7 on Webspectra (Intermediate I)

C_4H_6O

$C_nH_{2n+2+N-X}$ | $n = \#C$

$H_{2(4)+2} = H_{10}$

$-H_6$

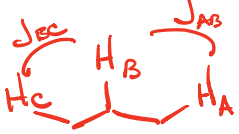
$2 \mid 4$

2 units

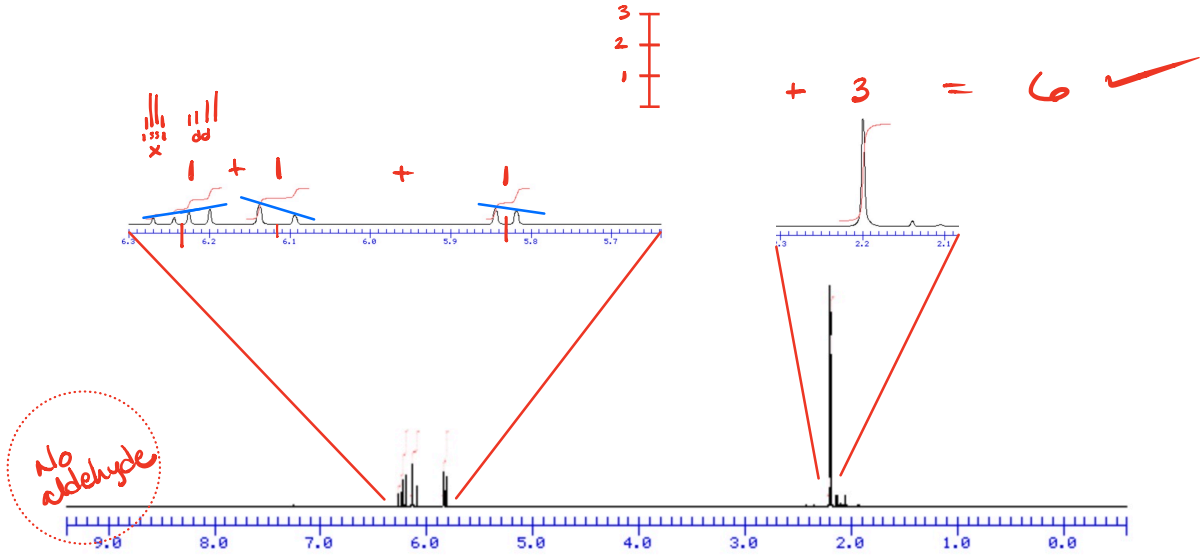
^{1}H-NMR Table

of H Environments = 4 ?

