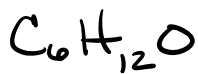


Issues w/ NMR

- Integration
- Wacky resolution
- Exchanges
- Assignments
- Asymboling

#11 webspectra



units of unsat

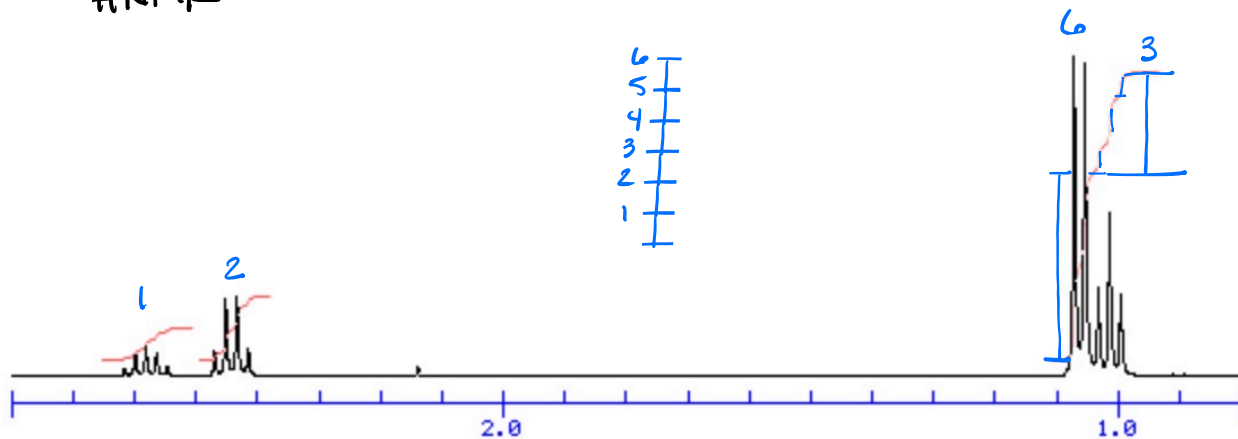
$$2(6) + 2 = 14$$

$$\underline{-12}$$

$$2 \quad \underline{2}$$

$$1 \text{ unit}$$

1H NMR



Chemical Environments = 4

ppm	Int	mult	#n	Assignment
1.01	<u>3</u>	triplet 1:2:1	<u>2</u>	CH_3-CH_2-
1.06	<u>6</u>	doublet 1:1	<u>4</u>	$2 \times CH_3-CH$
2.45	<u>2</u>	quartet 1:3:3:1	<u>3</u>	CH_3-CH_2-EWG
2.59	<u>1</u>	pentet? 1:4:6:4:1 septet 1:6:15:20:15:6:1	<u>4</u> <u>6</u>	$CH_2-CH(EWG)-CH_3$

pentet

$$\begin{matrix}
 & 1 & 1 & & & & \\
 & & 2 & 1 & & & \\
 & 1 & 3 & 3 & 1 & & \\
 1 & 4 & 6 & 4 & 1 & & \\
 1 & 5 & 10 & 10 & 5 & 1 & ? \\
 1 & 6 & 15 & 20 & 15 & 6 & 1
 \end{matrix}$$

←

septet

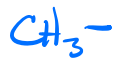
$$\begin{matrix}
 & 1 & 1 & & & & \\
 & & 2 & 1 & & & \\
 & 1 & 3 & 3 & 1 & & \\
 1 & 4 & 6 & 4 & 1 & & \\
 1 & 5 & 10 & 10 & 5 & 1 & ? \\
 1 & 6 & 15 & 20 & 15 & 6 & 1
 \end{matrix}$$

