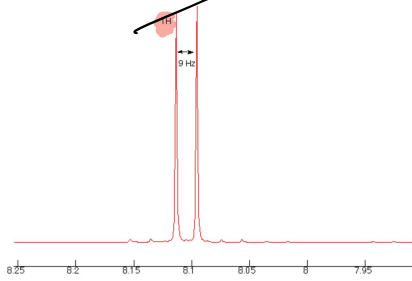
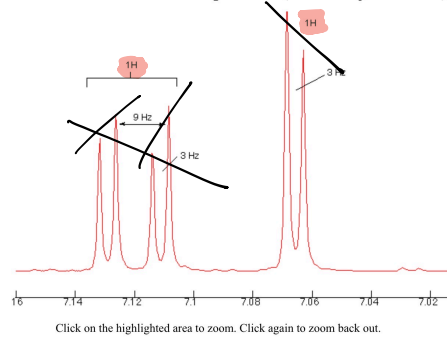


$$\begin{array}{c}
 (1 + 1) \\
 \uparrow \quad \uparrow \\
 \text{double doublet}
 \end{array}$$

Problem 12 - ^1H NMR spectrum (DMSO- d_6 , 500 MHz)



Problem 12 - ^1H NMR spectrum (DMSO- d_6 , 500 MHz)



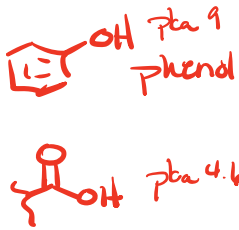
~~-SH~~

~~-NH~~

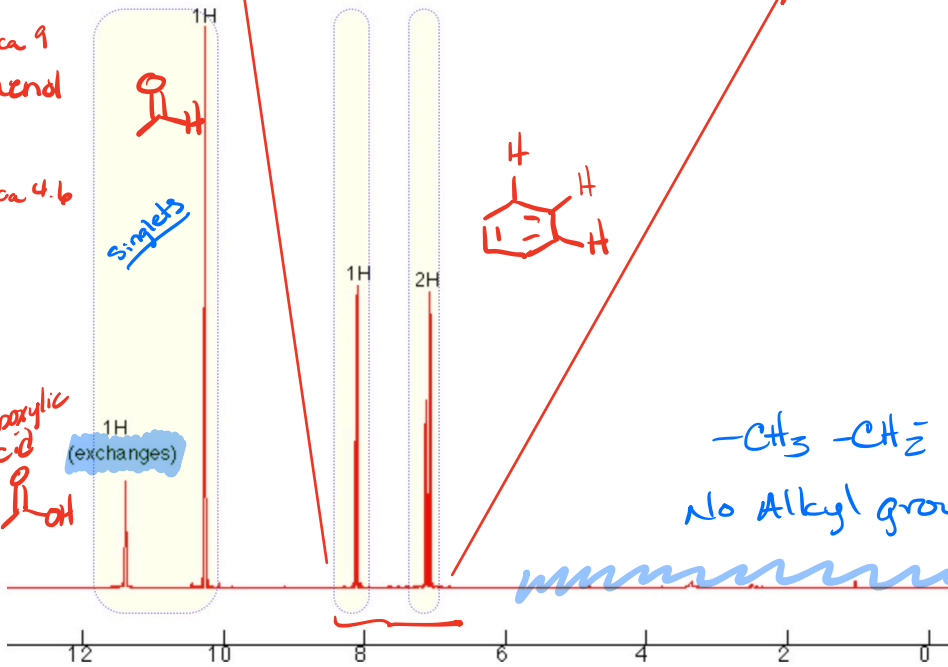
pKa 15.7

-OH Alcohol

Problem 12 - ^1H NMR spectrum (DMSO- d_6 , 500 MHz)



Carboxylic Acid



$-\text{CH}_3$ $-\text{CH}_2-$ $-\overset{|}{\text{C}}\text{H}$
 No Alkyl groups

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

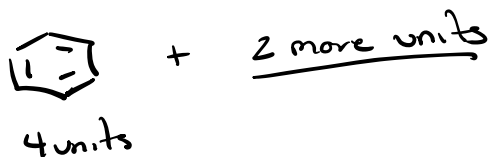
Number 12 webspectra

$C_7H_5NO_4$ units of unsaturation

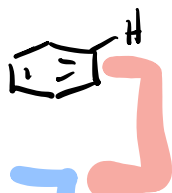

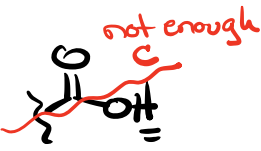
$$C_nH_{2n+2+N-x} \quad 2(7)+2+1 = \frac{17}{5}$$

