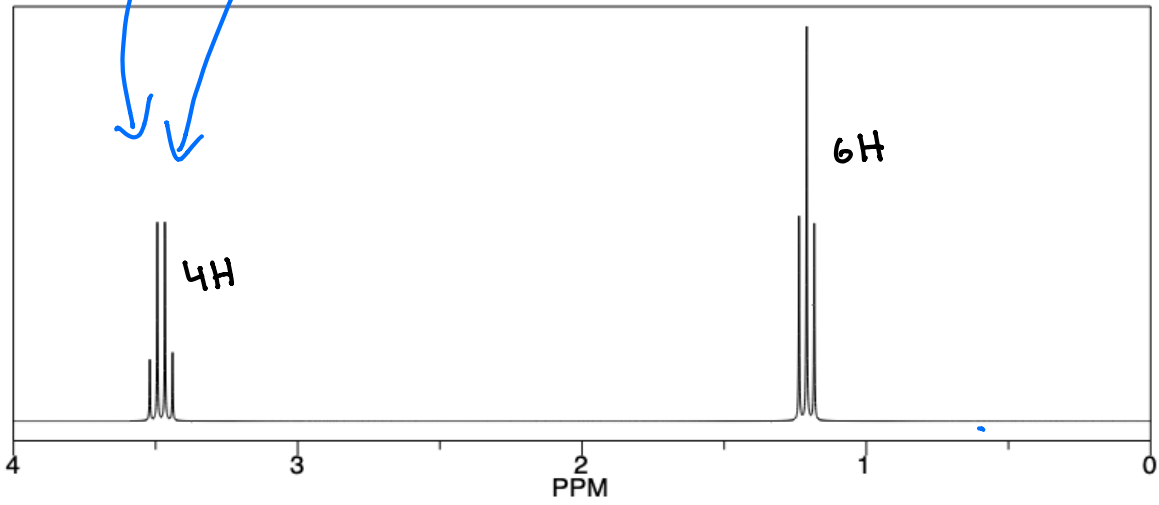


Estimation quality is indicated by color: **good**, **medium**, **rough**

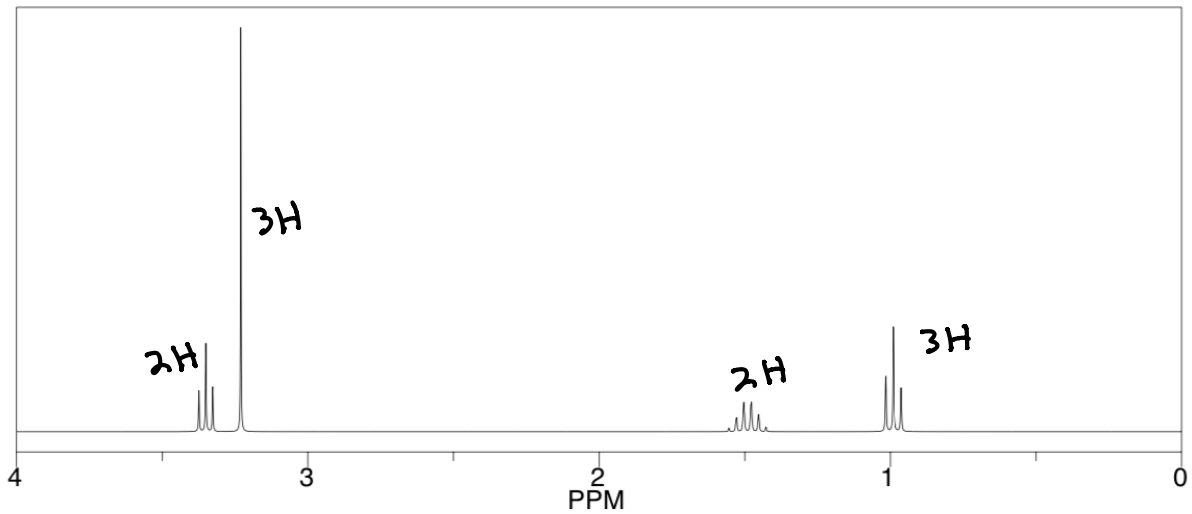