←

Int

Assignment

3



2



1



6



4



9

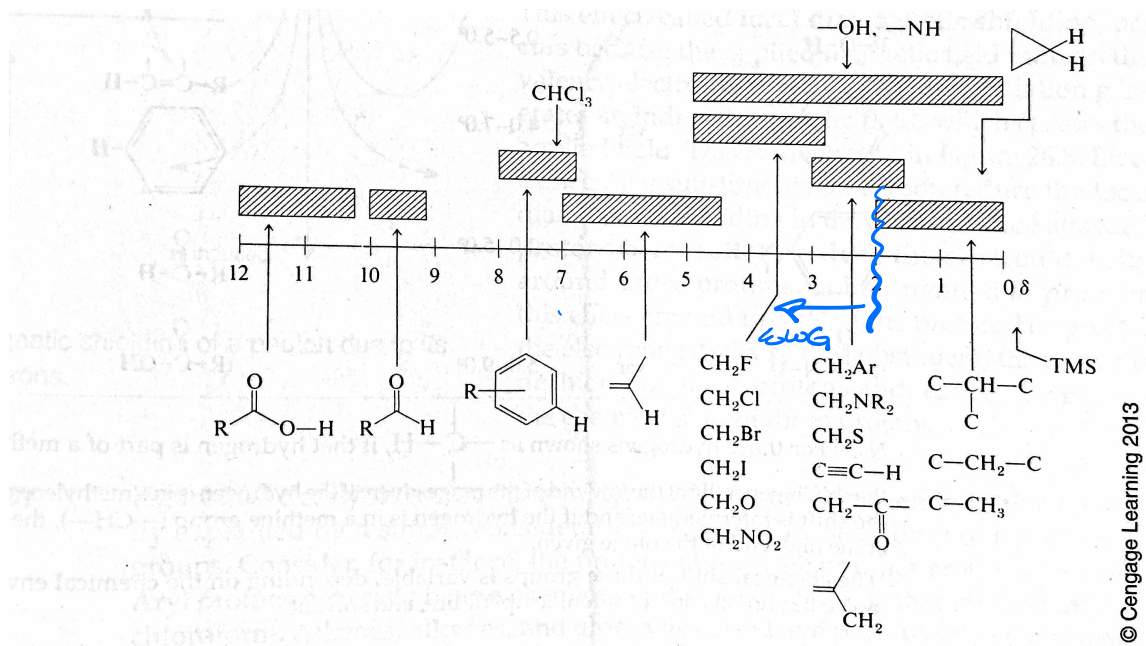
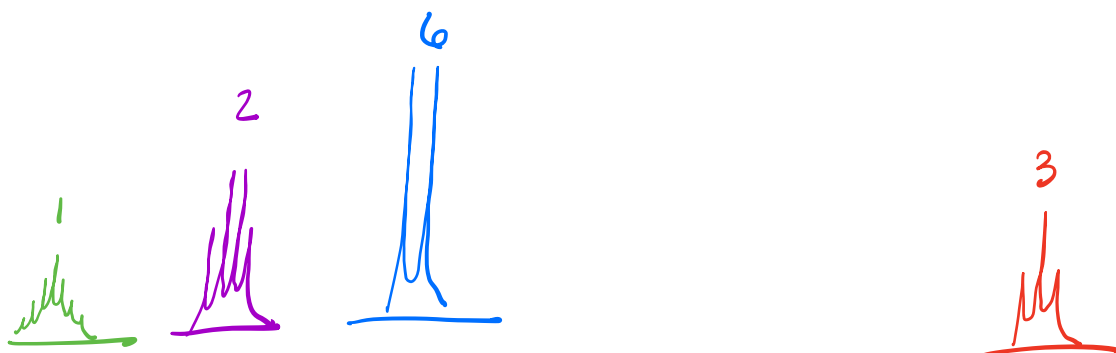
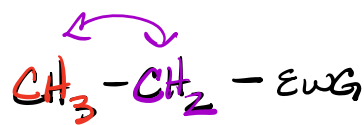
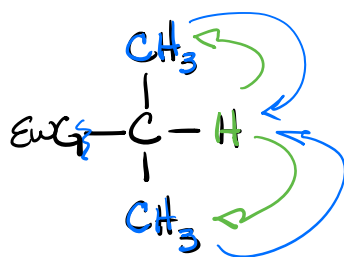


