

## NMR Problem Solving

① Data

- parse the  $^1\text{H}$ NMR &  $^{13}\text{C}$ NMR into table format

$^1\text{H}$ NMR # of Chemical Environments =

<u>ppm</u>	<u>Int</u>	<u>Multiplicity (Splitting)</u>	<u># neighbors</u>	<u>Assignment</u>
------------	------------	---------------------------------	--------------------	-------------------

$^{13}\text{C}$ NMR # of Chemical Environments =

<u>ppm</u>	<u>Assignment</u>
------------	-------------------

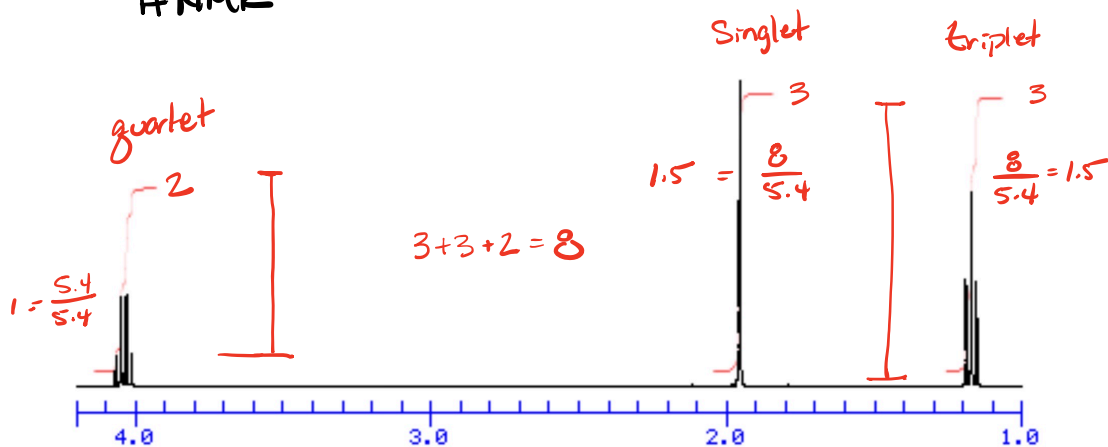
# WebSpectra problem 1 - $C_4H_8O_2$

9:41 AM Tue Jan 9

webspectra.chem.ucla.edu - Private

100%

$${}^1\text{H NMR } 2 \times [1:1.5:1.5] = 2:3:3$$



ppm

Zoom

Zo

[Back to WebSpectra Home Page](#)

Chemical Environments = 3

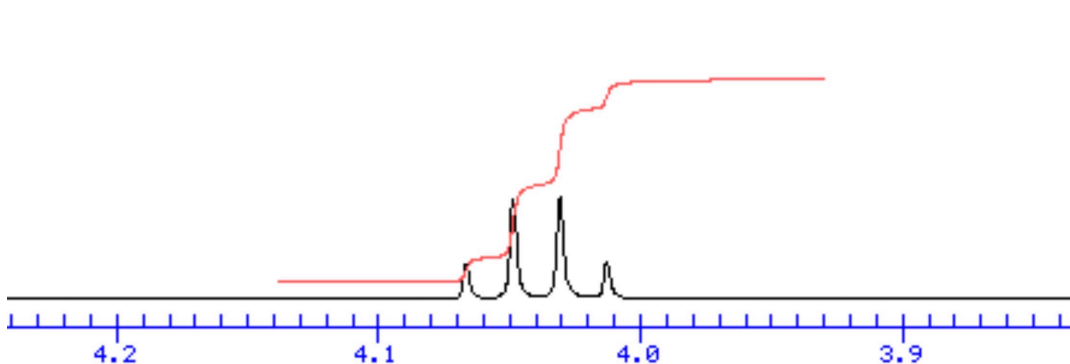
${}^1\text{H-NMR}$

ppm	Int	mult	# neighbors	Assignment
1.18	3	triplet	2 neighbors	Alkyl $\begin{array}{c} \text{H} \\   \\ \text{---C---H} \\   \\ \text{H} \end{array}$ methyl
1.96	3	Singlet	0 neighbors	Alkyl EWG $\begin{array}{c} \text{H} \\   \\ \text{---C---H} \\   \\ \text{H} \end{array}$
4.50	2	quartet	3 neighbors	Alkyl EWG $\begin{array}{c} \text{H} \\   \\ \text{---C---} \\   \\ \text{H} \end{array}$

