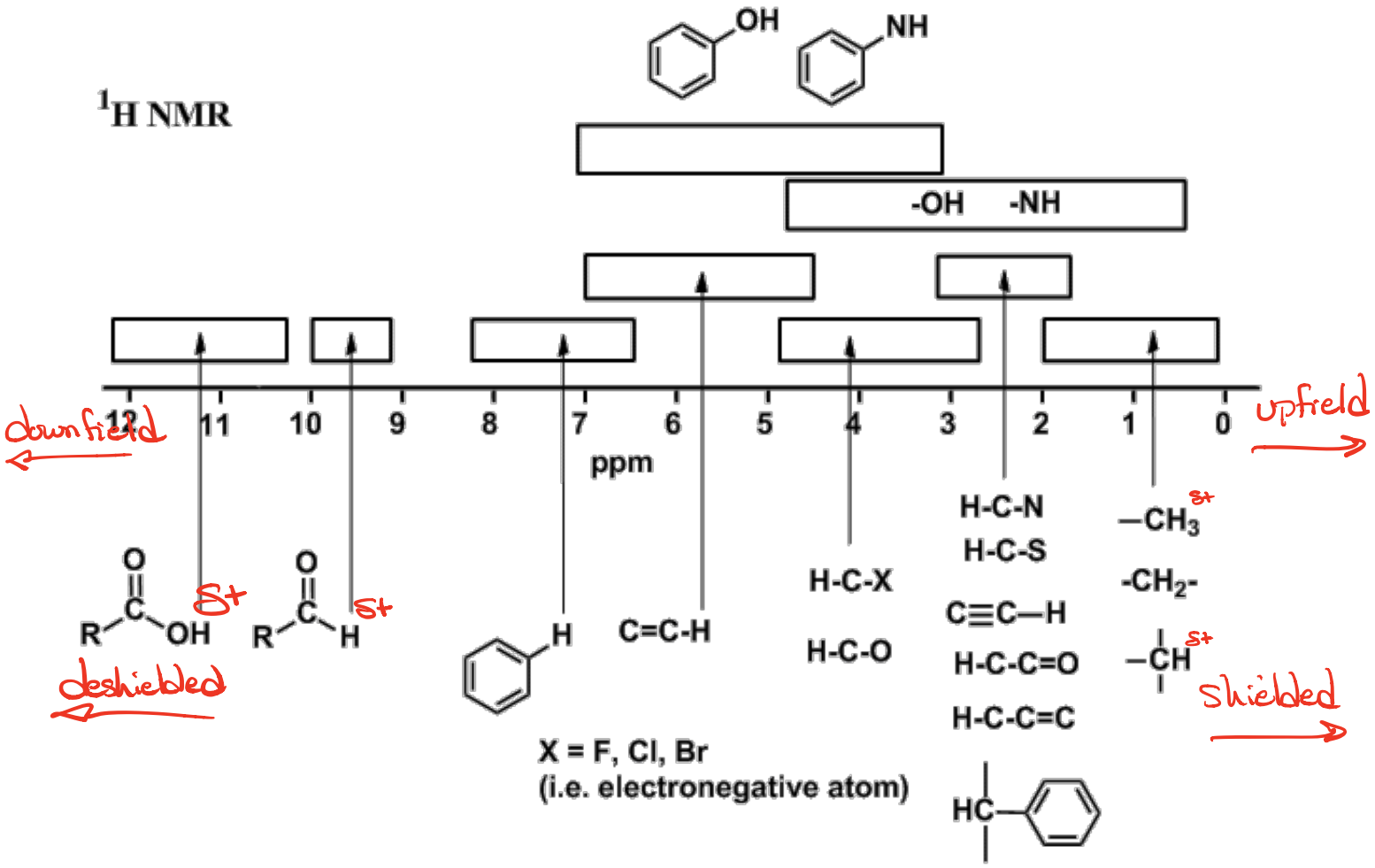
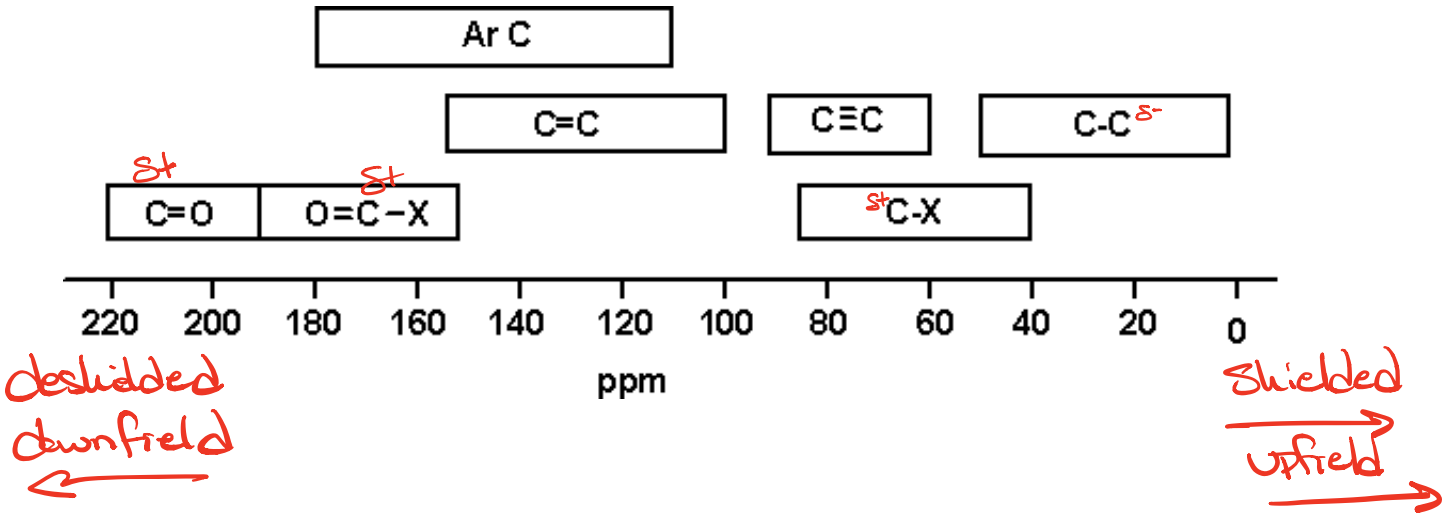
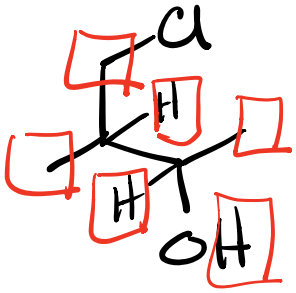
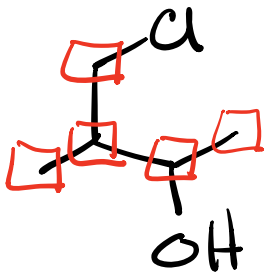
# $^1$H NMR