Figure 26.7

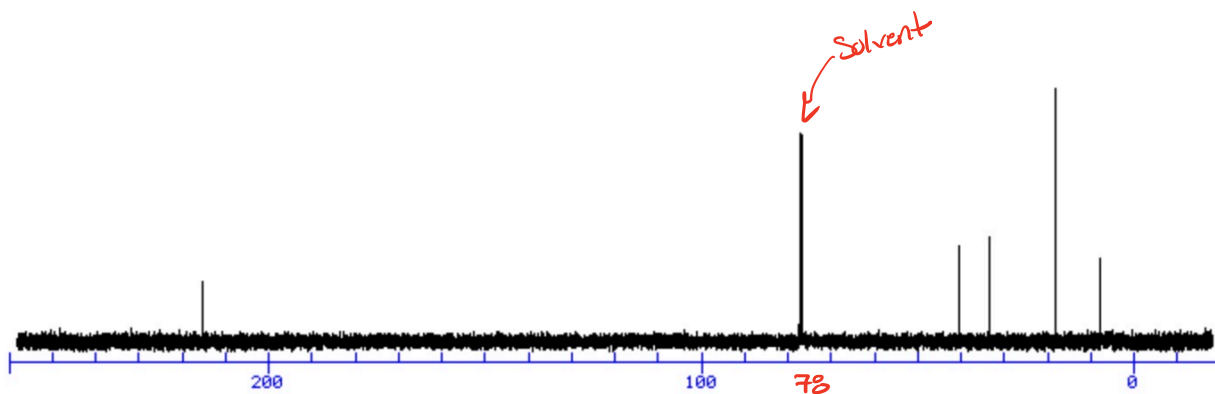
A simplified correlation chart for proton chemical shift values.



C_5H_{12} } missing is CO
 1 unit of unsat

$\text{C}=\text{O}$? CNMR ✓

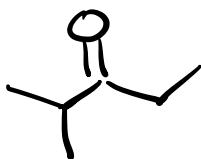
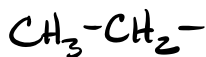
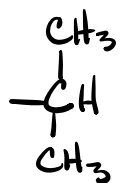
$^{13}\text{C-NMR}$



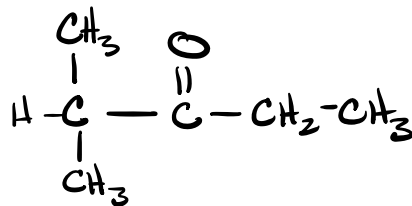
Environments 5

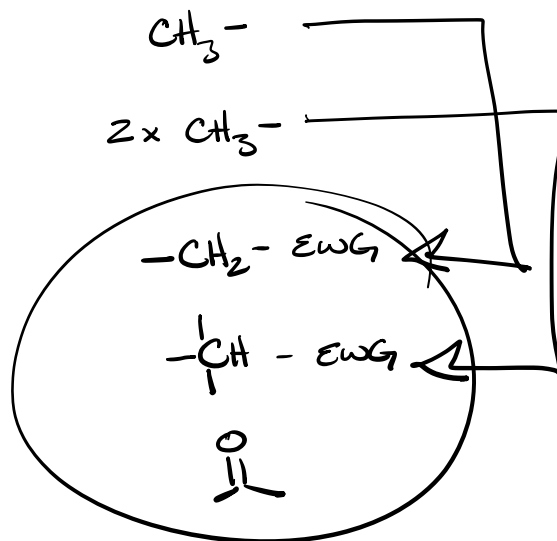
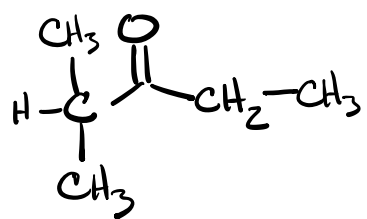
PPM