Estimation quality is indicated by color: good, medium, rough

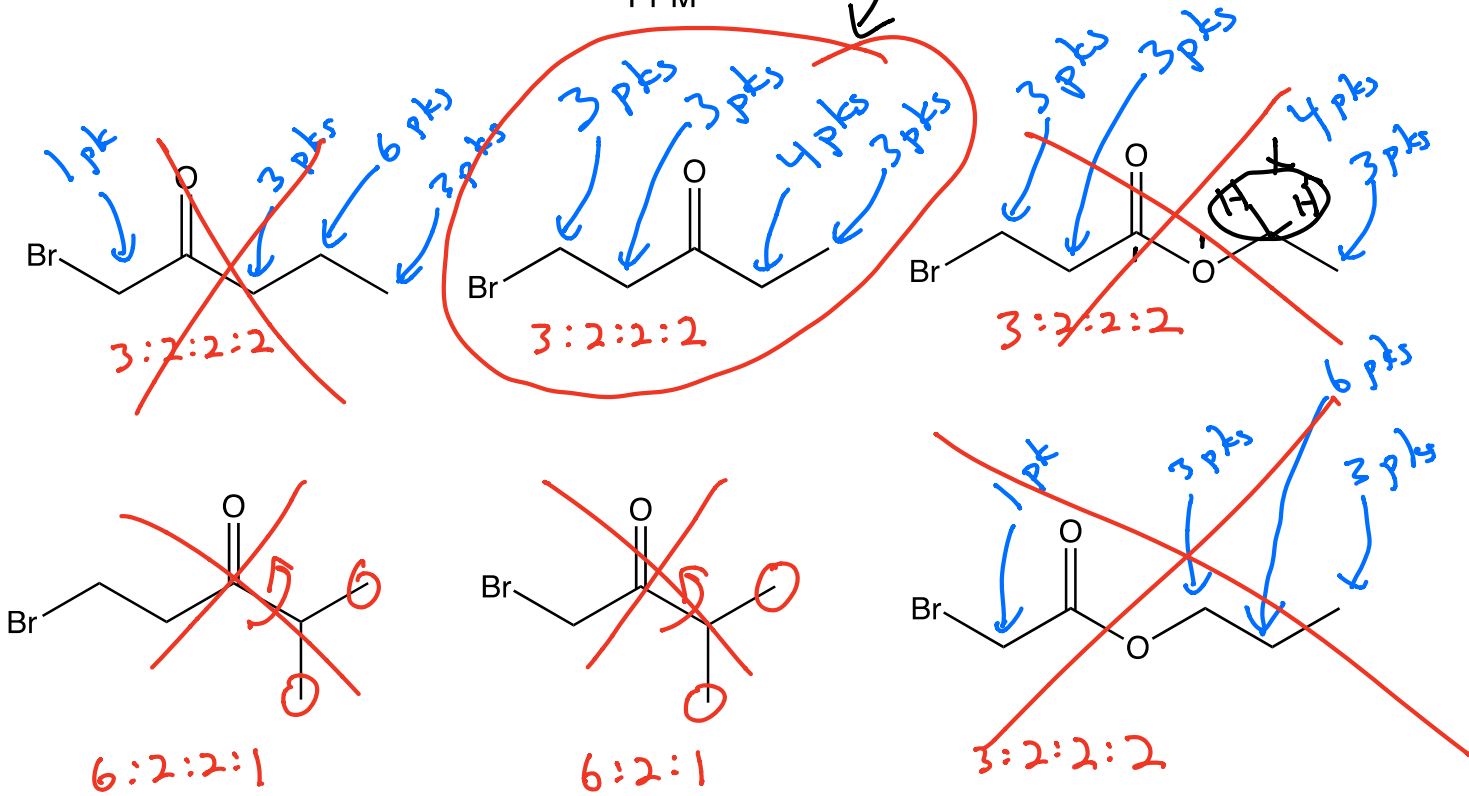
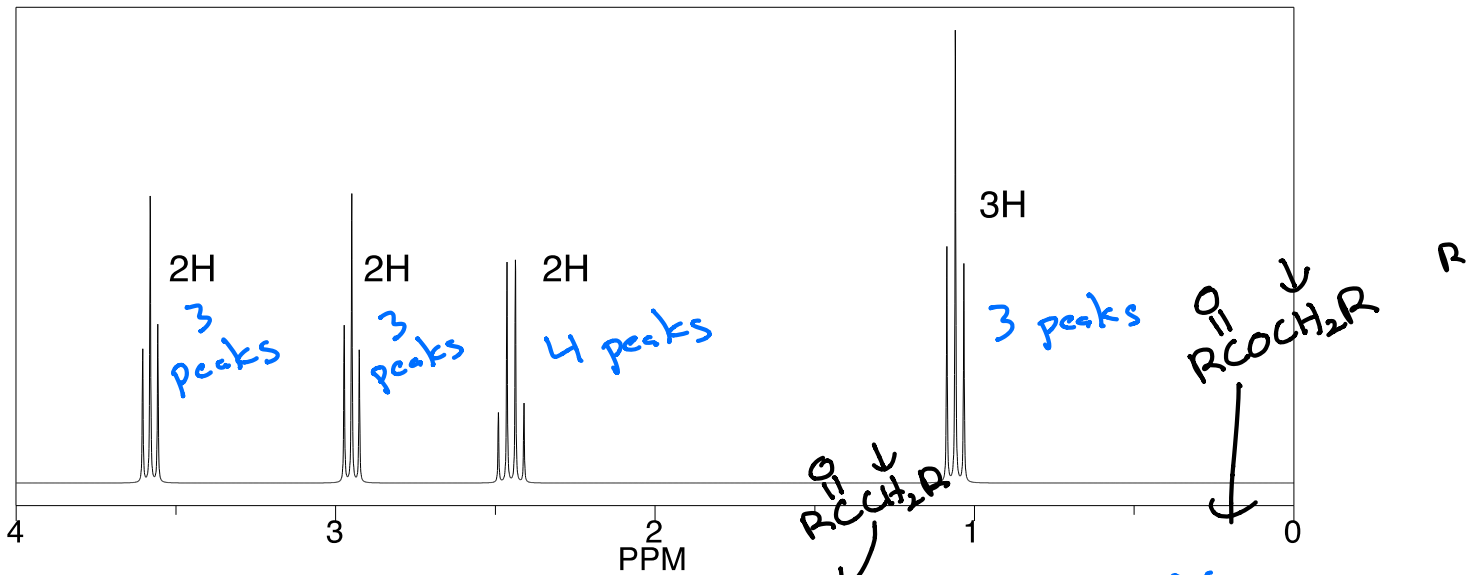