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



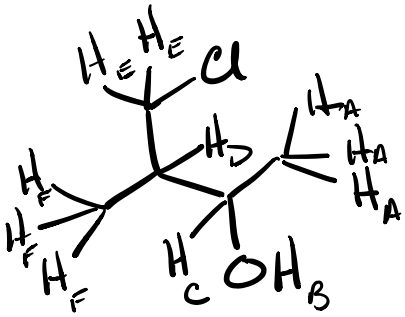



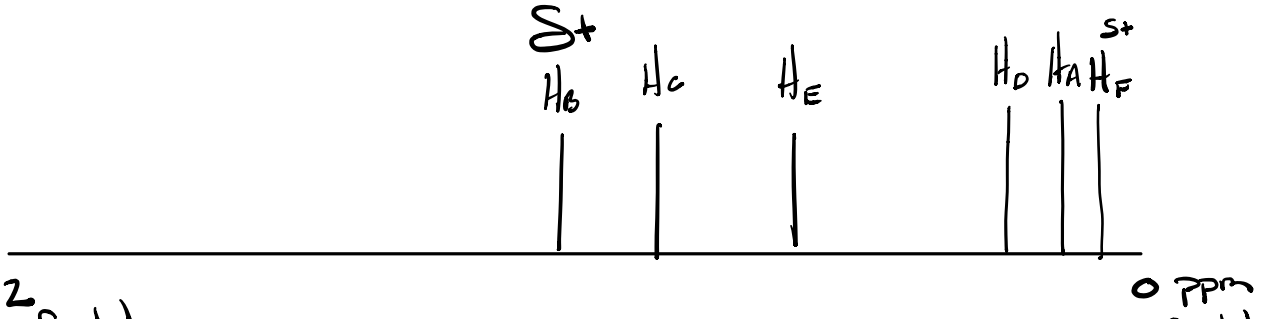
# H Environments 6



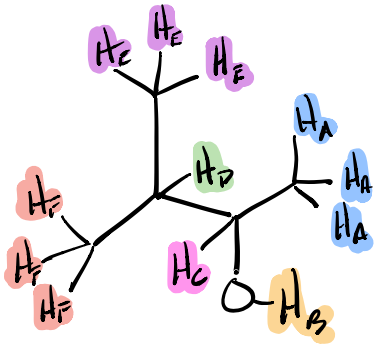
