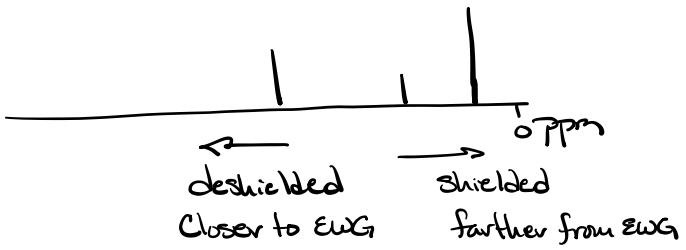
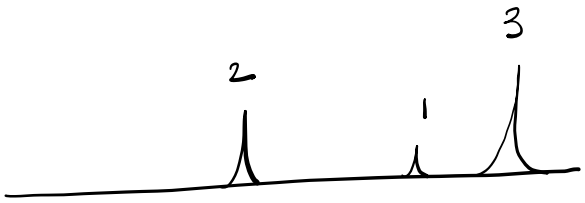
^{1}H-NMR

Rabbit Hole

Position

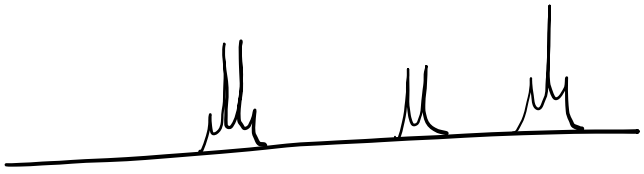


Integration



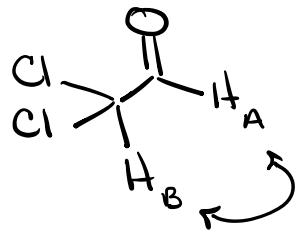
peaks have area to them
Integration ∝ # H's

Splitting

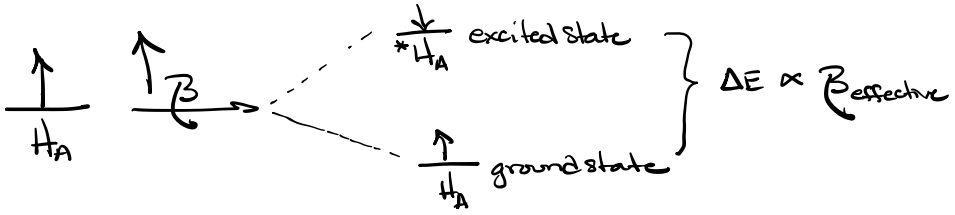


Spin-Spin Coupling
near neighbors cause peaks
to split into identifiable
pattern. pattern informs # of
neighbors