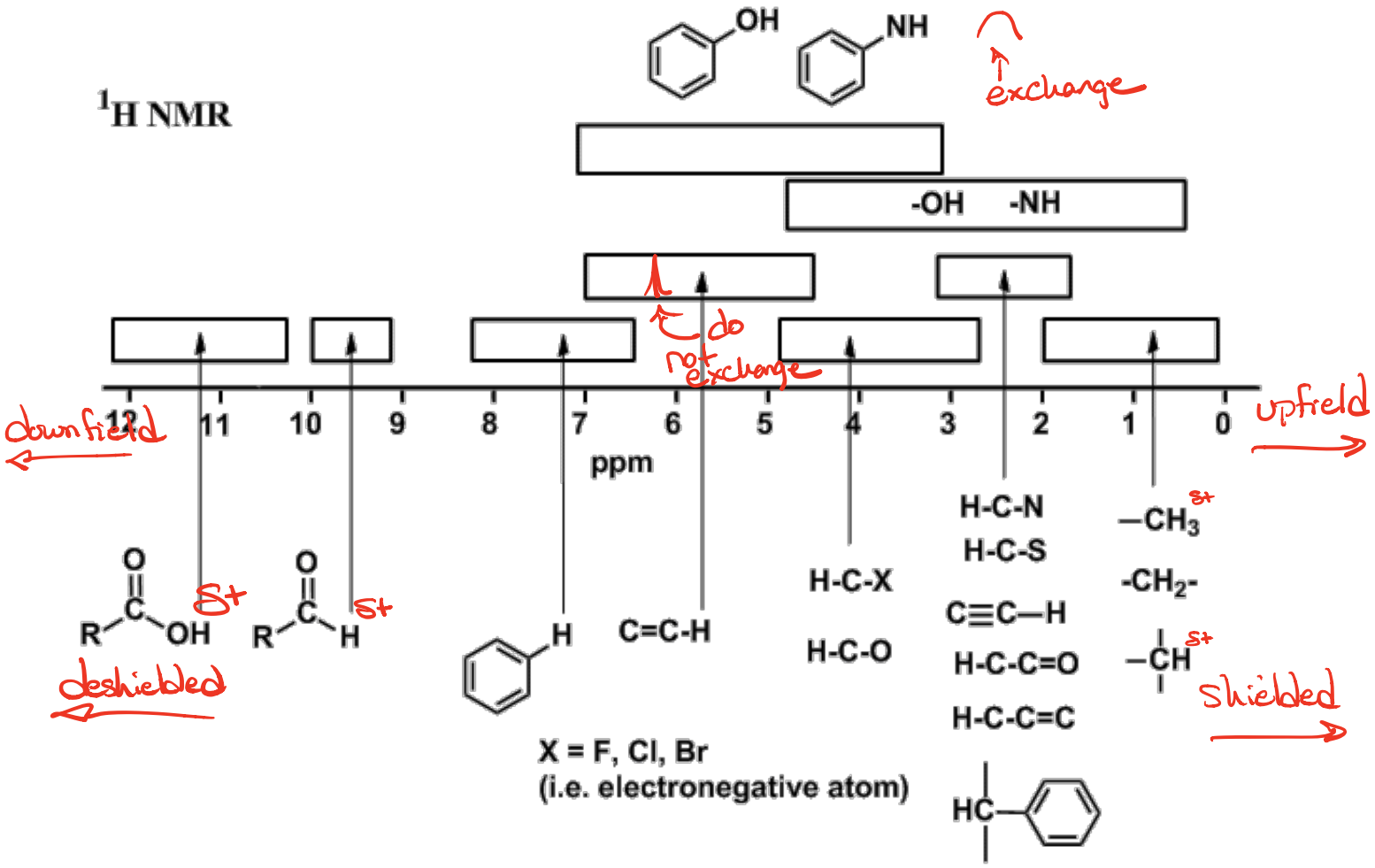
δ ppm	Int	(Spin) Mult	# of neighbors	assignment
2.2	3	s	∅	EWG – CH_3
5.83	1	d	1	$C=C^{H}$ × 3
6.12	1	d	1	
6.24	1	dd	2 (1+1)	



$J_{AB} \neq J_{BC}$ = double doublet



^{1}H NMR

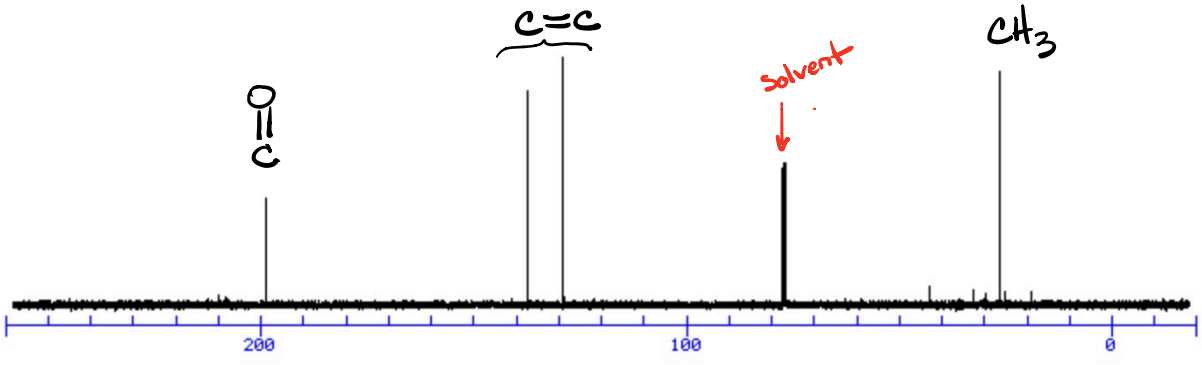

OH
NH
exchange
-OH -NH
do not exchange
downfield
upfield
12 11 10 9 8 7 6 5 4 3 2 1 0
ppm
H-C-N
H-C-S
—CH3
δ+
H-C-X
-CH2-
C≡C—H
H-C-O
H-C-C=O
—CH
δ+
H-C-C=C
C=C-H
H
R
OH
O
δ+
deshielded
shielded
X = F, Cl, Br
(i.e. electronegative atom)
HC