# C Environments 5

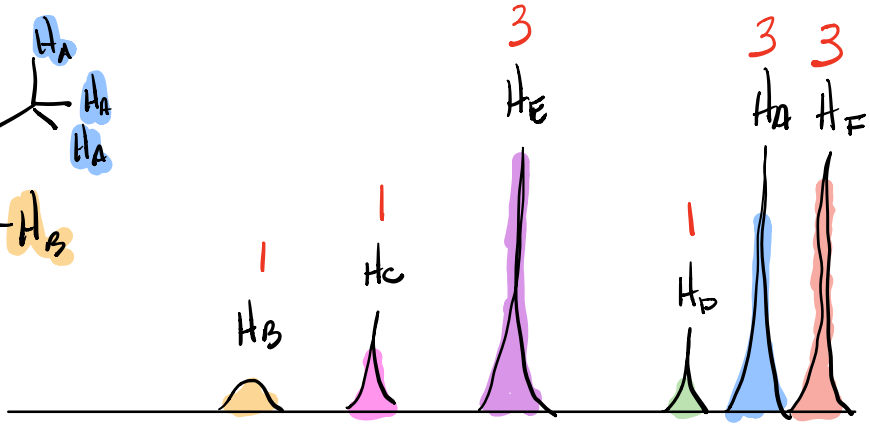
C 2.5 N 3.0 O 3.5 F 4.0 Cl 3.0 Br

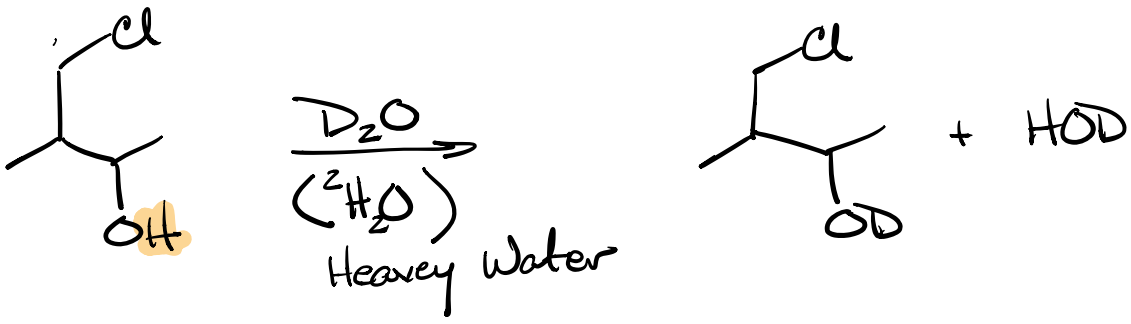




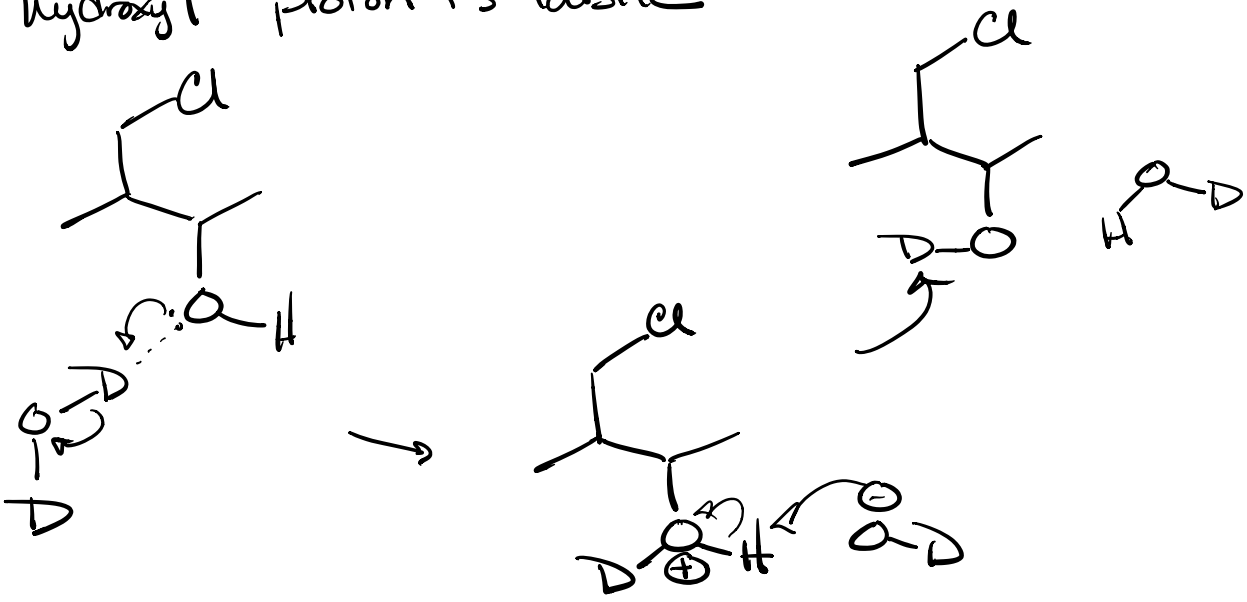
Integration - How many of each type of proton