$$2 \overline{) 12}$$

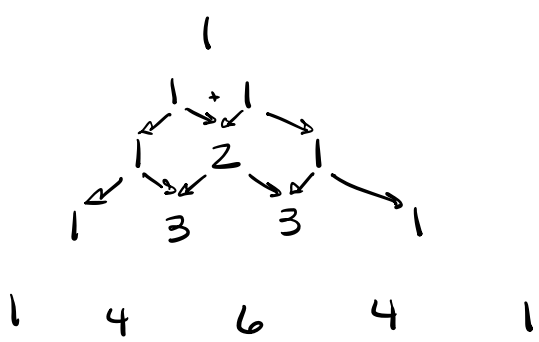
6 units



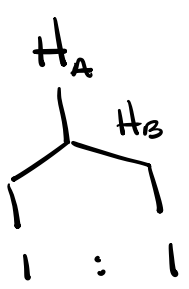
¹H NMR

<u>ppm</u>	<u>Int</u>	<u>mult</u>	<u># neighbors</u>	<u>Assignment</u>
7.06	1	doublet 3Hz	1	Ar-H, 
7.12	1	double-doublet 9Hz, 3Hz (1+1)		Ar-H 
8.1	1	doublet 9Hz	1	Ar-H 
10.3	1	Singlet	∅	
11.5	1	Singlet (exchanges)	∅	 Ar-OH

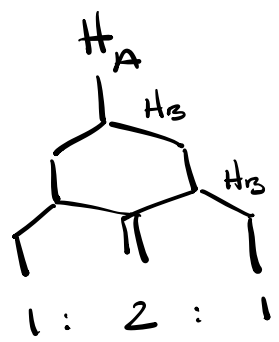
of neighbors



- ∅
- 1 when J-value is the same
- 2
- 3
- 4

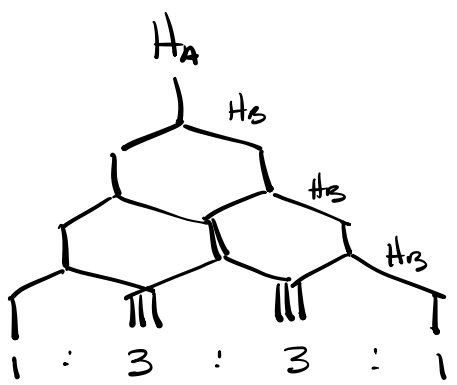


H_B
doublet



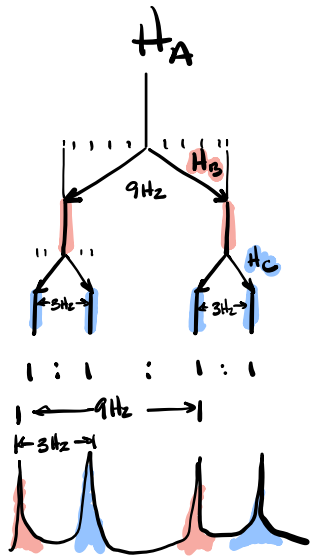
$2H_B$
triplet

J values all the same



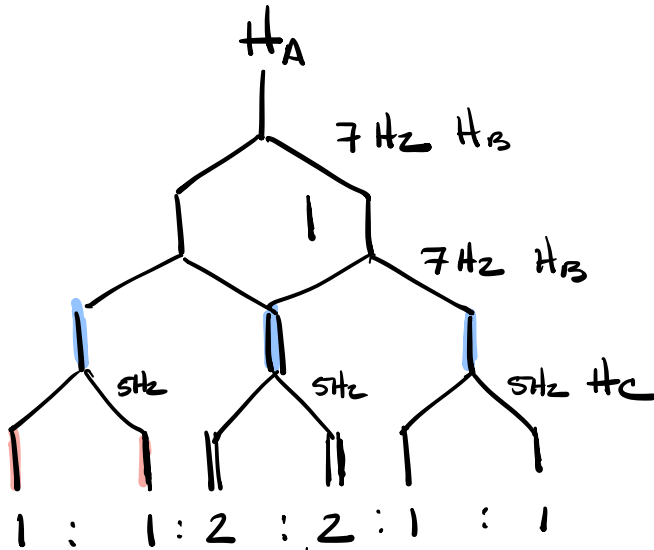
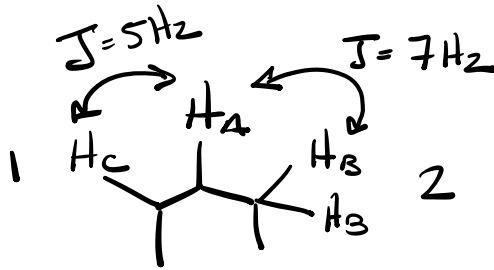
$3H_B$
quartet