$\rightarrow 3 = n+1 \text{ Rule } | n = \# \text{ neighbors}$

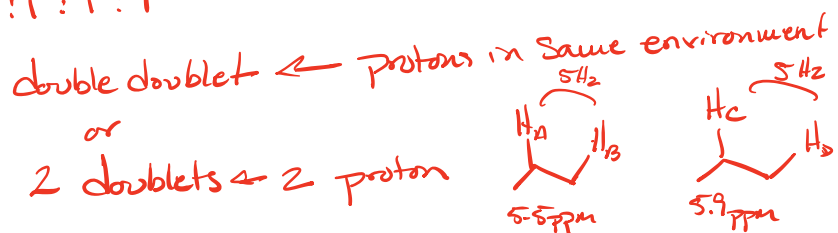
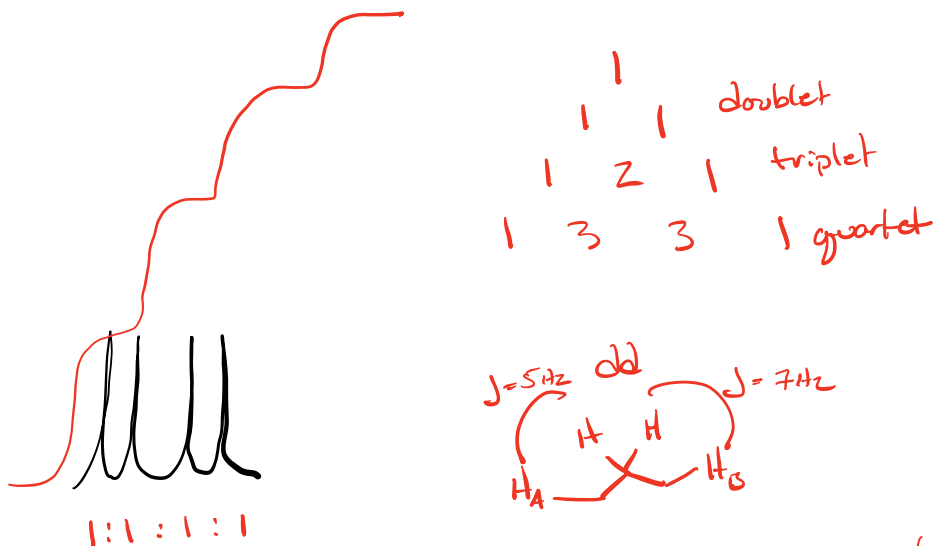
$\text{H}_8 \checkmark$