^{13}C-NMR Table

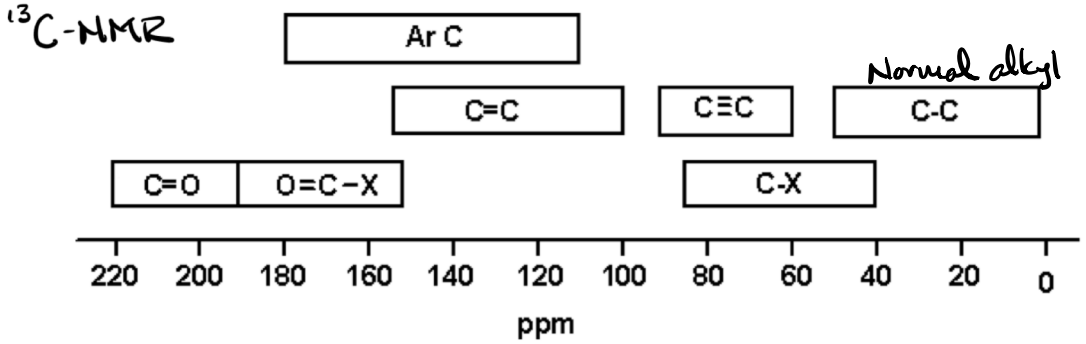
# of C Environments = 4

δ ppm	assignment
28	alkyl CH_3
129	C=C
138	C=C
200	C=O

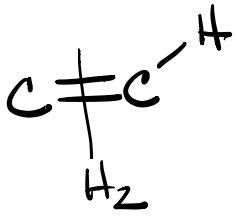
} 2 units of unsaturation

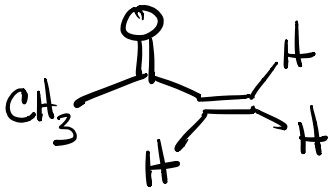


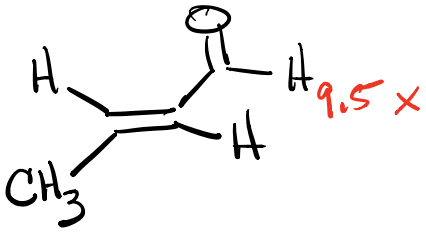
^{13}C-NMR

