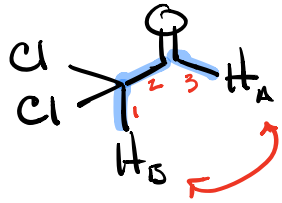
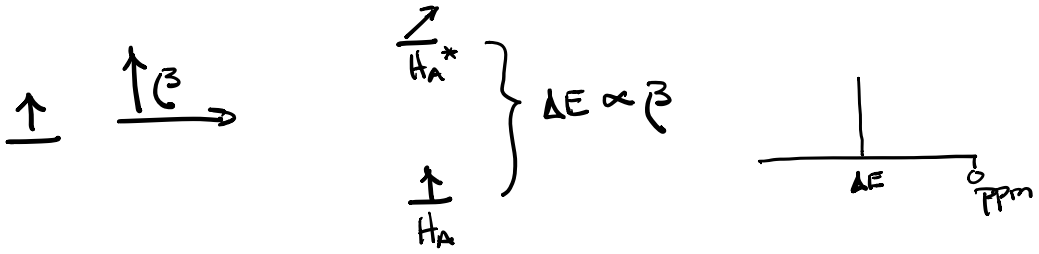
NMR Spin-Spin Coupling

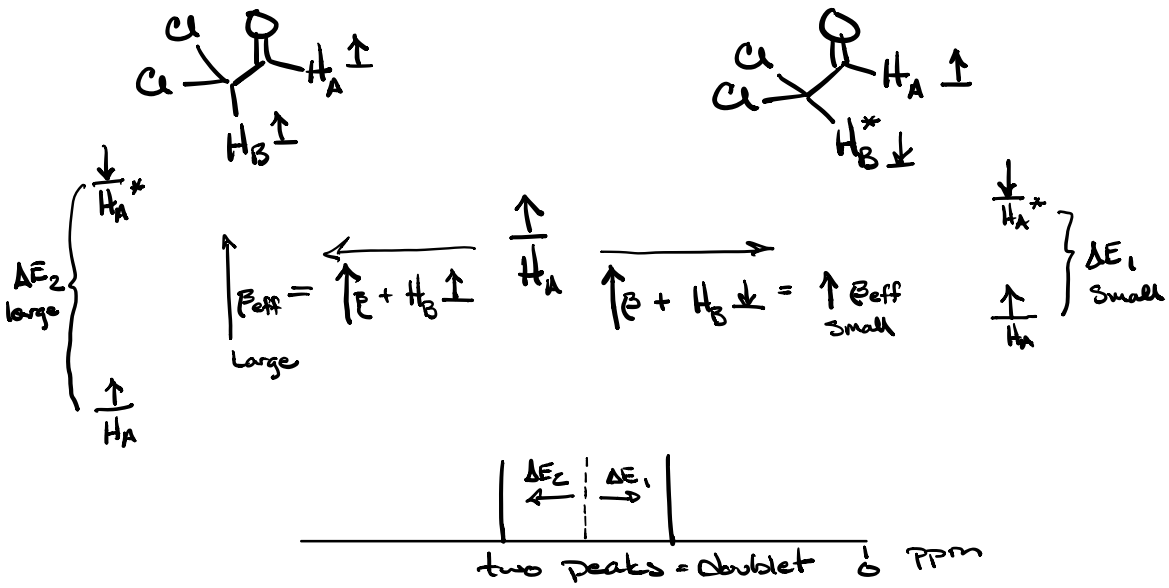


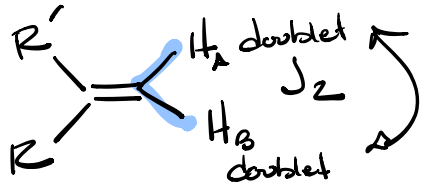
3 Bonds apart = J_3

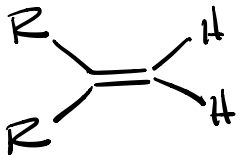
H_A By itself



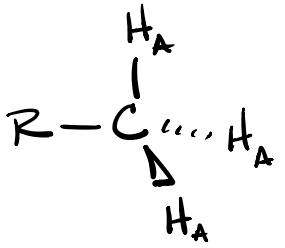
H_A is affected by H_B (Near Neighbors)