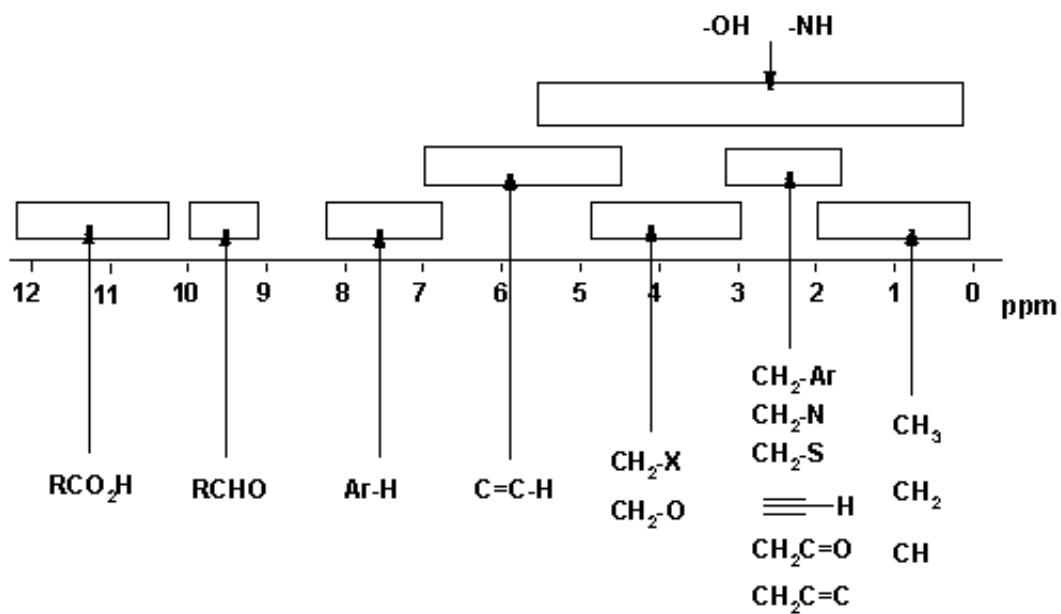
1 : 3 : 3 : 1



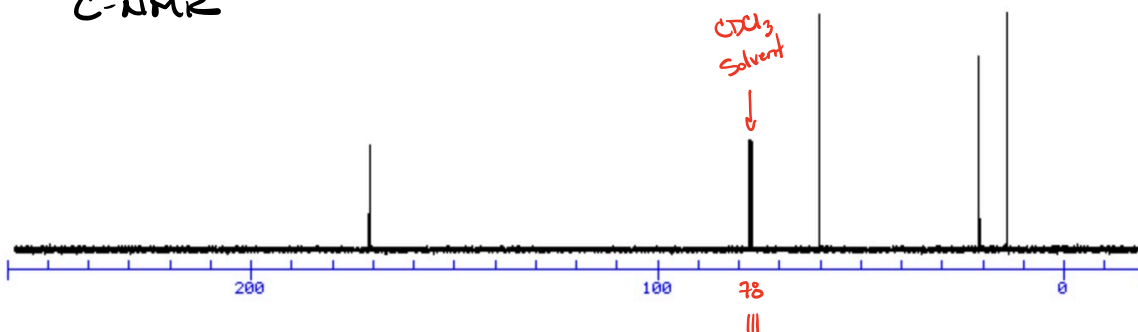
to  ppm [Zoom](#)

[Back to WebSpectra Home Page](#)





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



Chemical Environments = 4 (Count peaks)

PPM

Assignment

13

Alkyl C-C

21

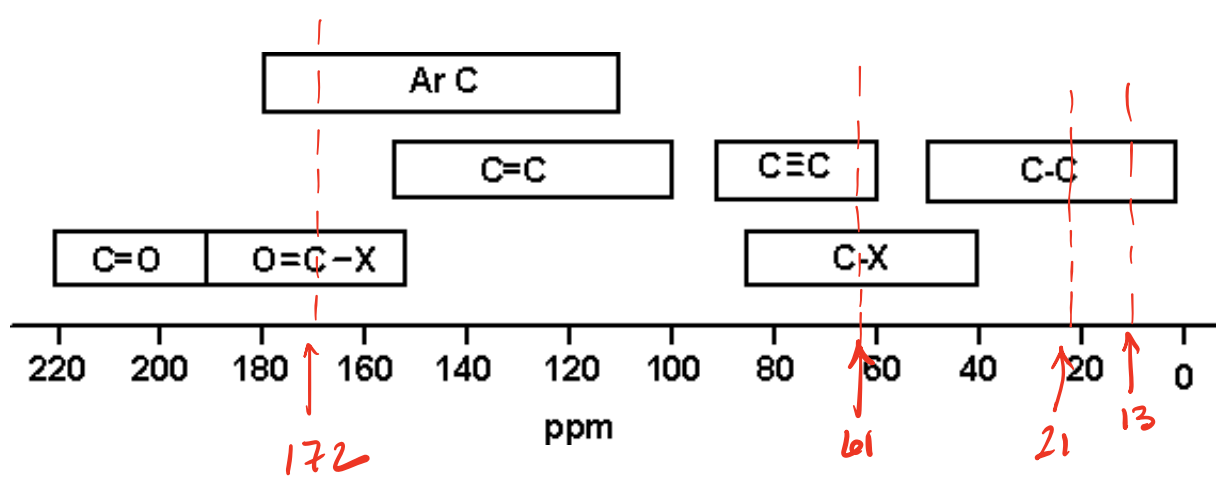
Alkyl C-C

61

Alkyl C-ENG

172

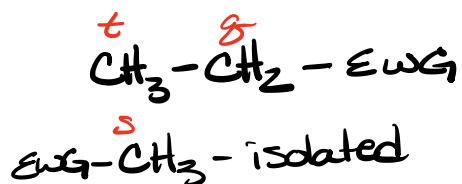
$\text{C}_x$  |  $x = \text{O or Cl, Br, N}$