J-values Different

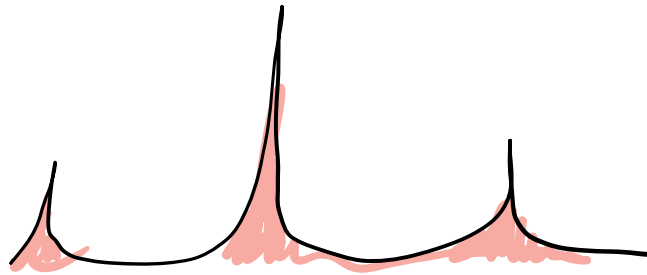
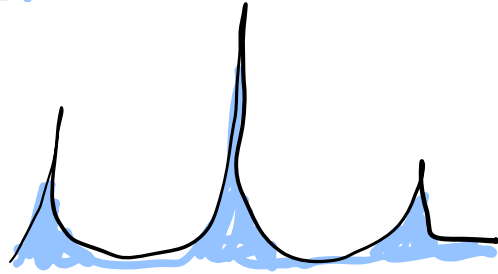
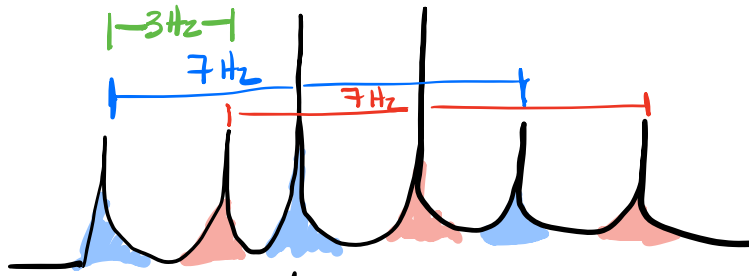


H_B 9 Hz
 H_C 3 Hz
 } Two neighbors
 in different
 environments

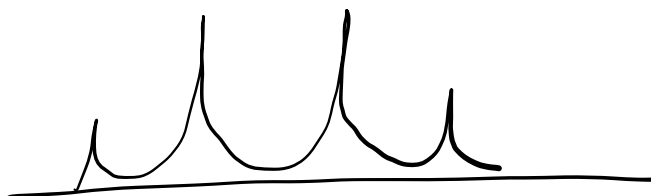
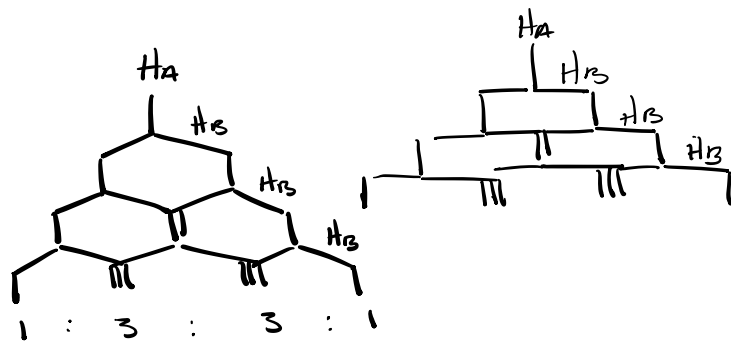
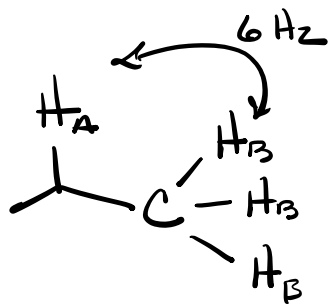
double doublet



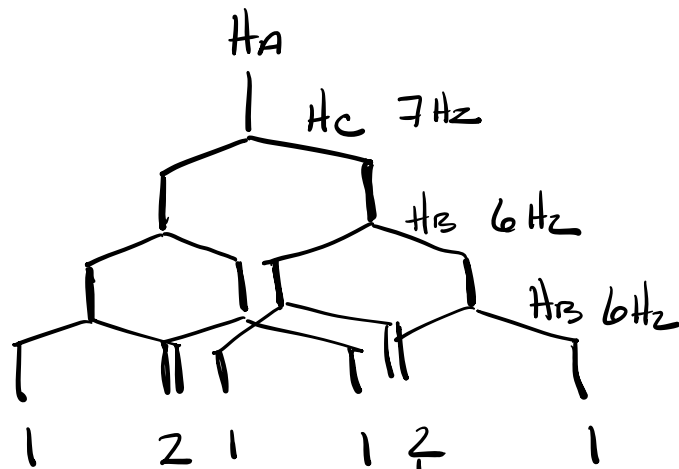
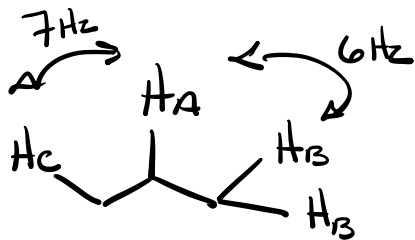
$2 + 1$
 \downarrow \downarrow
 triplet doublet
 double-triplet