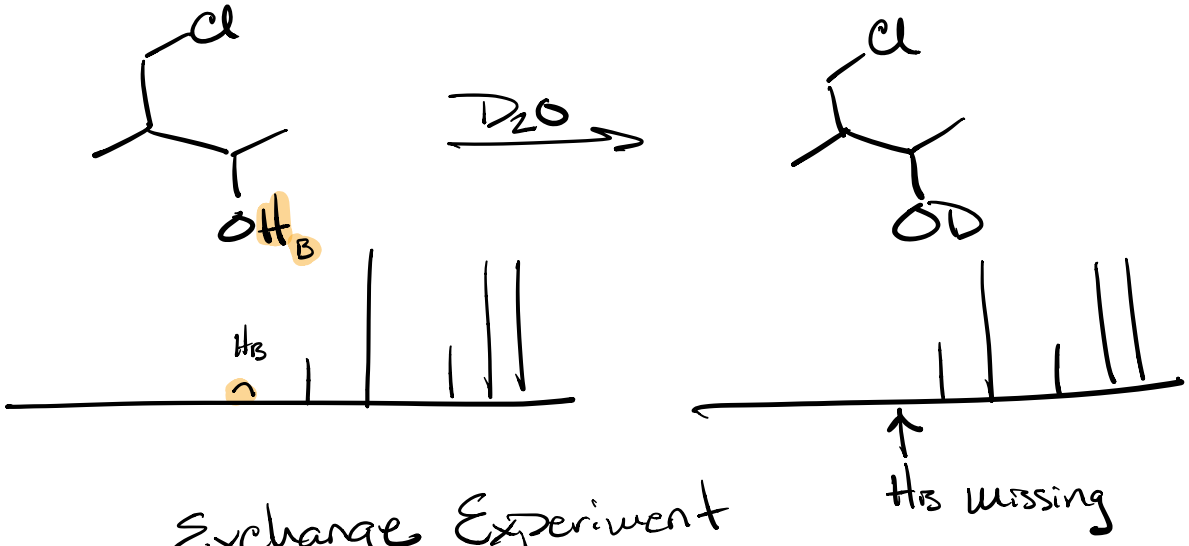



Hydroxyl Proton is labile





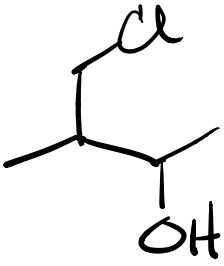

Exchange Experiment

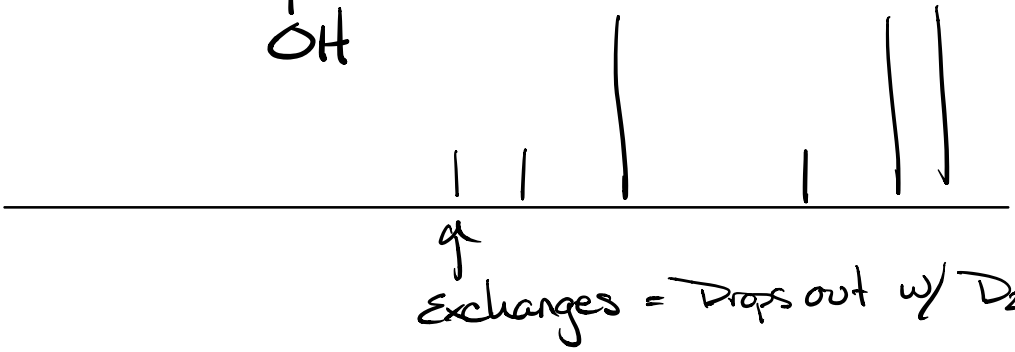
Test for protic hydroges

R-OH

R-NH

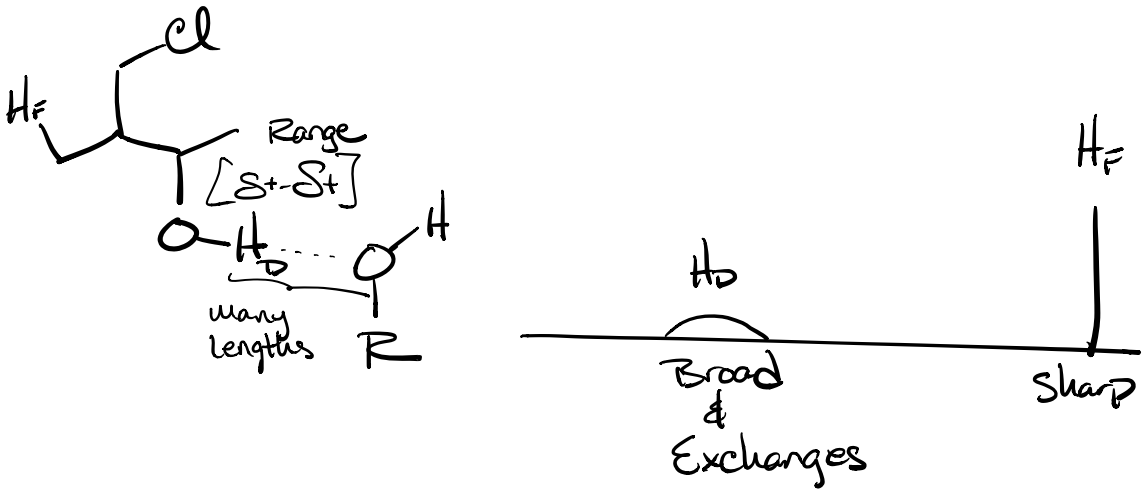
R-SH



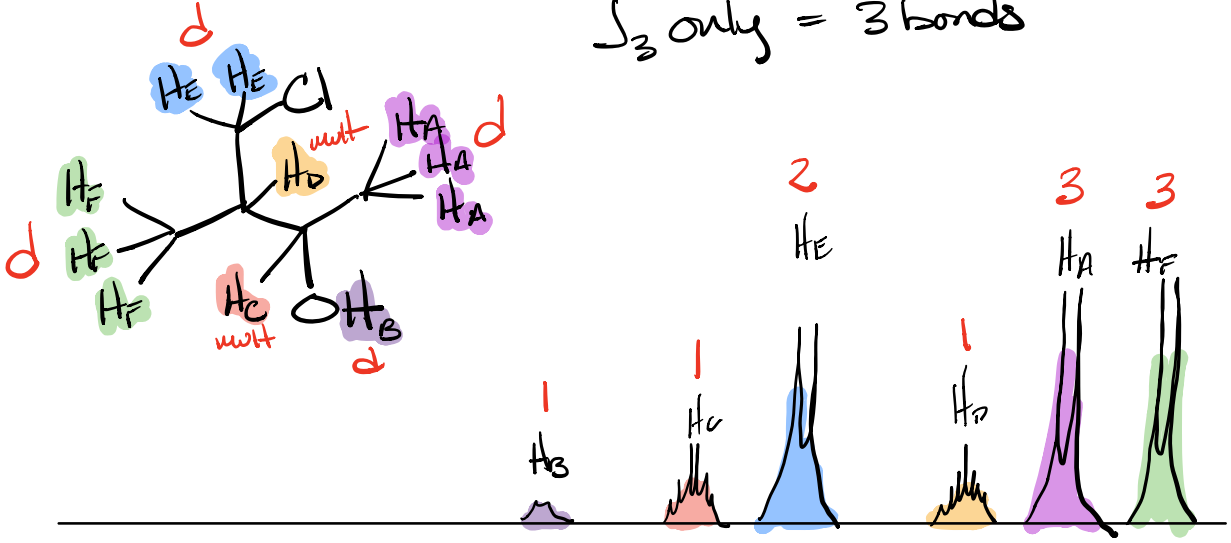
q

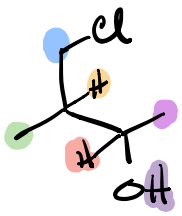
Exchanges = Drops out w/ $D_2O$



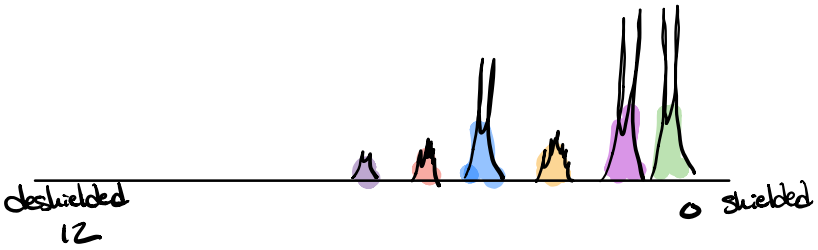

# Multiplicity - Spin-Spin Coupling

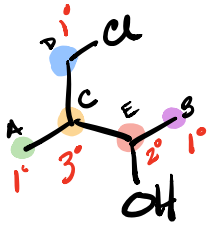