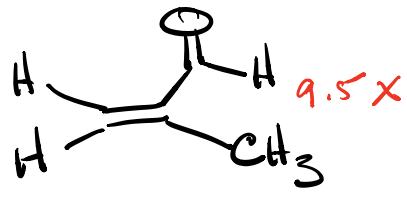


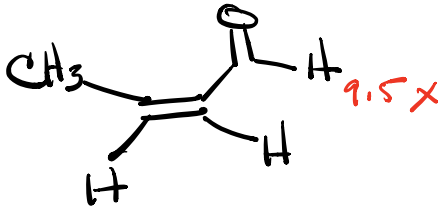
Pieces

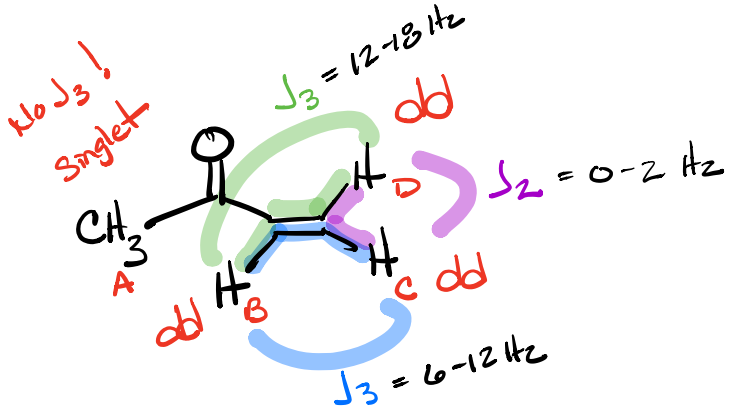


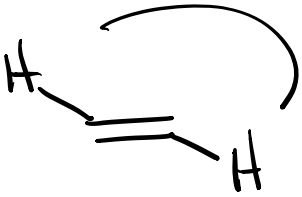






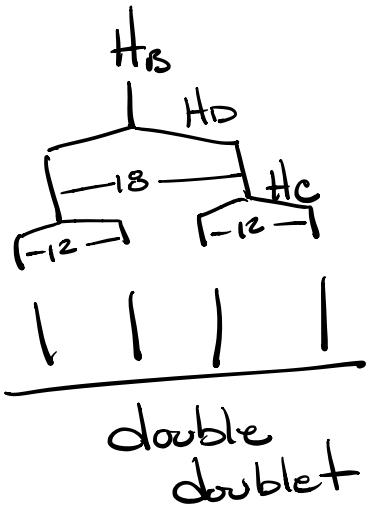


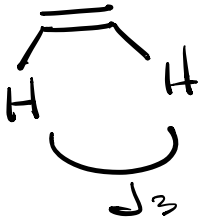




J_3 = 12-18 Hz