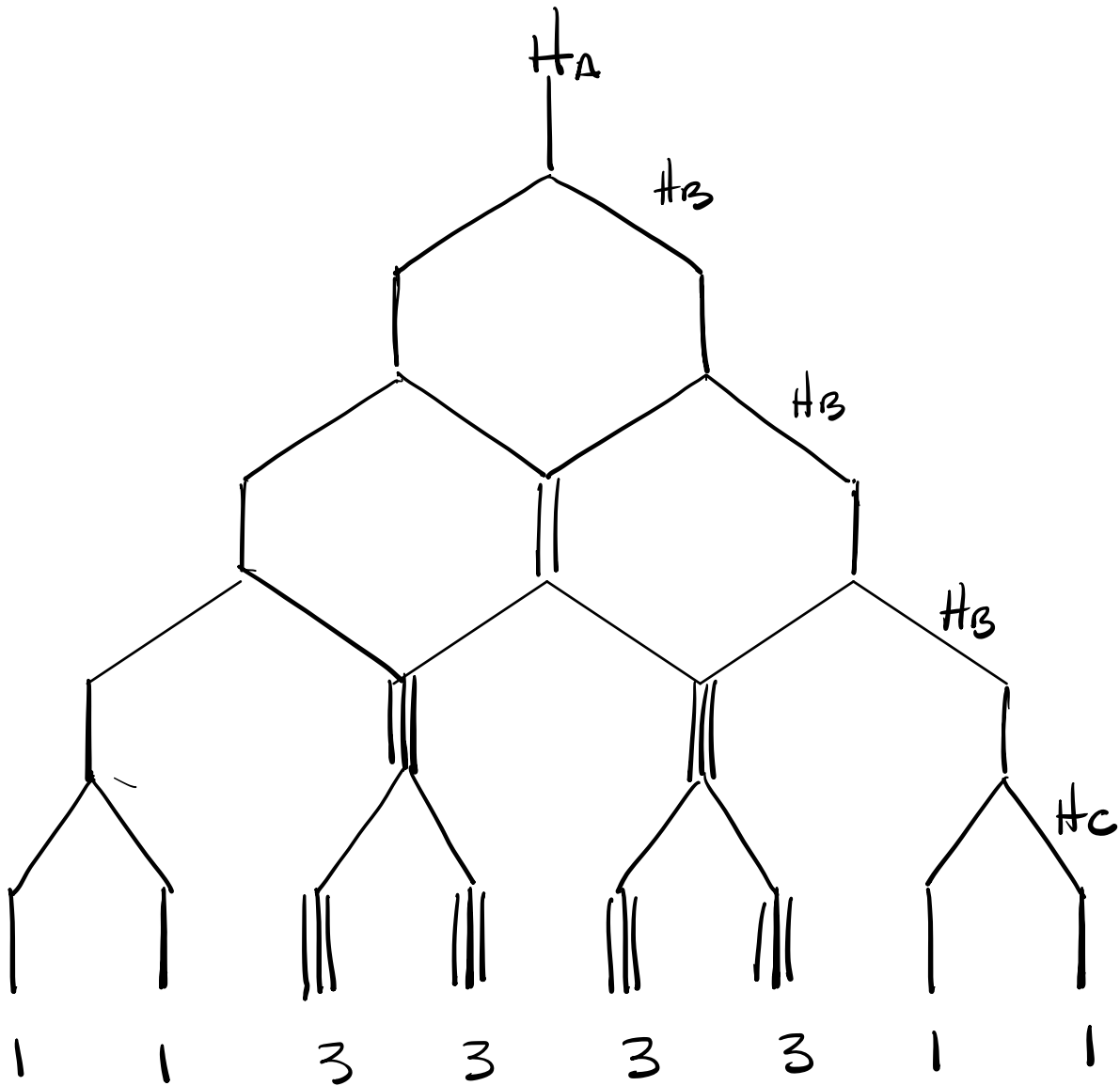
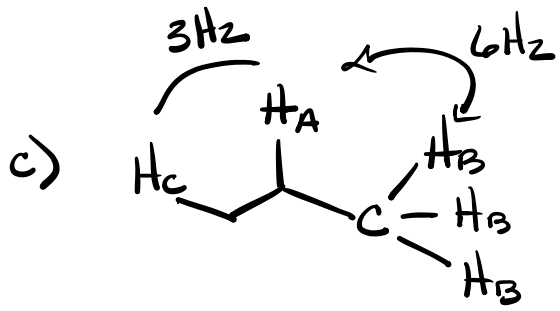
A)