$J_3$ only = 3 bonds



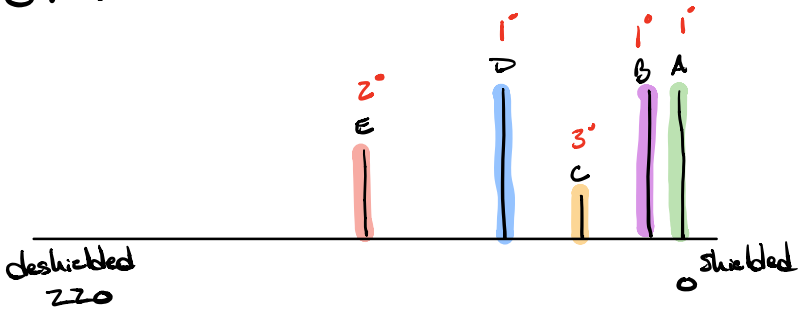



$^1$H-NMR

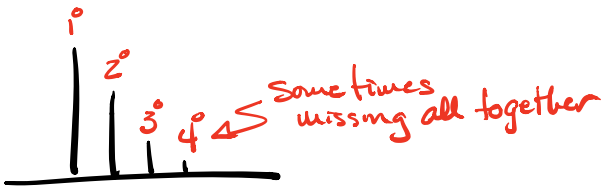



$^{13}$C-NMR




$^{13}$C NMR



#16 on WebSpectra

$C_7H_7OBr$

units of unsaturation

$C_nH_{2n+2+N-X}$

$C_7H_{2(7)+2+0-1}$

$H_{15}$ for saturation

$-H_7$

$2|8$

4 units of unsaturation

C ≤ 12 units unsat ≥ 4 = aromatic Ring

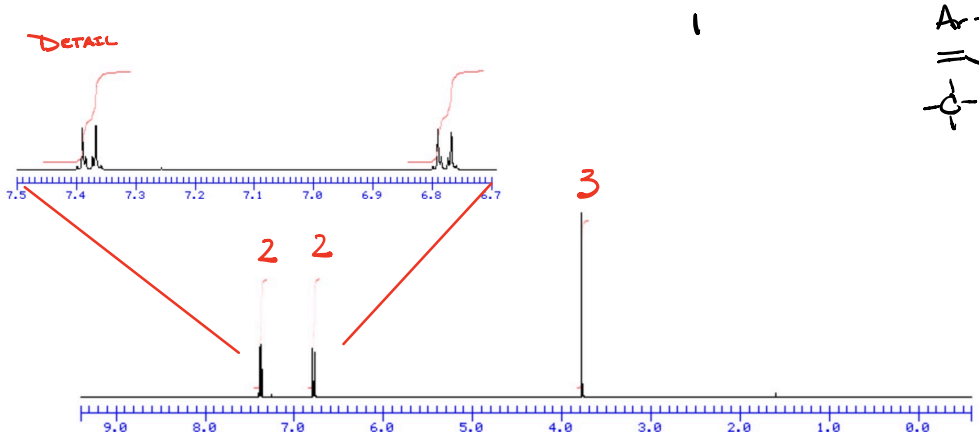
Int

3, 6, 9 ... $-CH_3$

2, 4, 6 ... $-CH_2-$

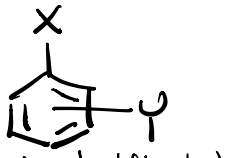
1 Ar-H, $=H$, $-\overset{|}{C}-H$