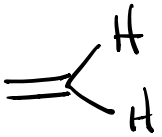
Trans





J_3 = 6-12 Hz

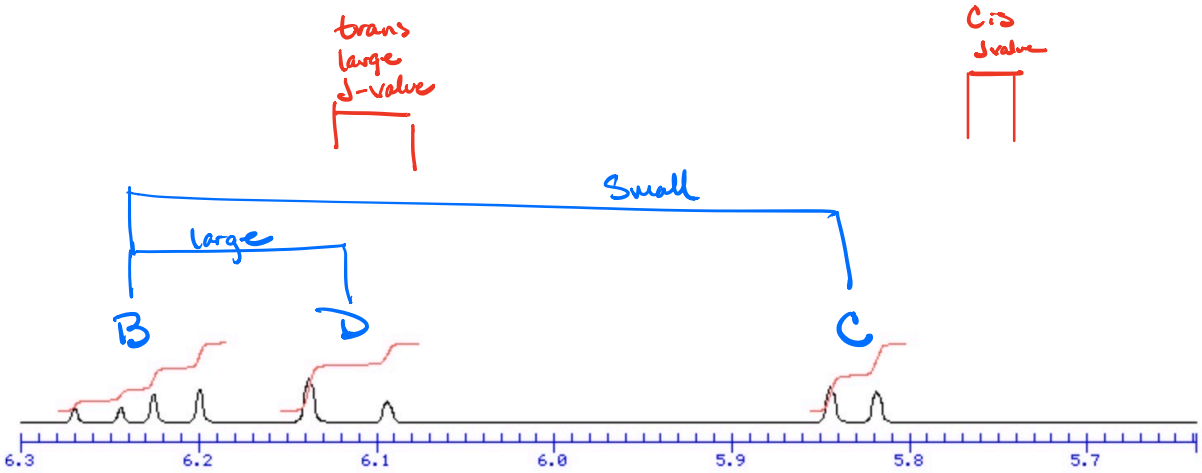
Cis

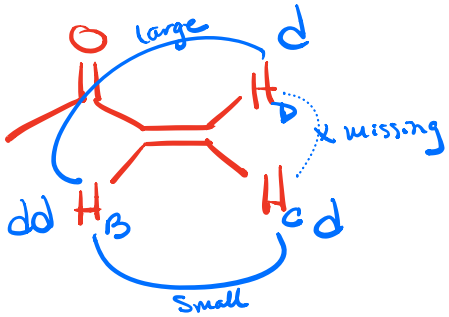


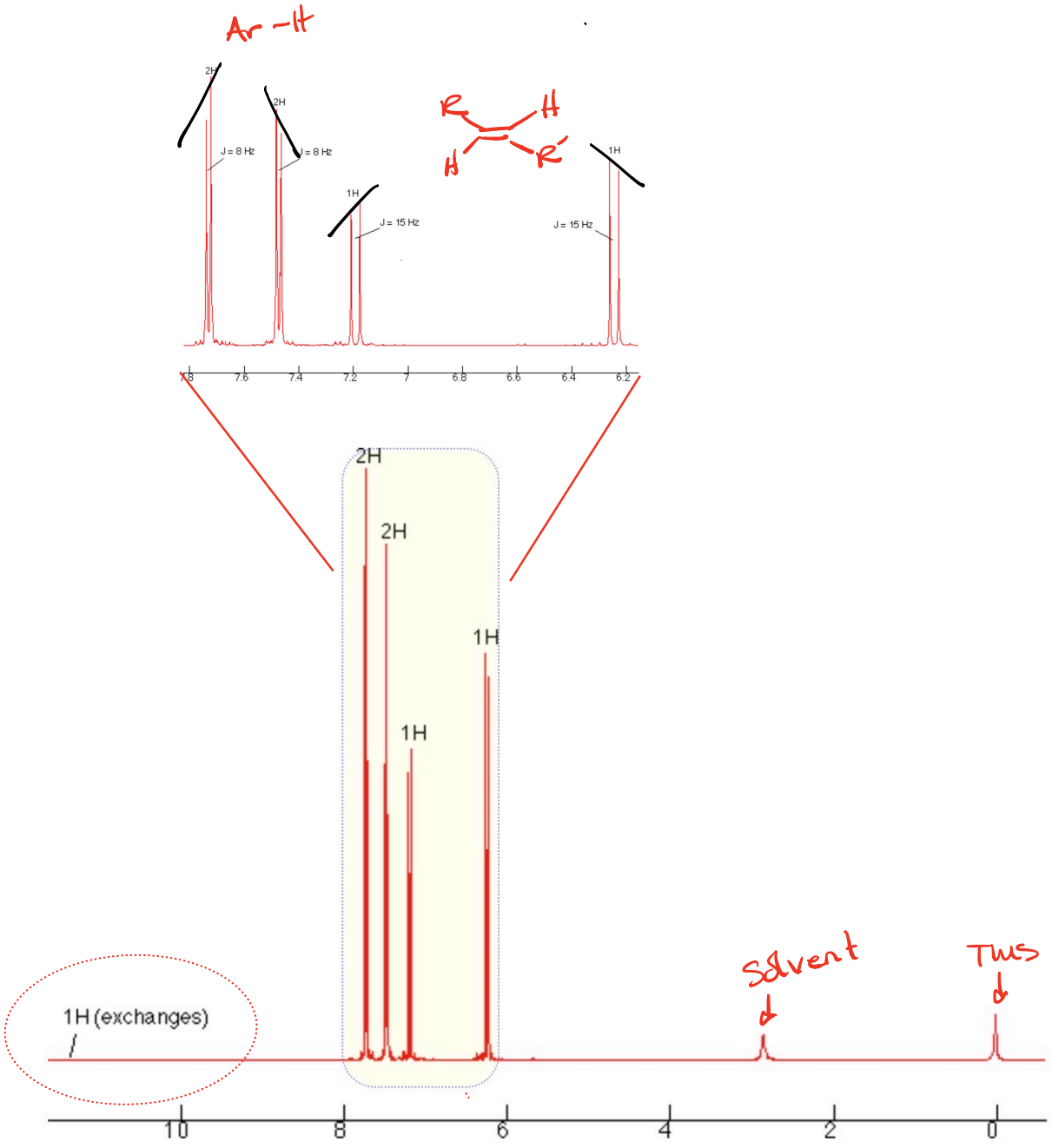
J_2 = 0-2 Hz

geminal

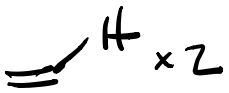
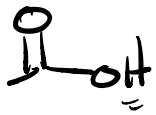
The alkene System