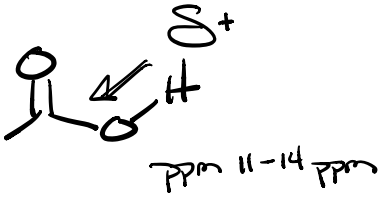




Chemically Equivalent
No Splitting

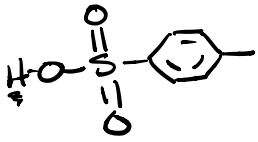


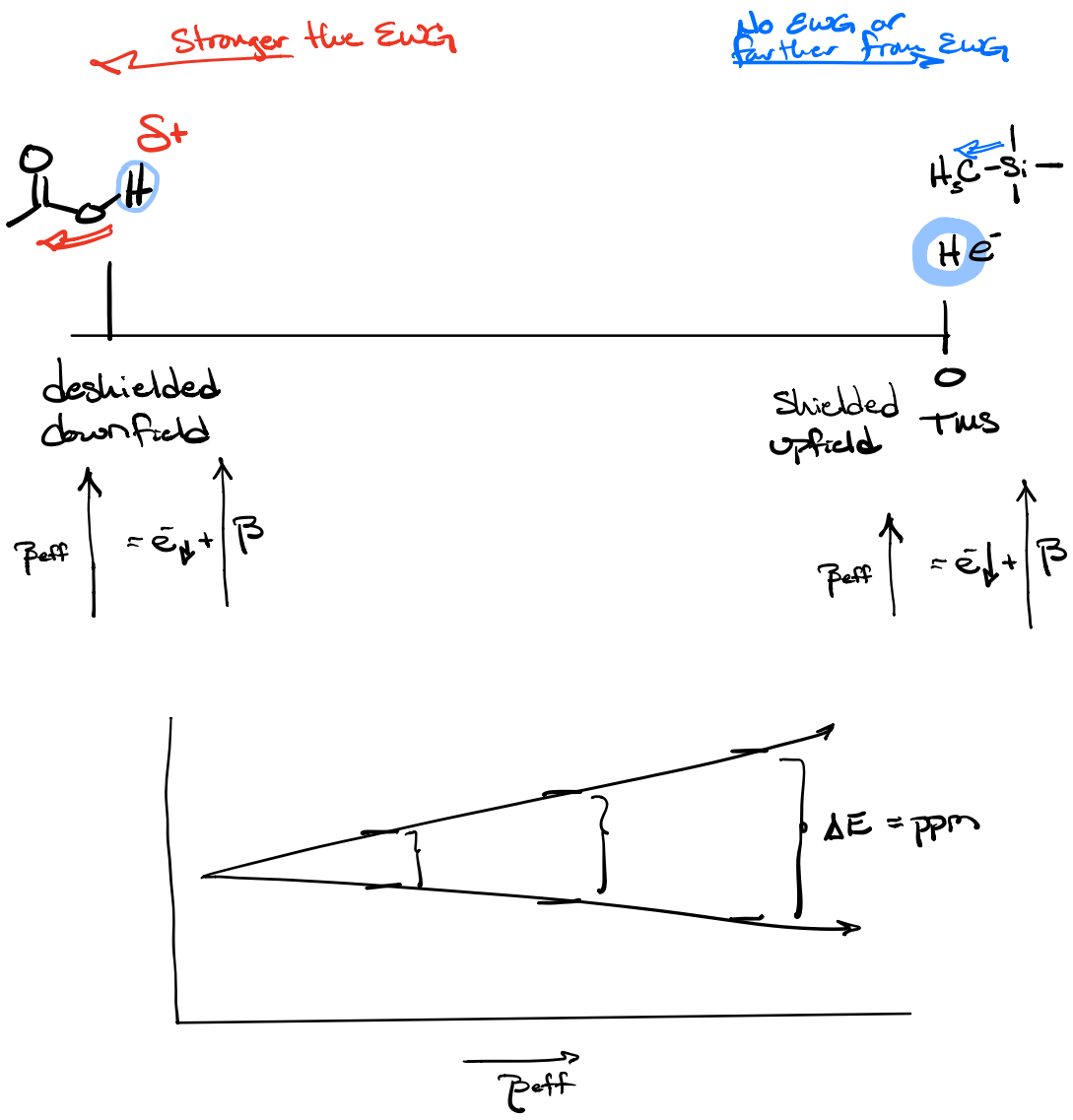
All Chemically Equivalent
⇒ no Splitting