$^1$H-NMR




$^1$H-NMR

| ppm | Int | mult | # of N | assignment |
|---|---|---|---|---|
| 3.8 | 3 | s | 0 | $-O-CH_3$ |
| 6.8 | 2 | ? | ? | Ar-H |
| 7.4 | 2 | ? | ? | Ar-H |

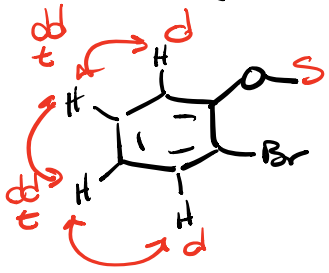


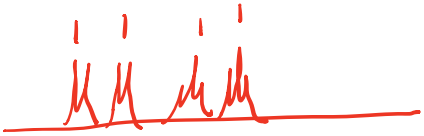

disubstituted


$-O-CH_3$

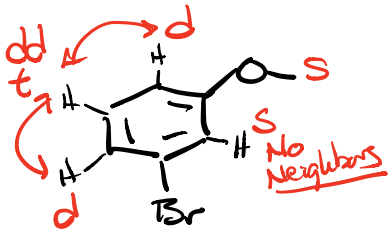
$-Br$

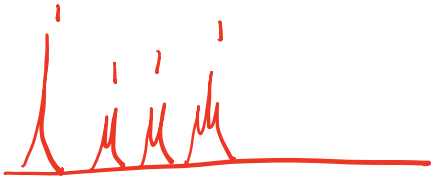
ortho (1,2)



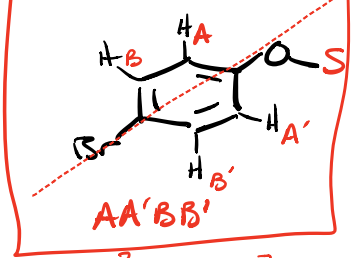
meta (1,3)



Match ✓

para (1,4)





Inverted Quartets