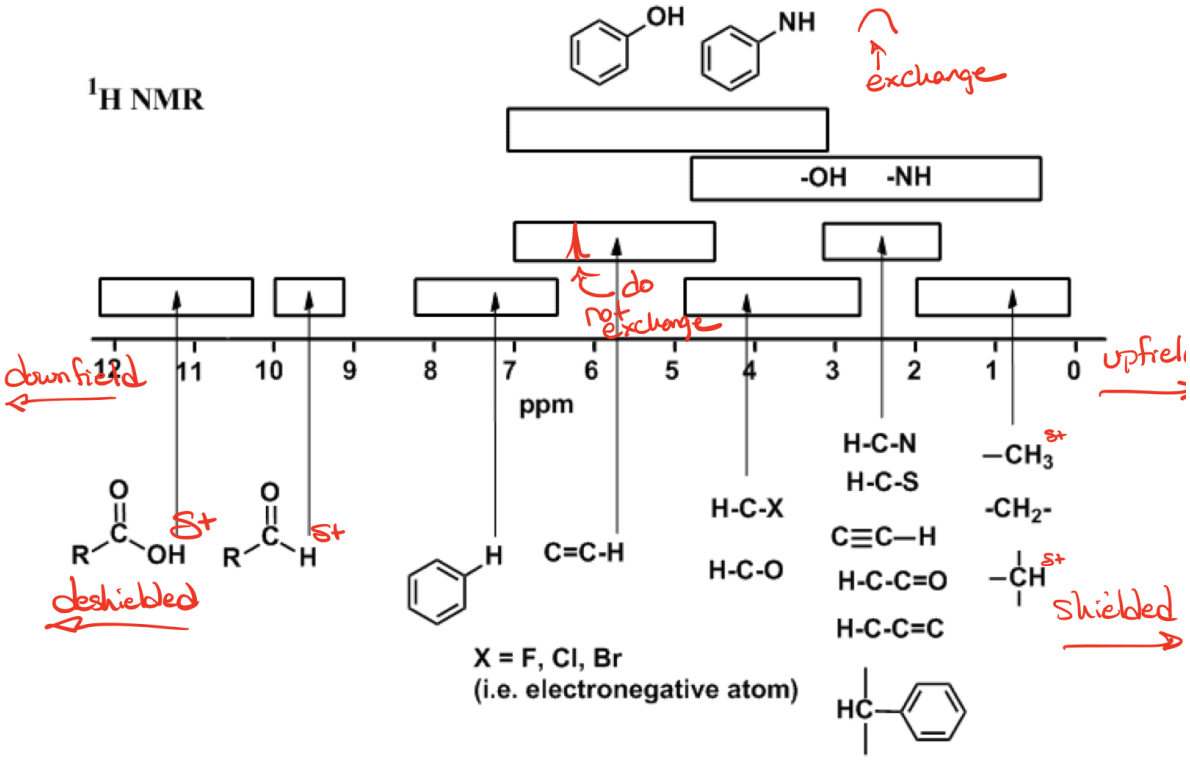


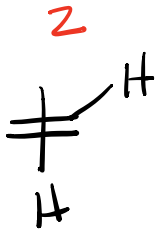



Ar-H
2H
2H
J = 8 Hz
J = 8 Hz
1H
J = 15 Hz
1H
J = 15 Hz
R
H
H
R'
7.8
7.6
7.4
7.2
7
6.8
6.6
6.4
6.2
2H
2H
1H
1H
1H (exchanges)
solvent
TMS
10
8
6
4
2
0

HNMR Table 5 Environments

ppm	Int	mult	# n	assignment
6.2	1	d 15Hz	1	 x2
7.2	1	d 15Hz	1	
7.44	2	d 8Hz	1	Ar-H x4
7.66	2	d 8Hz	1	
11.5	1	s exchanges		