ppm 11-14 ppm

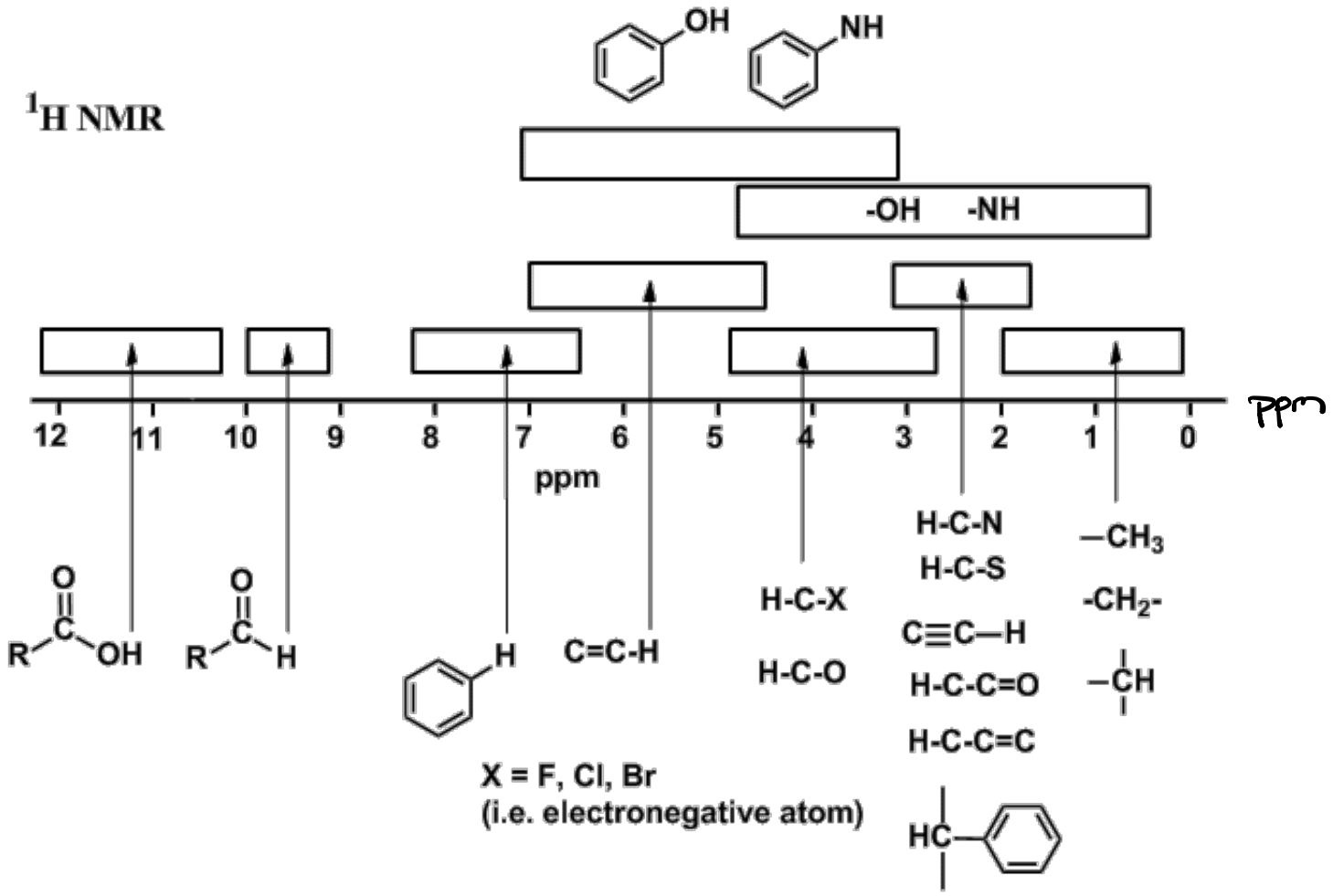
pka 4.5

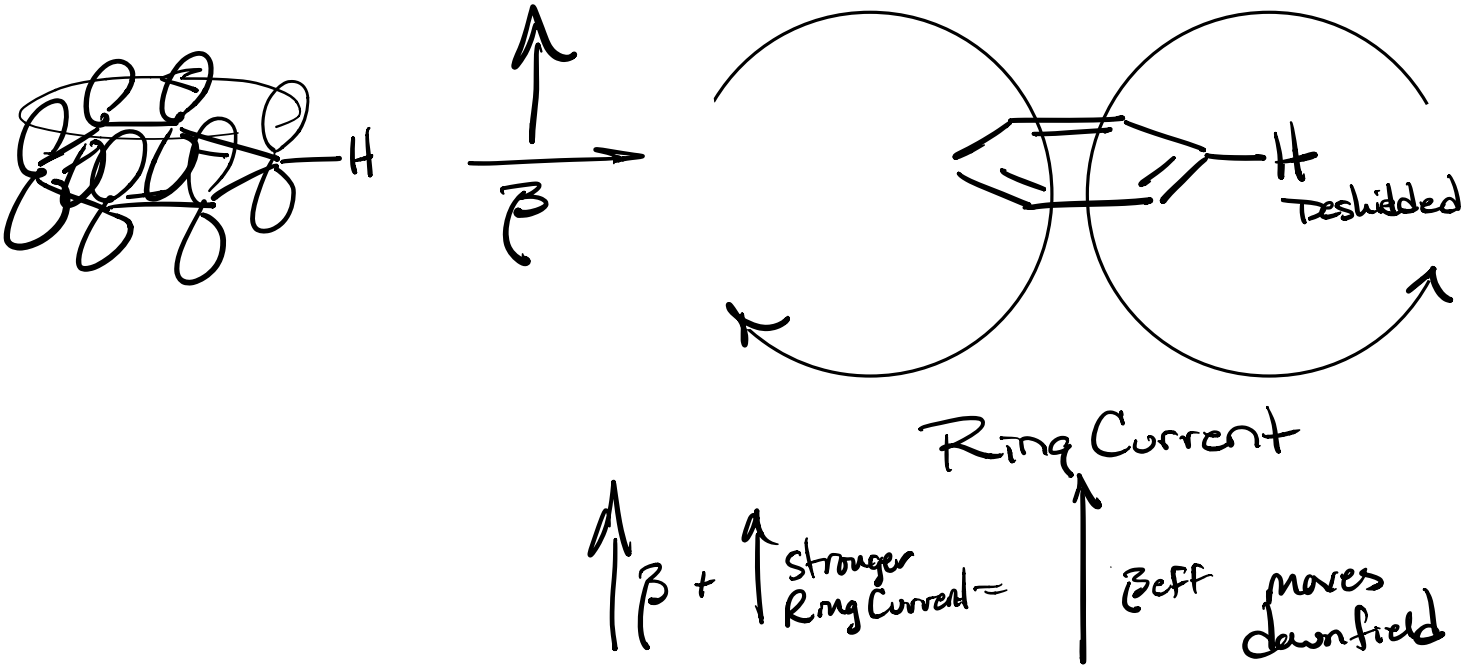


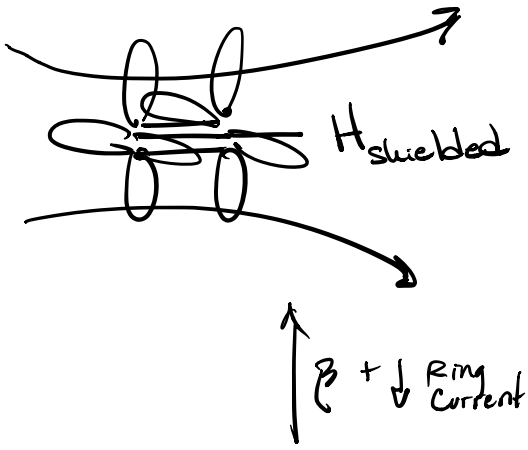

Stronger the EWG
No EWG or farther from EWG
δ+
H
H_3C-Si-
He^-
deshielded
downfield
Shielded
upfield
0
TMS
B_{eff}
$= \bar{e}_\downarrow +$
B
B_{eff}
$= \bar{e}_\downarrow +$
B

ΔE = ppm
B_{eff}

^{1}H NMR


OH
NH
-OH -NH
12 11 10 9 8 7 6 5 4 3 2 1 0
ppm
ppm
H-C-N
H-C-S
—CH3
-CH2-
H-C-X
C≡C—H
H-C-O
H-C-C=O
H-C-C=C
C=C-H
X = F, Cl, Br
(i.e. electronegative atom)
HC


H
B
H
Deshielded
Ring Current
B + Stronger Ring Current = Beff moves downfield



$B + \Delta B_{Ring\ Current} = B_{eff}$

moves upfield

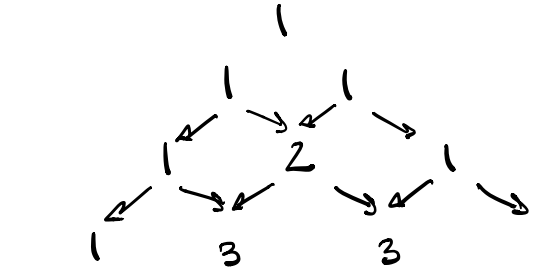
Use ^{1}H-NMR & ^{13}C-NMR table from the NMR section in your lab book (Pavia).