10	}	Alkyl CH
20		
32	}	Alkyl - EWG
40		
217		



\equiv

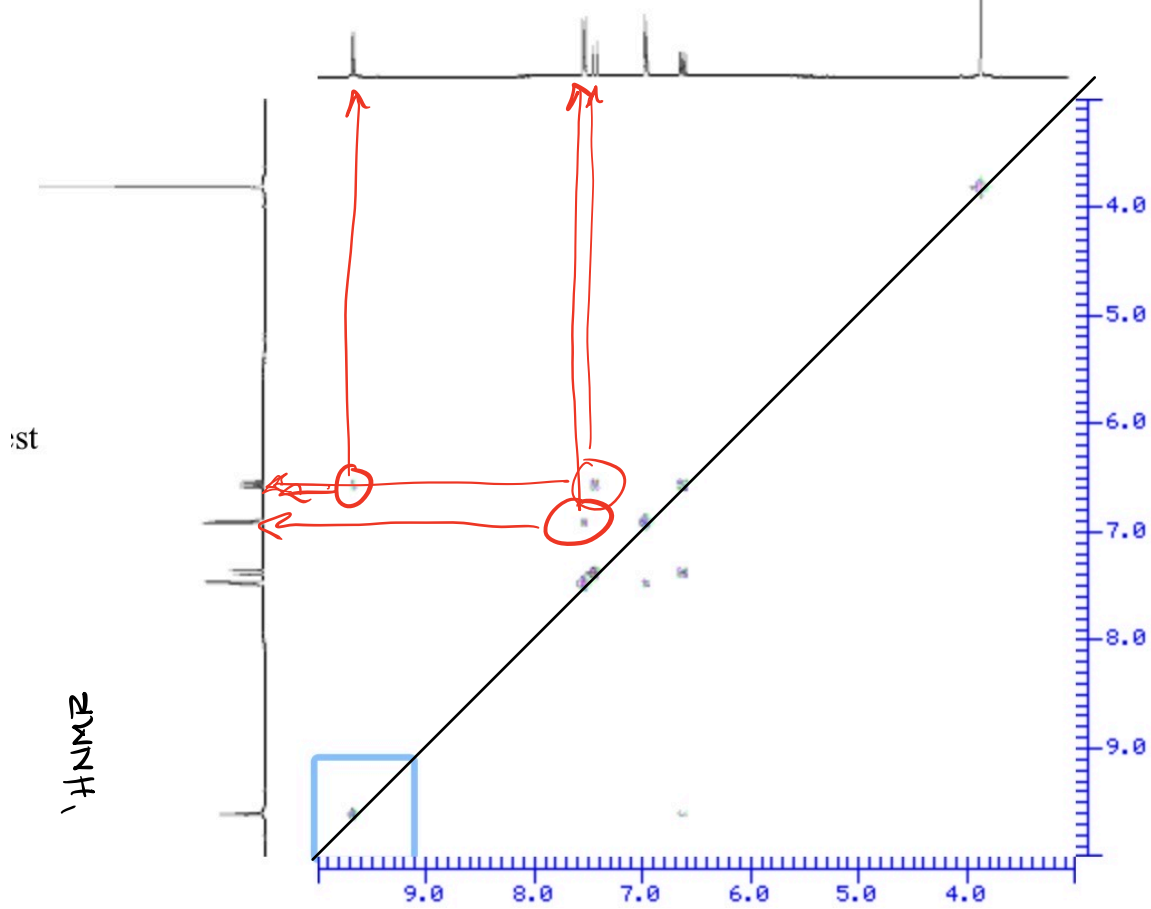




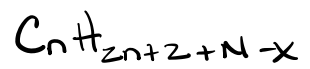
2D-NMR
COSY

¹H NMR

δ

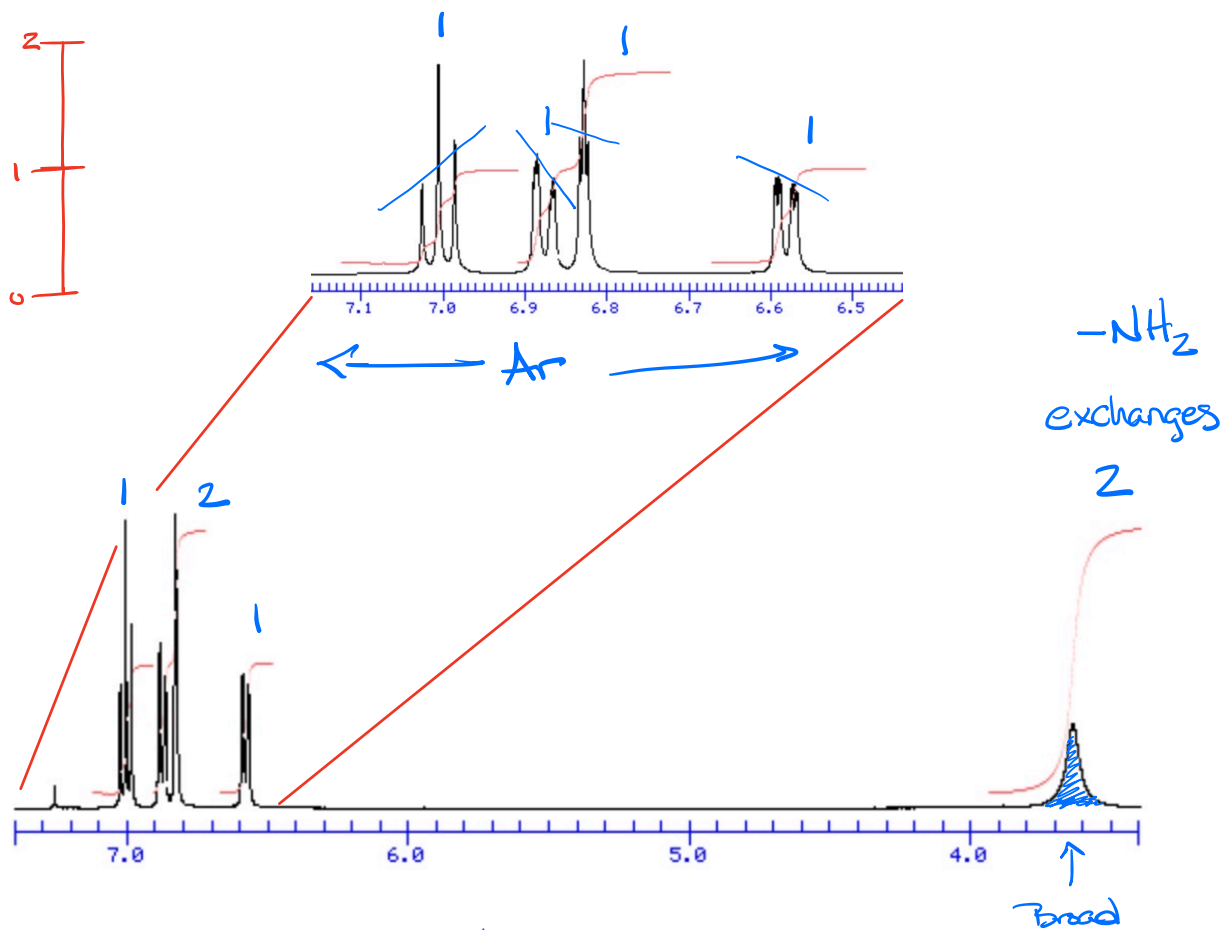


#14 Webspectra



$$2(6) + 2 + 1 - 1 = 14 \text{ for sat}$$

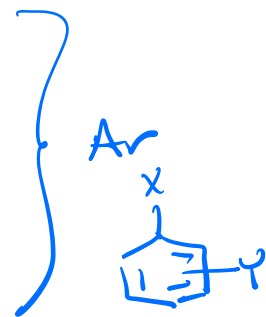
$$\begin{array}{r} 14 \\ - 6 \\ \hline 2 \overline{) 8} \\ 4 \text{ units} \end{array}$$



Environments δ

<u>ppm</u>	<u>Int</u>	<u>mult</u>	<u>#n</u>	<u>Assignment</u>
3.6	2	S(exchange)	?	-NH ₂

6.58	1	d	1	Small J-value
6.84	1	S(t) \swarrow long Range \searrow J4	ϕ (2)	
6.88	1	d	1	
7.00	1	t	2	