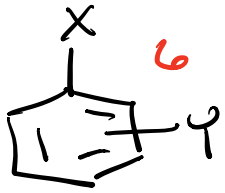




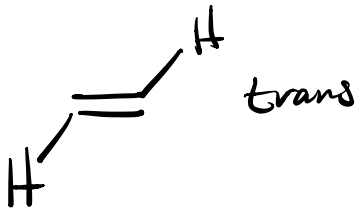
2

15Hz

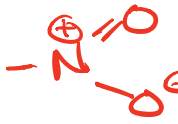
1



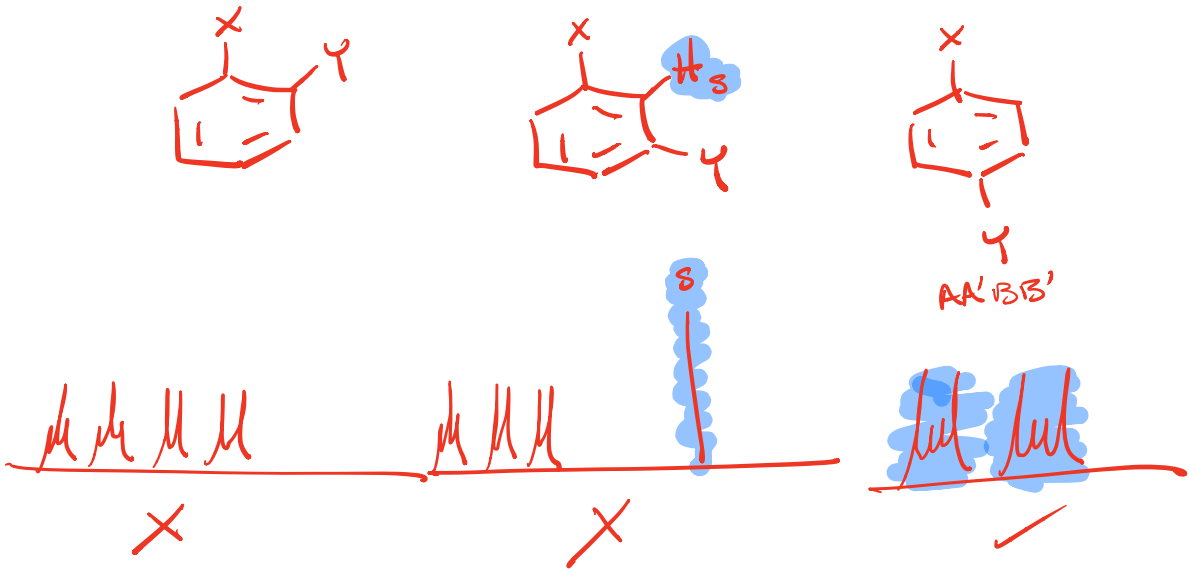
4 = 7 ✓

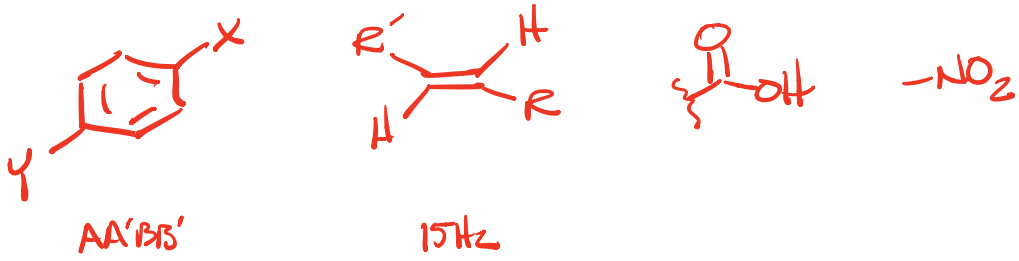


$C_9H_7O_2$ $C_9H_7NO_4$?