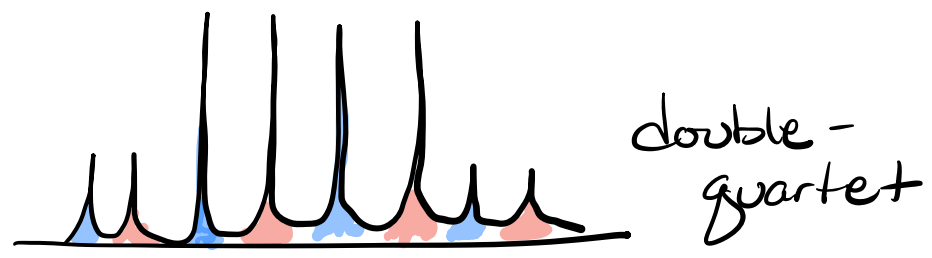
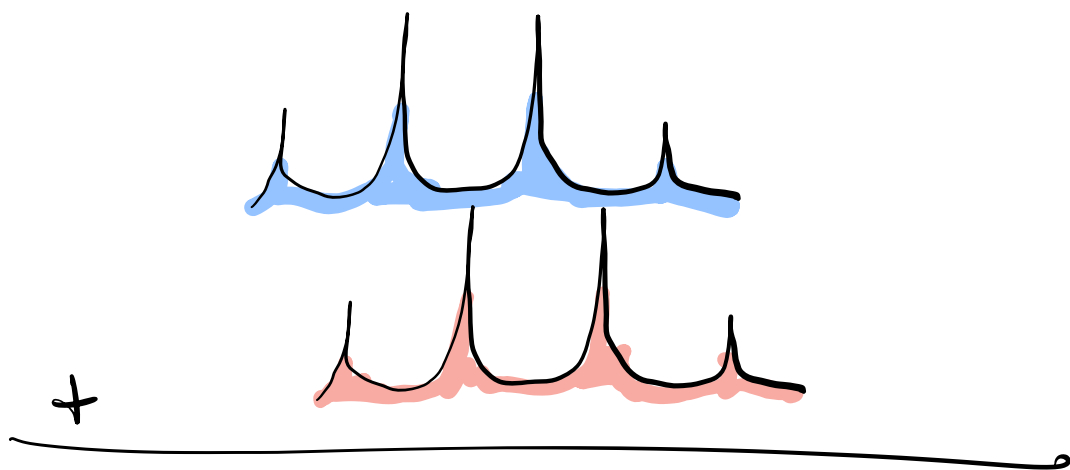


B)