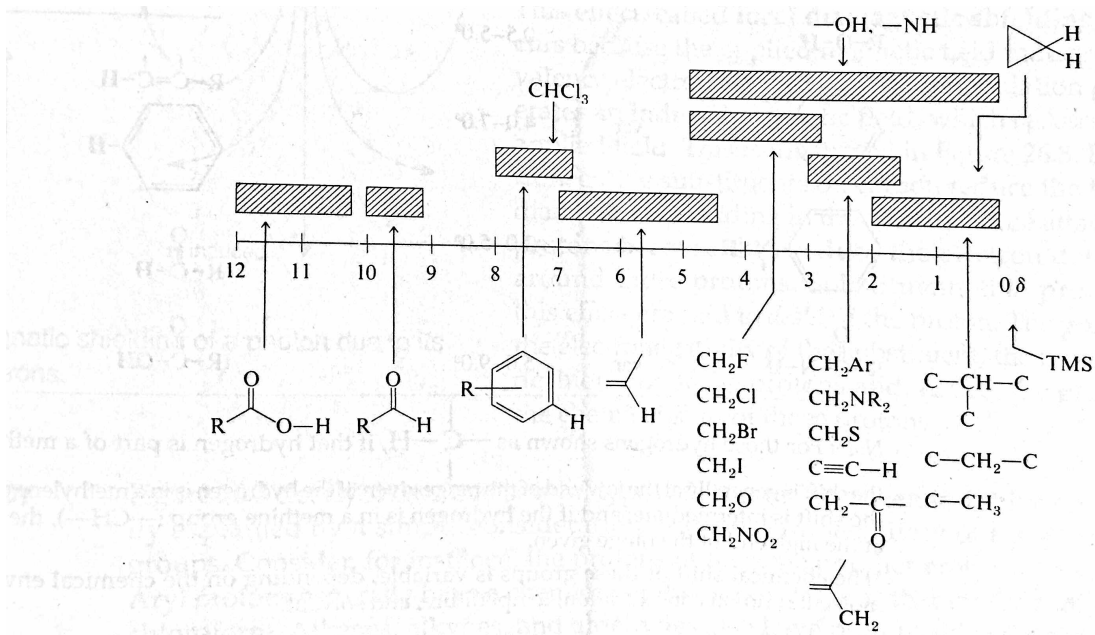
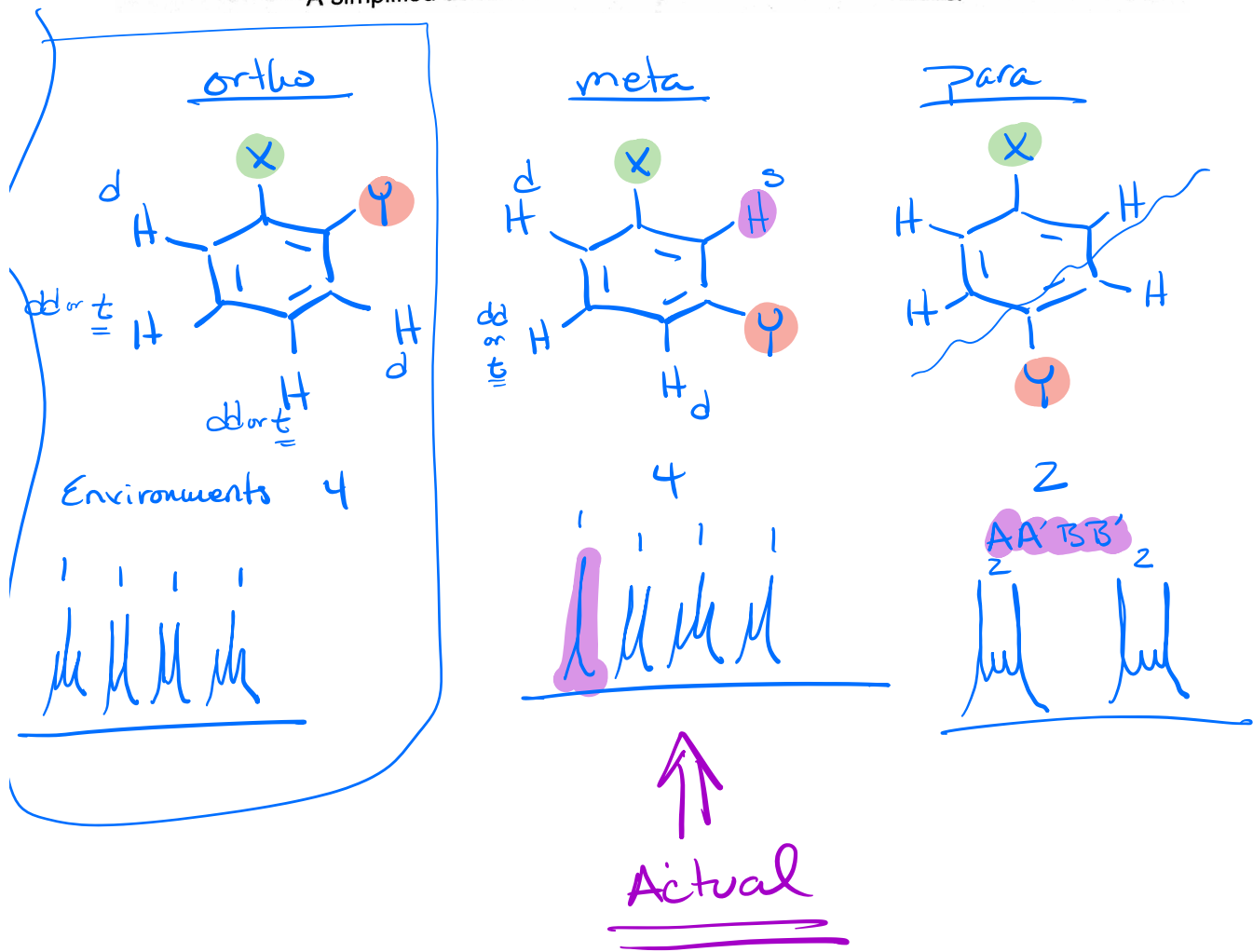
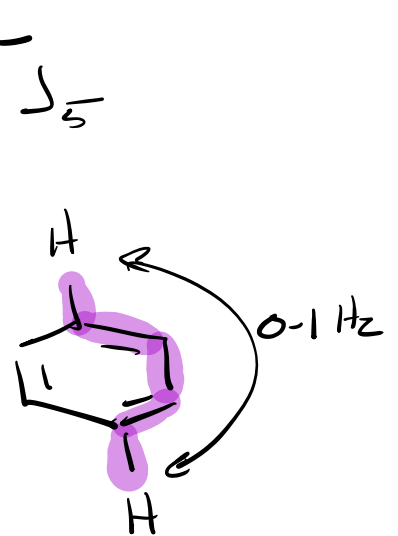
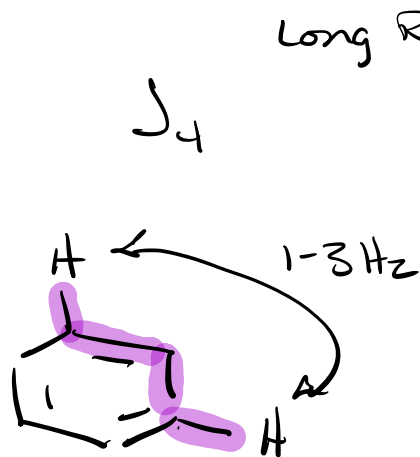
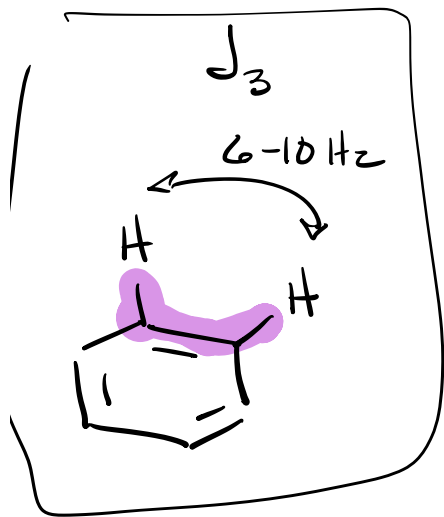
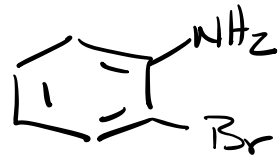
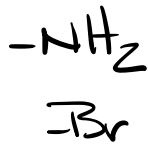
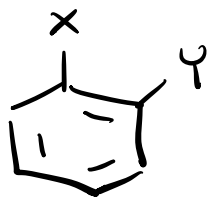


Figure 26.7
A simplified correlation chart for proton chemical shift values.





Smaller
J-value