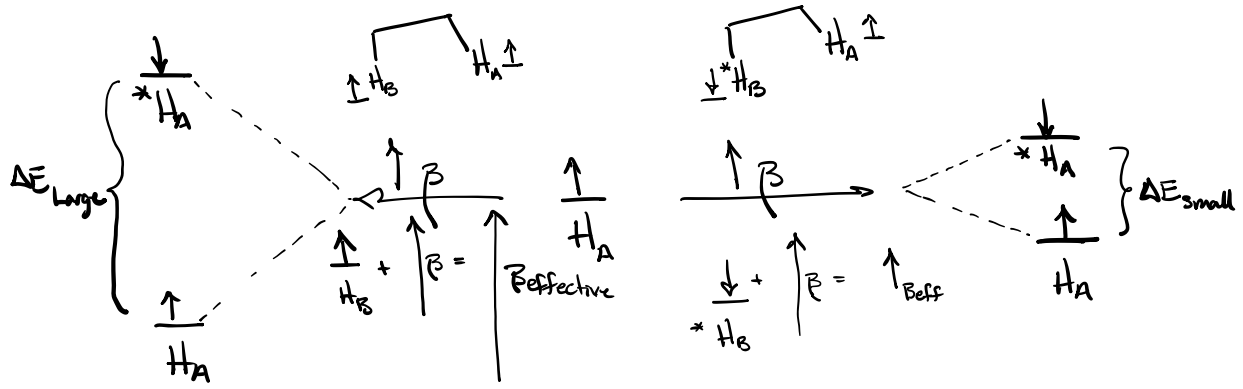
Spin - Spin Coupling

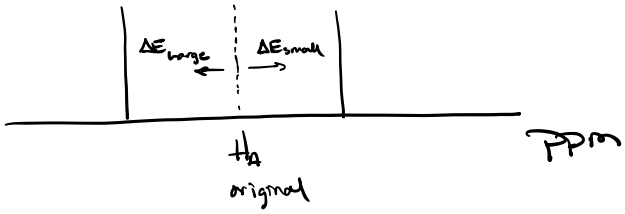


H_A by itself

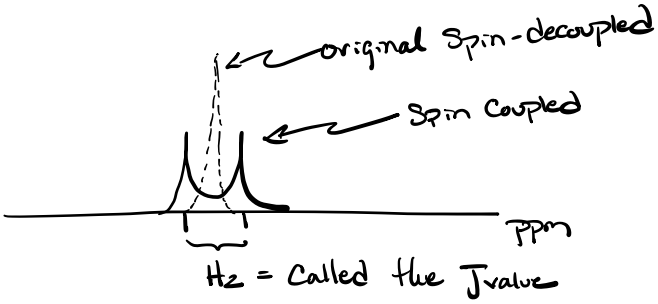


H_A affected by H_B (Near Neighbor)

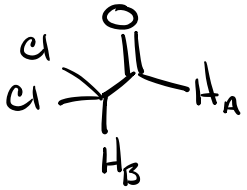




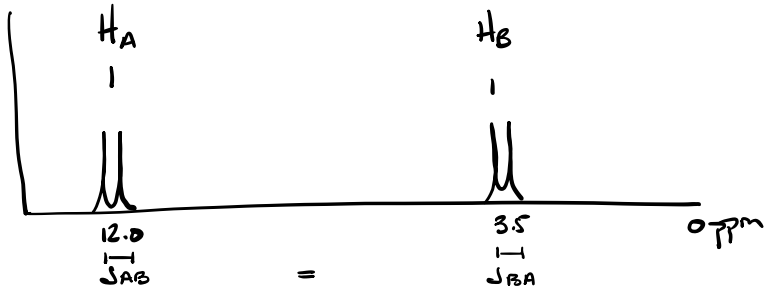
doublet



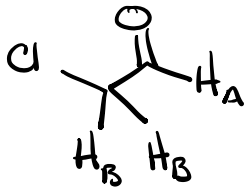
$$\frac{\nu_{signal} - \nu_{ref}}{\nu_{field}} \times 10^6 = ppm$$



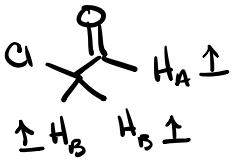
$J_{AB} = J_{BA}$ = Coupling Constant
& is measured in Hz



Neighbors that split each other will always have same J value

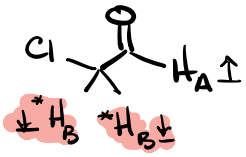


Focus on H_A

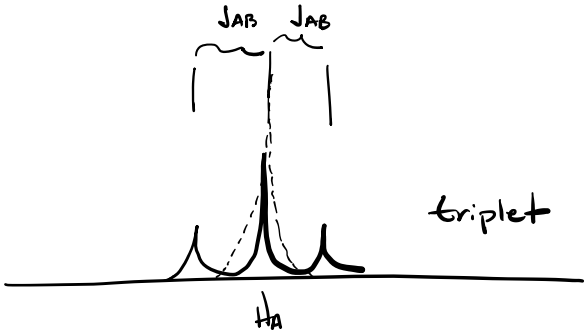


$\Delta E_{large\ H_A}$

2x ΔE unchanged



$\Delta E_{small\ H_A}$



Pattern follows n+1 rule | n = # of neighbors

Pascals Triangle

# of neighbors							
0			1				
1		1		1			
2	1		2		1		
3		1	3	3	1	quartet	1:3:3:1
4	1	4	6	4	1	pentet	1:4:6:4:1
5	1	5	10	10	5	1	sextet 1:5:10:10:5:1