What we have

<sup>1</sup>H NMR

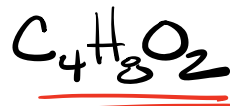
3 environments



<sup>13</sup>C NMR

4 environments

- 2 Alkyl
- 1 Alkyl-EWG



units of unsaturation

$$C_n H_{2n+2+N-x}$$

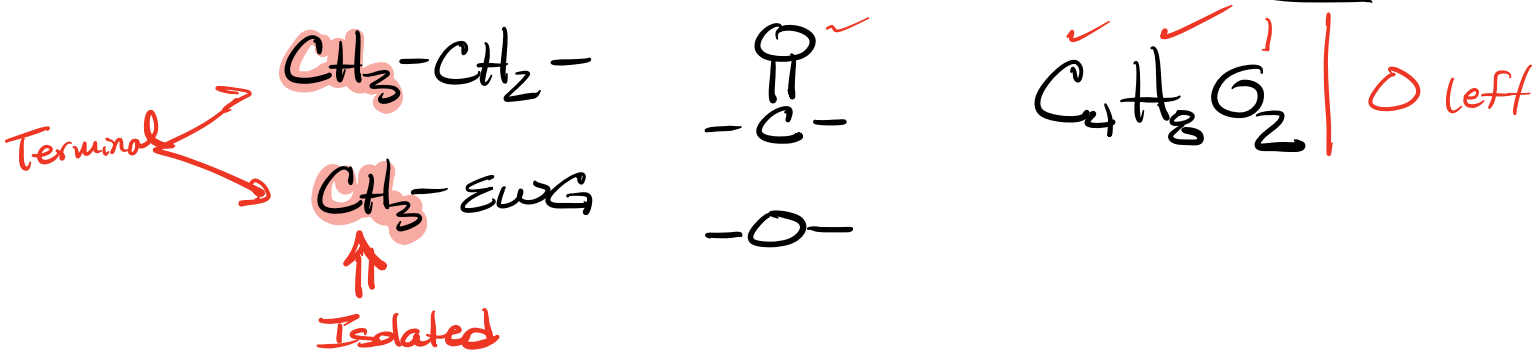
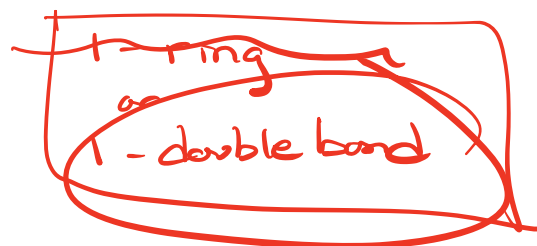
for saturated

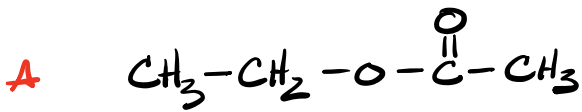
$$H_{2(4)+2+0-0}$$

$H_{10}$  saturated  
 $- H_8$  in formula

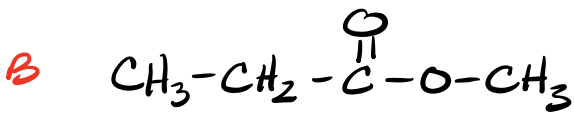
$$2 \mid 2 \text{ missing}$$

1 unit unsaturation

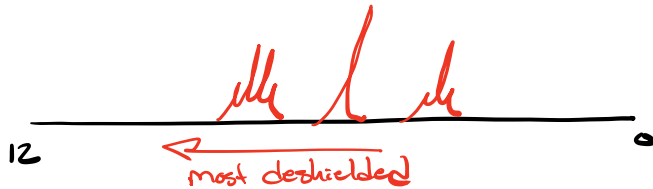
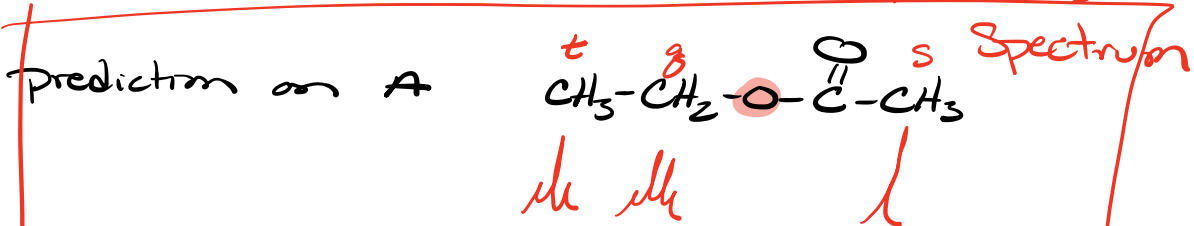