Estimation quality is indicated by color: good, medium, rough



V. When solving NMR spectra problems:

- 1) Determine number and relative integrations of signals predicted for a given structure ✓
- 2) Make sure the splitting pattern matches with the spectrum for each signal and ✓
- 3) If the number and relative integrations as well as splitting patterns match with the spectra, compare expected chemical shifts with those of the signals in the spectra. ✓



Type of Hydrogen (R = alkyl, Ar = aryl)	Chemical Shift (δ)*	Type of Hydrogen (R = alkyl, Ar = aryl)	Chemical Shift (δ)*
R_2NH	0.5-5.0	RCH_2OH	3.4-4.0
ROH	0.5-6.0	RCH_2Br	3.4-3.6
RCH_3	0.8-1.0	RCH_2Cl	3.6-3.8
RCH_2R	1.2-1.4	$\begin{array}{c} O \\ \\ RCOCH_3 \end{array}$	3.7-3.9
R_3CH	1.4-1.7	$\begin{array}{c} O \\ \\ RCOCH_2R \end{array}$	4.1-4.7
$R_2C=CRCHR_2$	1.6-2.6	RCH_2F	4.4-4.5
$RC\equiv CH$	2.0-3.0	$ArOH$	4.5-4.7
$\begin{array}{c} O \\ \\ RCCH_3 \end{array}$	2.1-2.3	$R_2C=CH_2$	4.6-5.0
$\begin{array}{c} O \\ \\ RCCH_2R \end{array}$	2.2-2.6	$R_2C=CHR$	5.0-5.7
$ArCH_3$	2.2-2.5	$\begin{array}{c} O \\ \diagup \quad \diagdown \\ H_2C \quad CH_2 \end{array}$	3.3-4.0
RCH_2NR_2	2.3-2.8	$\begin{array}{c} O \\ \\ RCH \end{array}$	9.5-10.1
RCH_2I	3.1-3.3	$\begin{array}{c} O \\ \\ RCOH \end{array}$	10-13
RCH_2OR	3.3-4.0		

* Values are relative to tetramethylsilane. Other atoms within the molecule may cause the signal to appear outside these ranges.

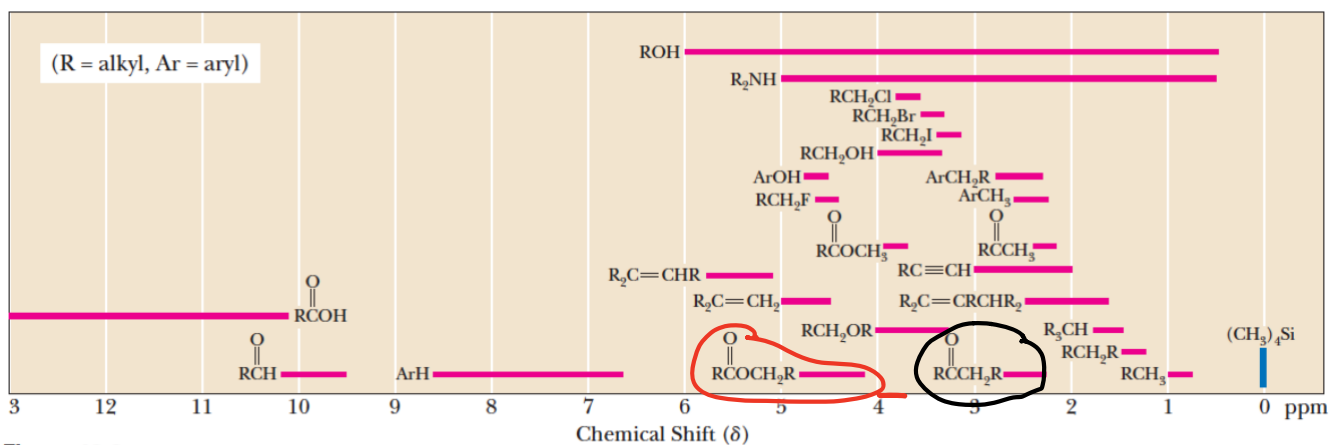


Figure 13.8

Average values of chemical shifts of representative types of hydrogens. These values are approximate. Other atoms or groups in the molecules may cause signals to appear outside of these ranges.