Predicts Relative Intensities for number of neighbors

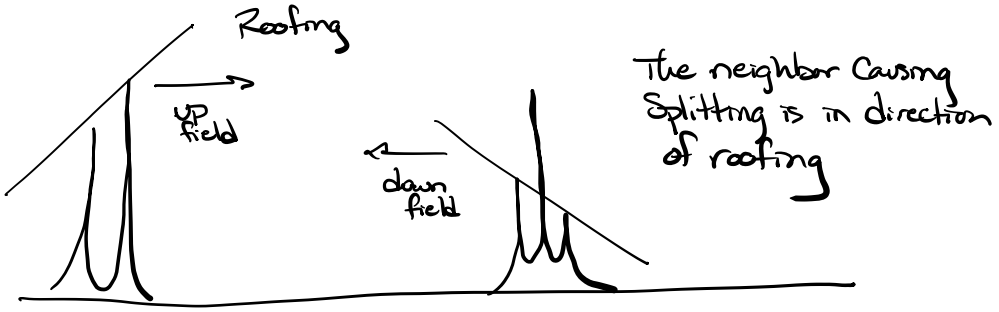
doublet 1:1

triplet 1:2:1

- Pattern tells # of neighbors
- Integration tells how many of each proton
- ppm tells Chemical environment
- J-value whom is connected to whom