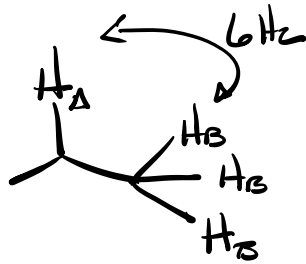


double-triplet

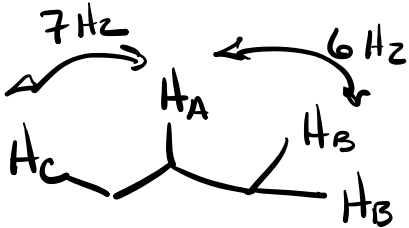




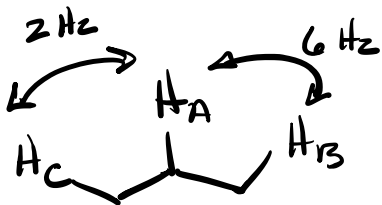
of neighbors



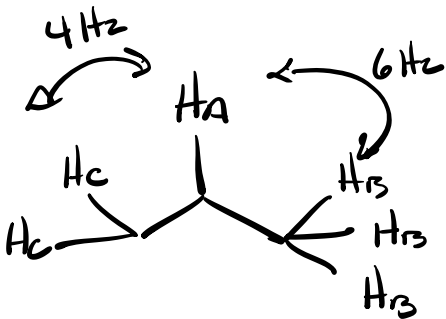
3 neighbors
quartet



3 neighbors ($1+2$)
↓ double
↓ triplet

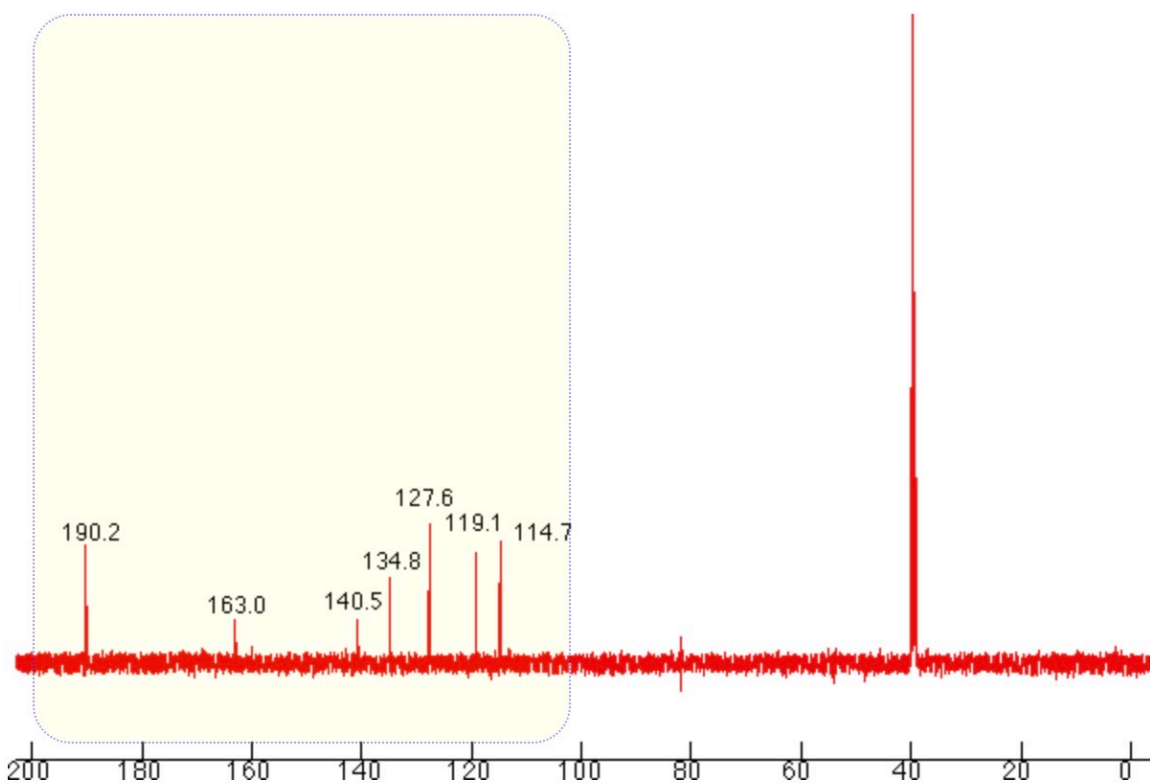


2 neighbors ($1+1$)
↓ double
↓ doublet



5 neighbors ($2+3$)
↓ triplet
↓ quartet

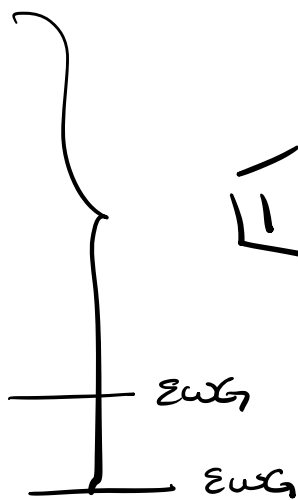
Problem 12 - ^{13}C NMR spectrum (DMSO- d_6 , 125 MHz)

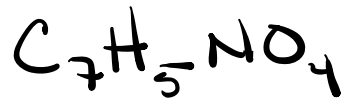
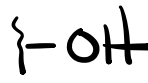
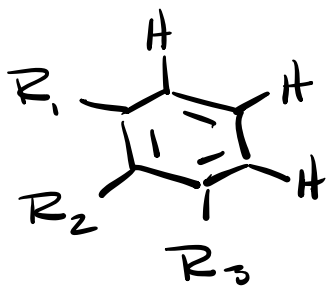


Click on the highlighted area to zoom. Click again to zoom back out.