Spin-Spin Coupling follows an N+1 Rule where N = # of neighbors

# of neighbors	Splitting	N+1 Rule
0	1	
1	2	
2	3	
3	4	

The signals have different intensity patterns.

Pascal's Triangle



1 4 6 4 1

1 5 10 10 5 1

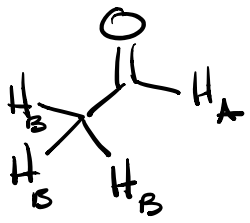
1:1 doublet

1:2:1 triplet

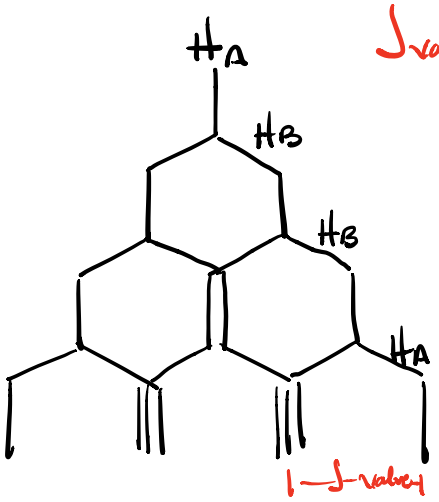
1:3:3:1 quartet

1:4:6:4:1 pentet

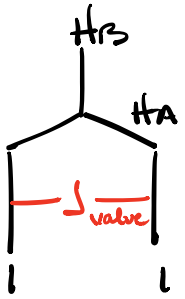
Sextet

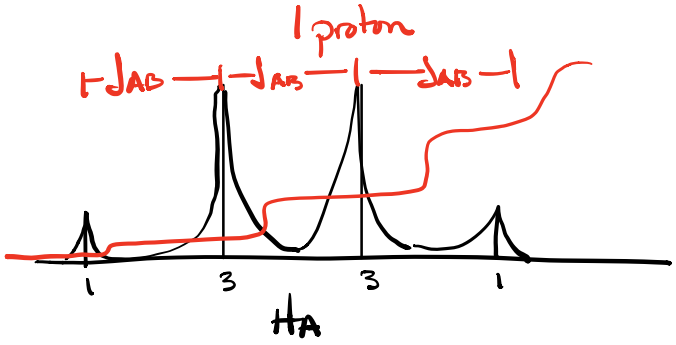