  Identical J-values ID's neighbors

- Roofing helps to find neighbors



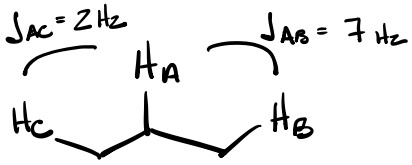
Symmetrical Roofing

doublet

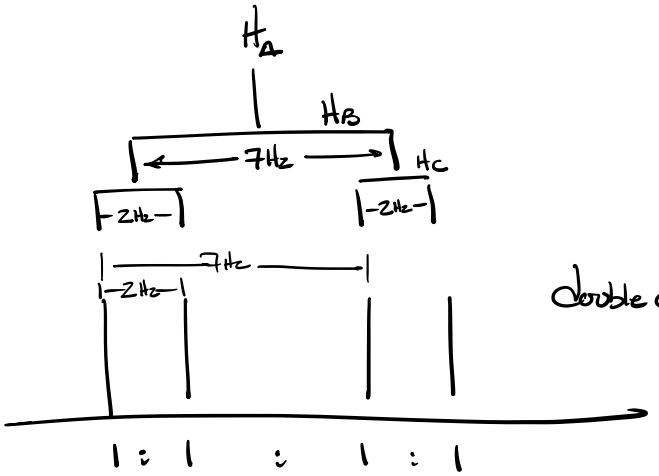
triplet

quartet

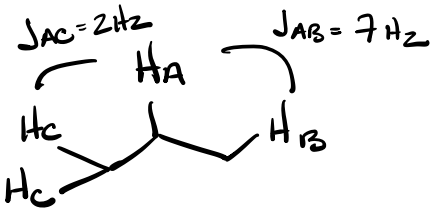
Inequivalent Neighbors

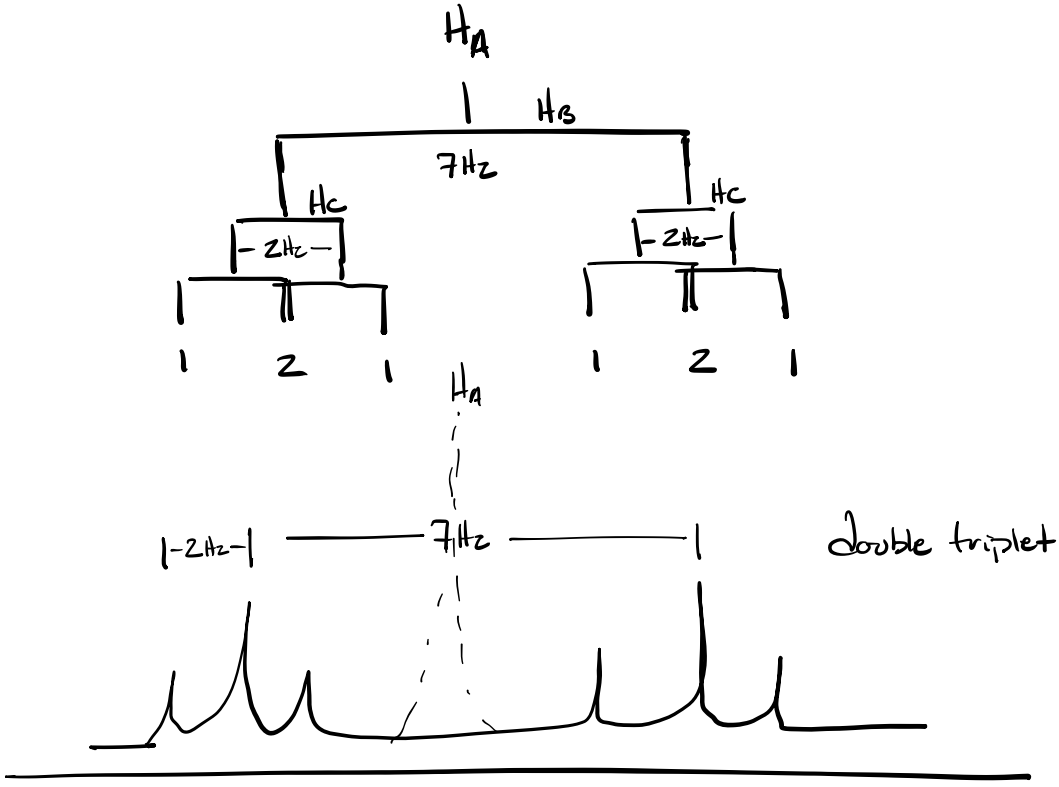


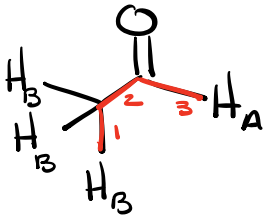
Tree diagram

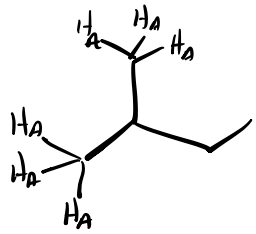


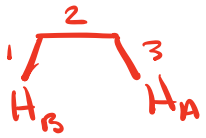
double doublet