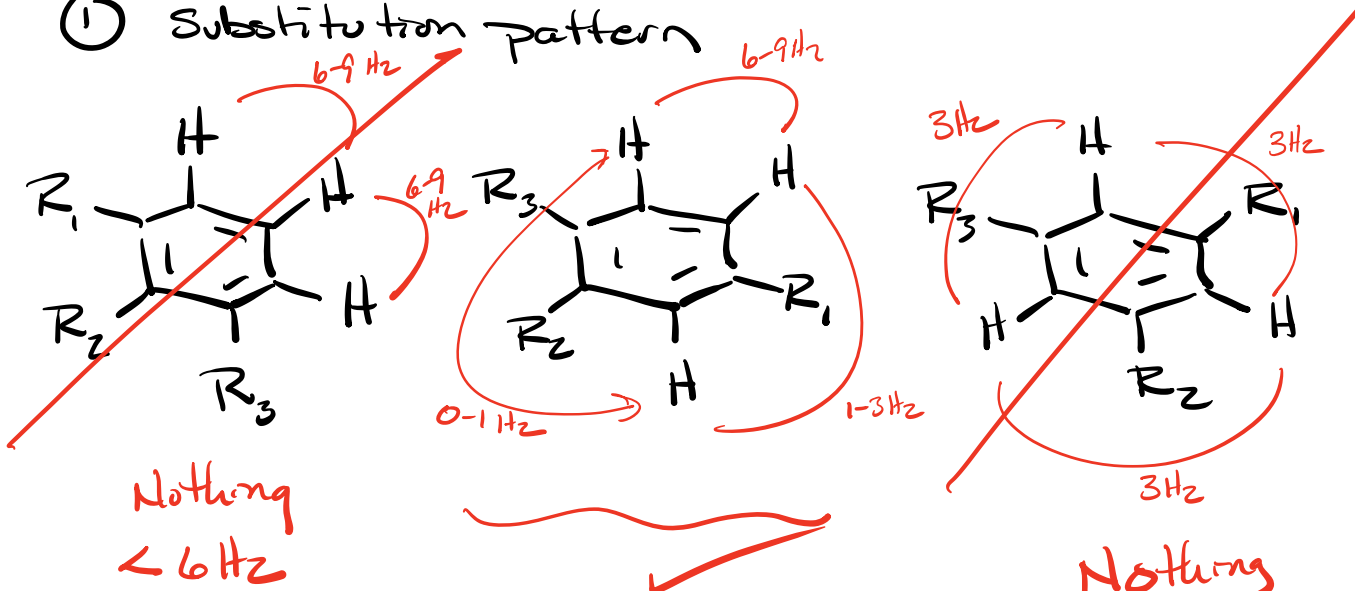
^{13}C -NMR Environments 7

114.7
119.1
127.6
134.8
140.5
163.0
190.2



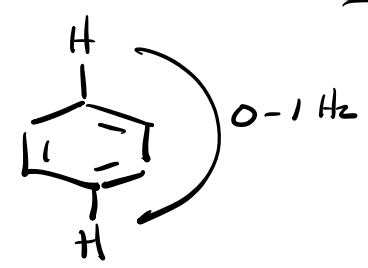
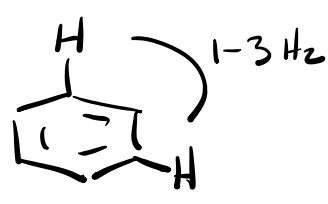
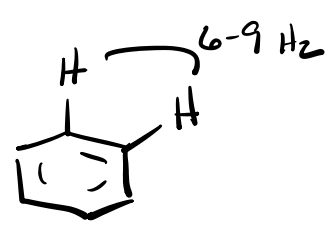
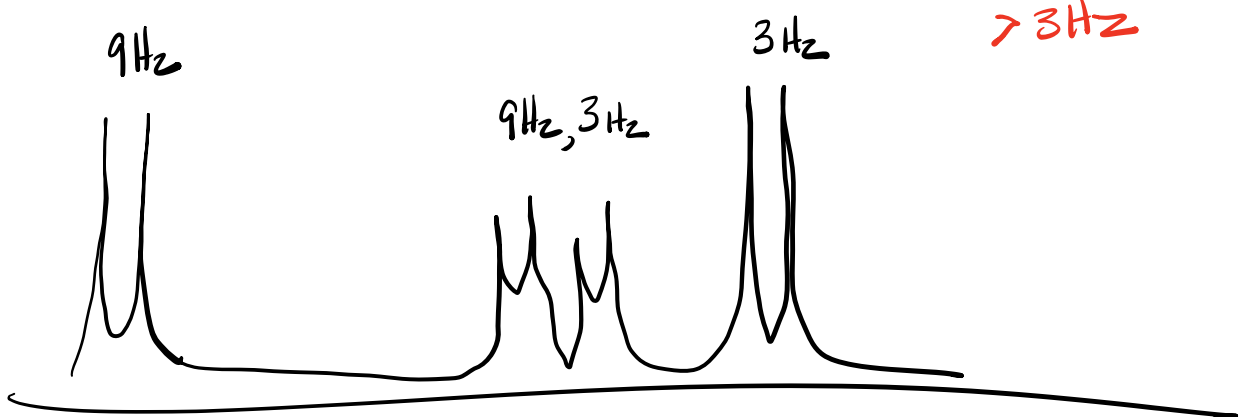