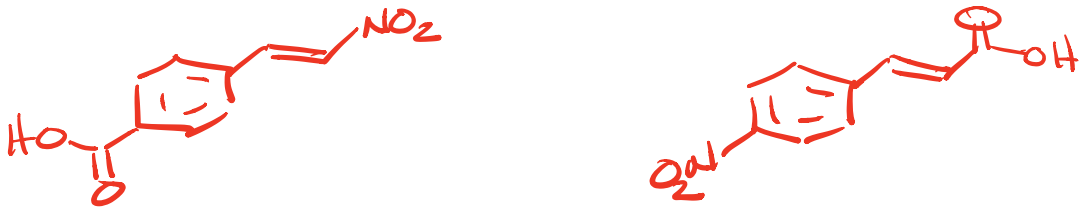
missing NO_2 =  = $-NO_2$

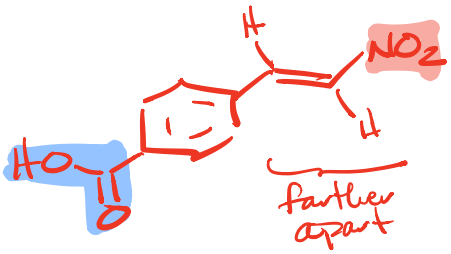
Nitro group

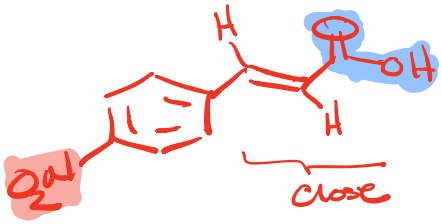




No CH_3's

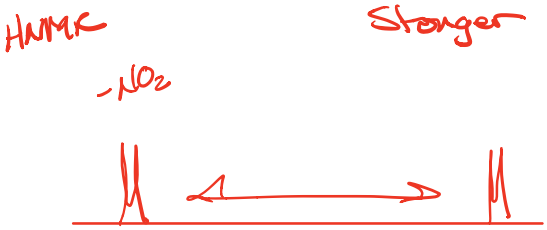


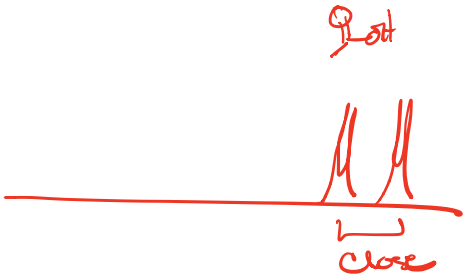

H
NO2
H
HO
O
farther apart


H
OH
H
O2N
close

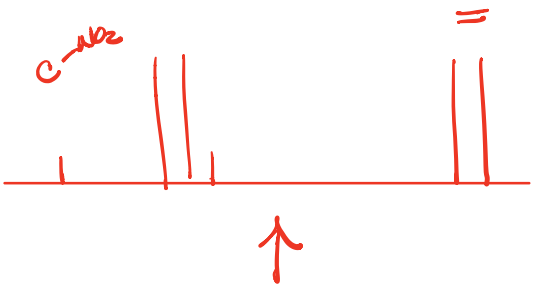

Stronger

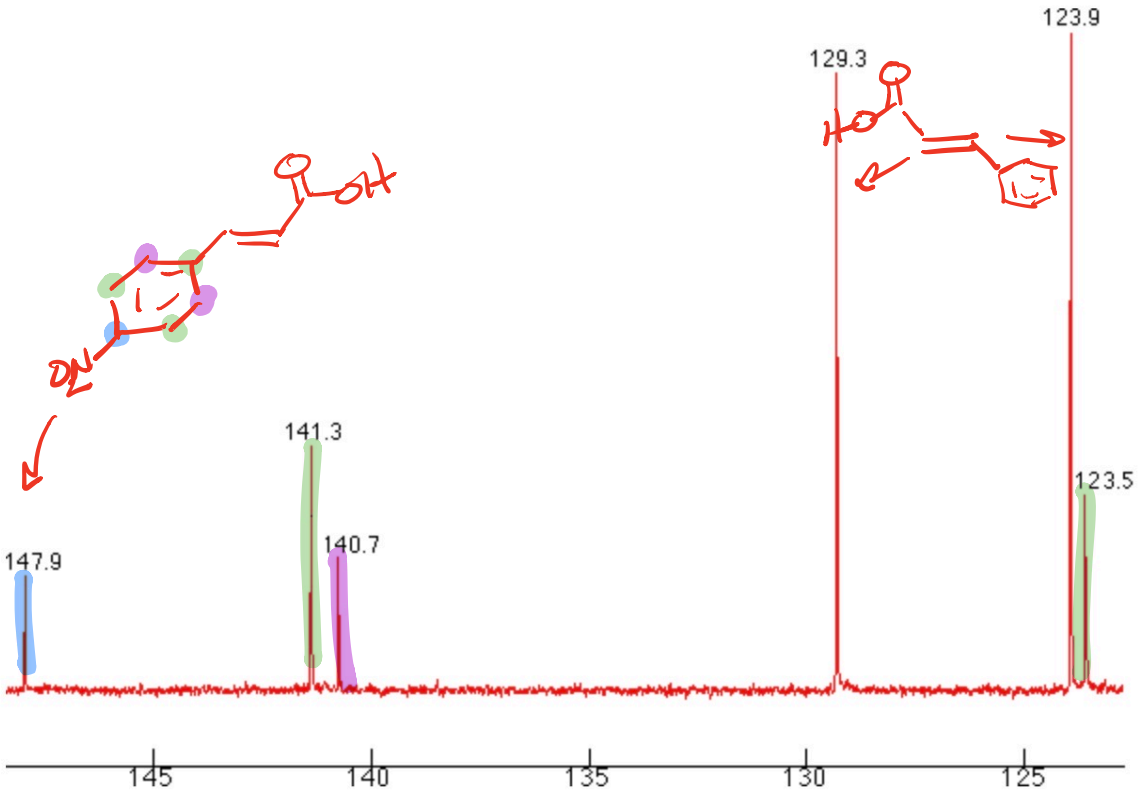

OH


HNMR
-NO2


OH
close


CNMR
Ar
NO2
X


C-NO2
=



Click on the highlighted area to zoom. Click again to zoom back out.