$J_{AC} = 2Hz$
$J_{AB} = 7Hz$
H_A
H_C
H_C
H_B

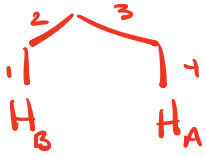

H_A
H_B
7Hz
H_C
2Hz
H_C
2Hz
1 2 1
1 2 1
H_A
2Hz
7Hz
Double triplet



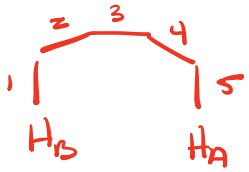




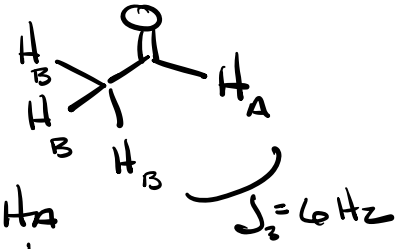
J_3 = 3 bonds apart 6-8 Hz



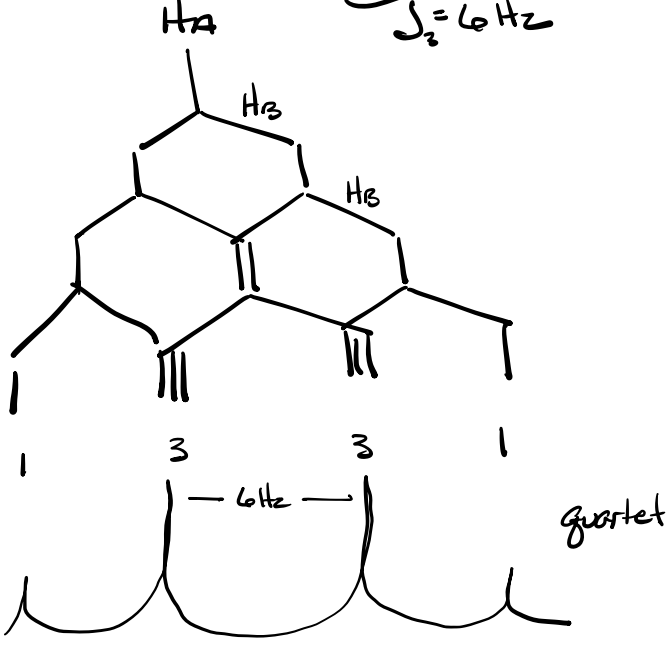
J_4 = small 1-3 Hz

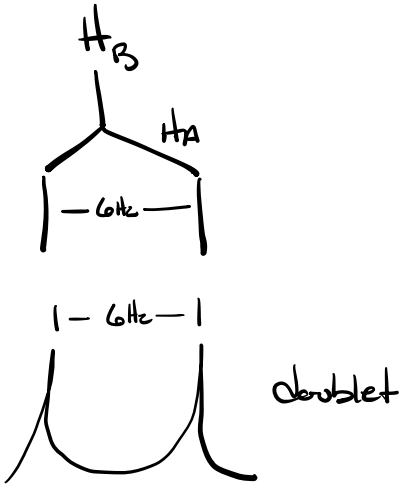


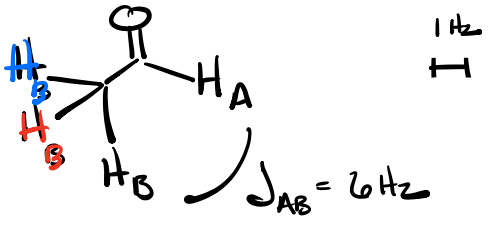
J_5 = tiny if visible 0-1 Hz