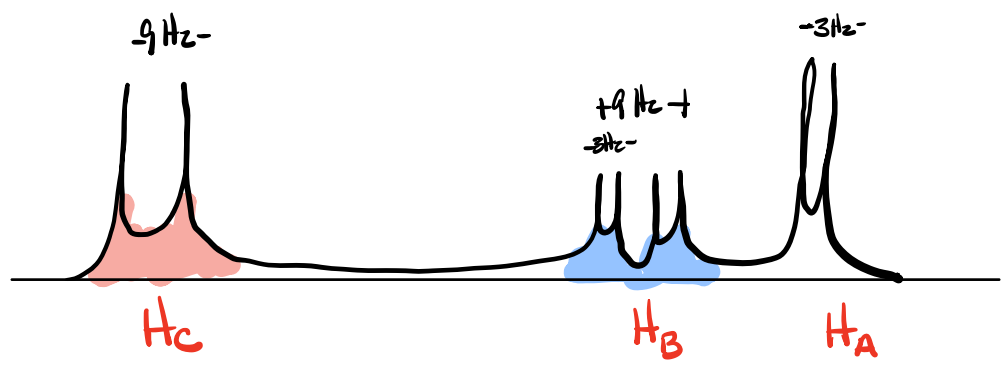
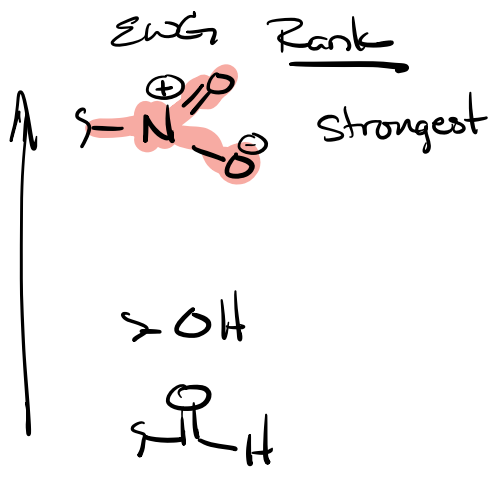
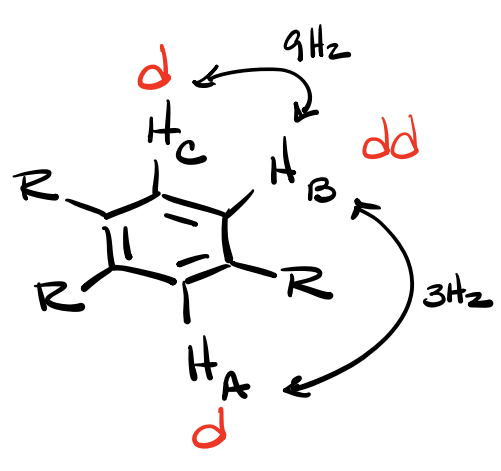
① Substitution pattern



Nothing
< 6 Hz

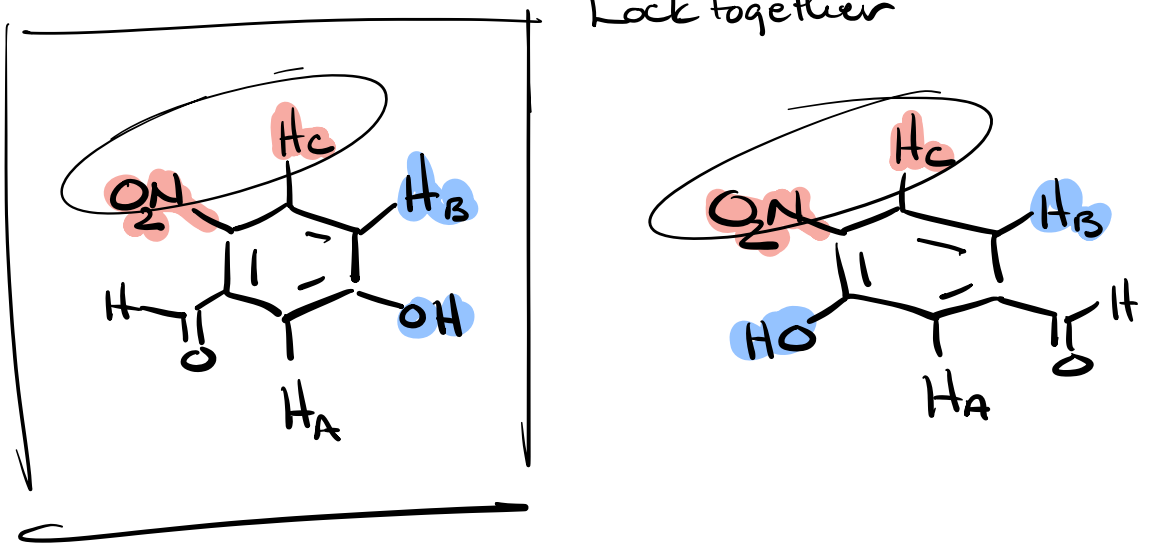
Nothing
> 3 Hz





desielded

Lock together



Either molecule would be correct