Tree diagram

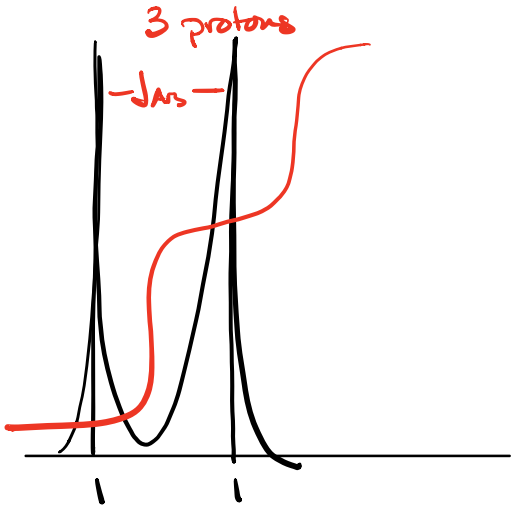


$J_{value} = J_{AB}$

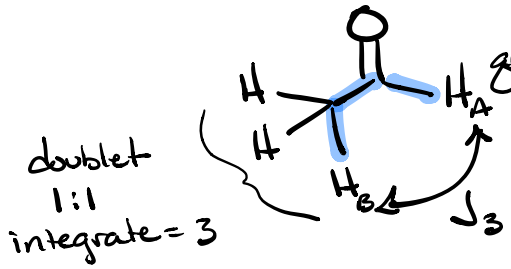




quartet = 3 neighbors

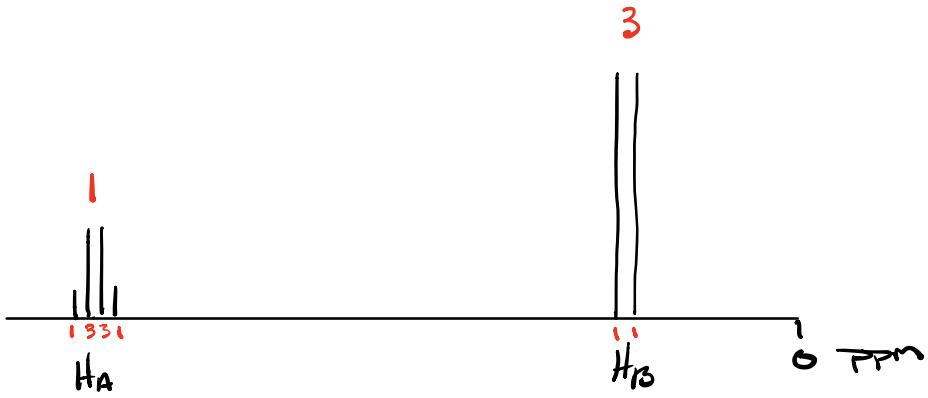


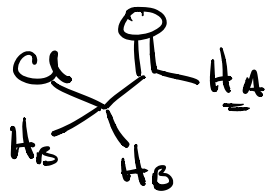
doublet = 1 neighbor



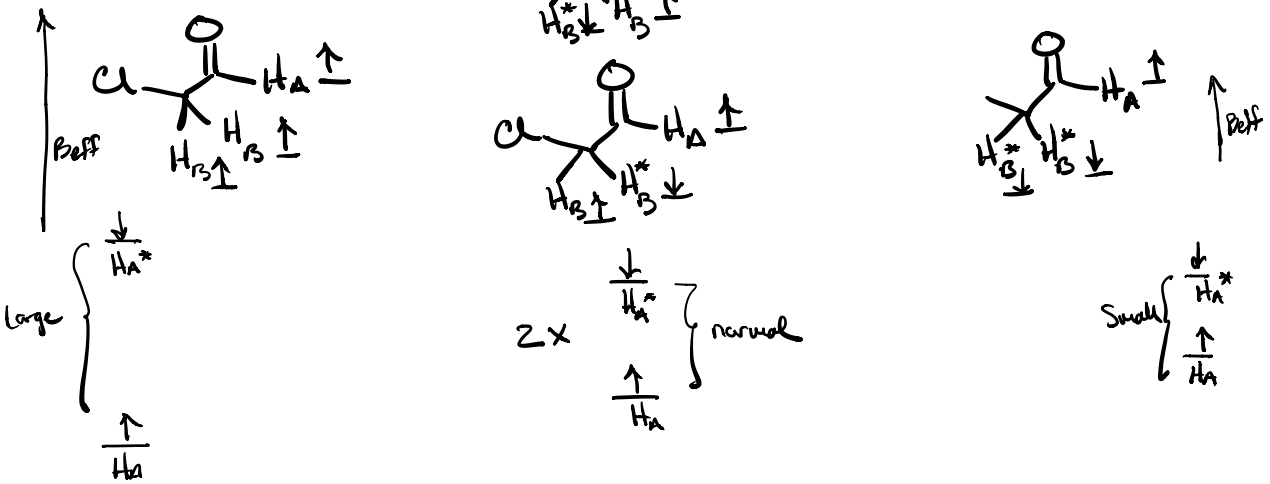
doublet
1:1
integrate = 3

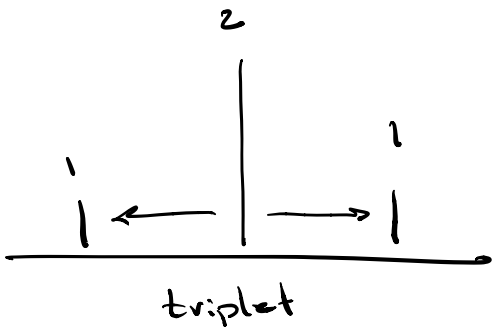
quartet 1:3:3:1
integrate = 1





Three Spin System




2
1
1
triplet