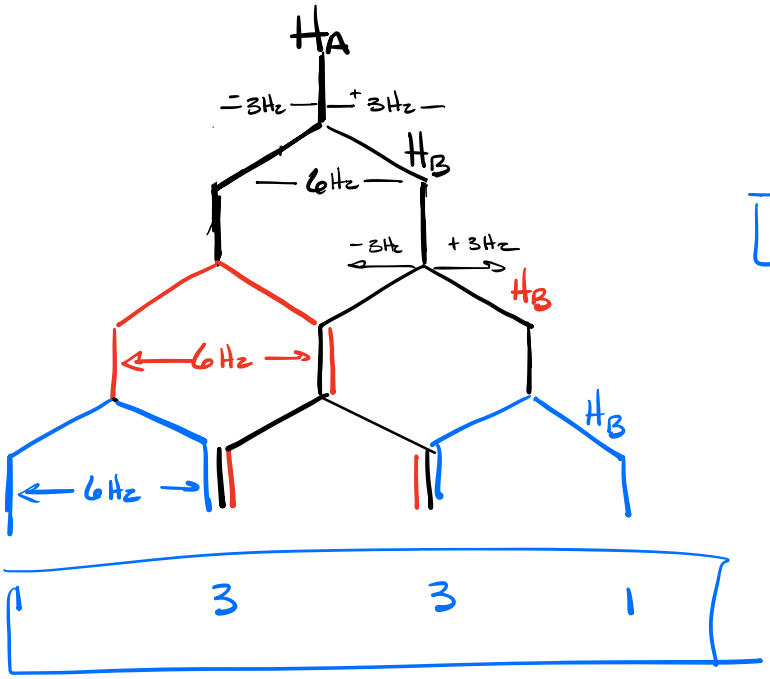


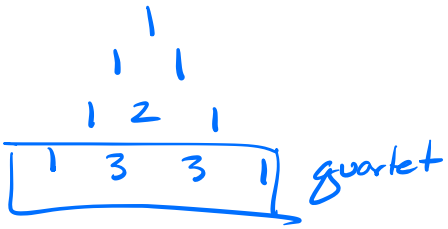
Give tree-diagram for H_A & H_B









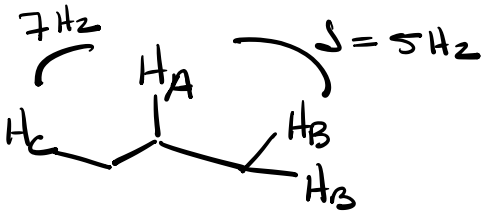


Coupling Constant = J_{AB} = Hz

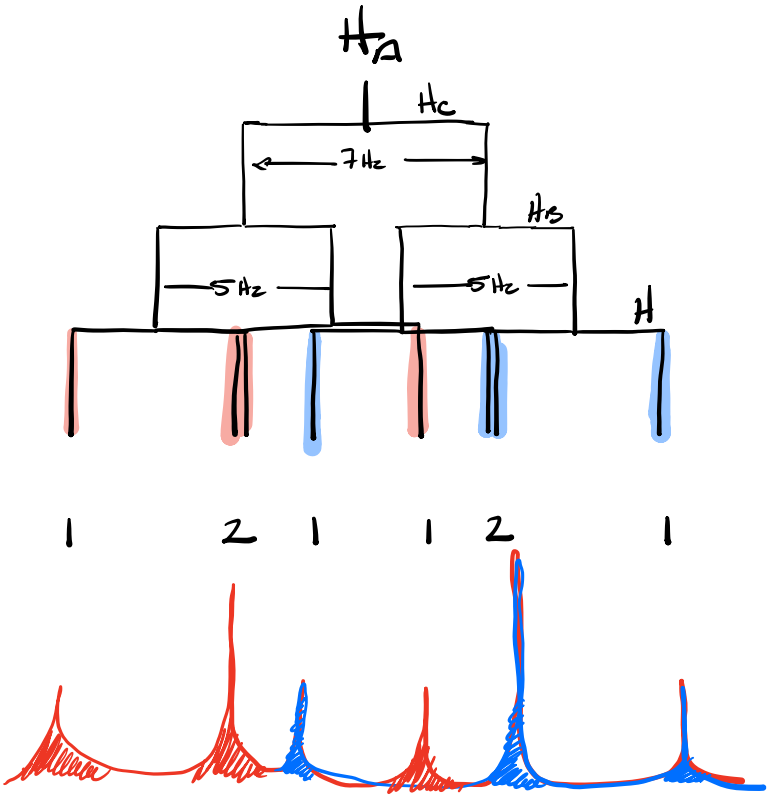
distance of neighbor in bonds = J_3 or J_4 or J_5

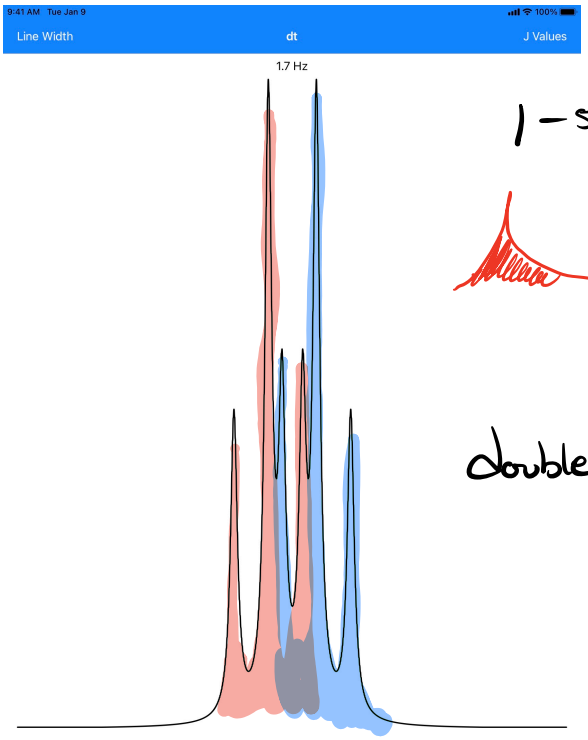
J_3 or J_{AB} description or type

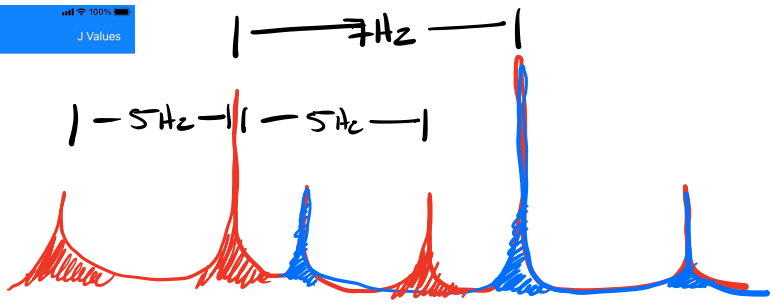
$J = 6\,Hz$ value



draw H_A, H_B, H_C







double triplet