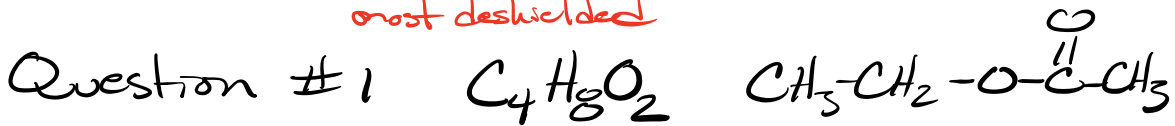
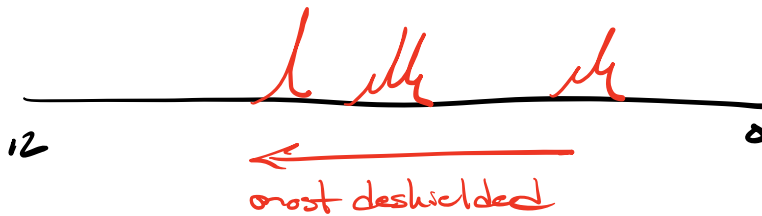
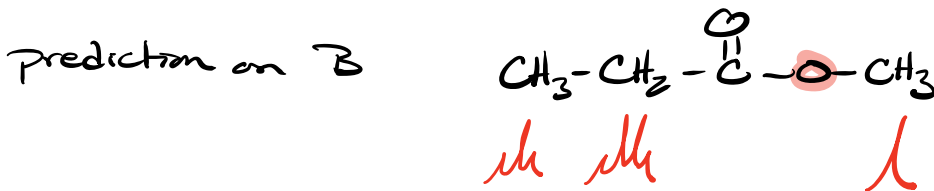
only 2 possible structures



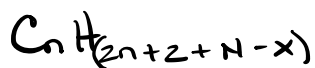
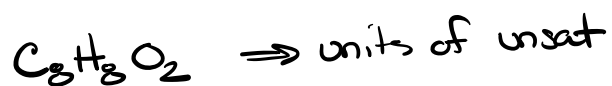
Matches



what is more EW, the  $\text{-C(=O)-}$  or  $\text{-O-}$



Problem #2 Webspectra



$$2(8) + 2 + 0 - 0 = 18$$

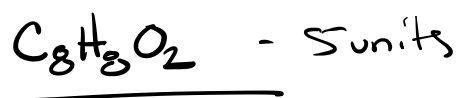
$$\begin{array}{r} - 8 \\ \hline 2 \overline{) 10} \end{array}$$

5 units of unsat

5 units w/ Less 10 Carbons



3 double bonds + 1 ring = 4 units



=

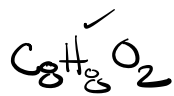


or

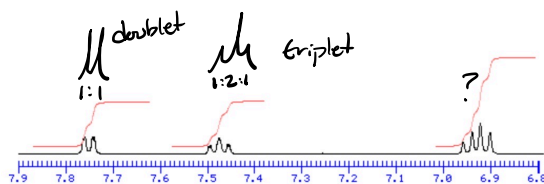
additional Ring



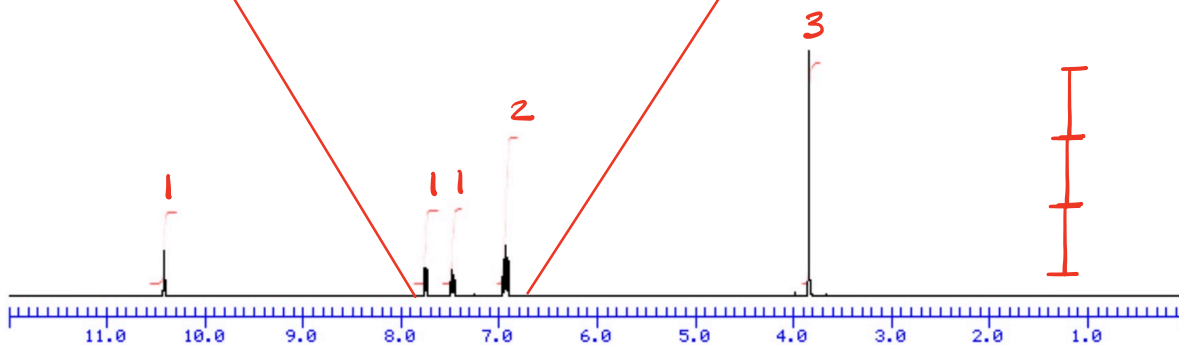
<sup>1</sup>H NMR



Singlet  
doublet  
triplet  
quartet

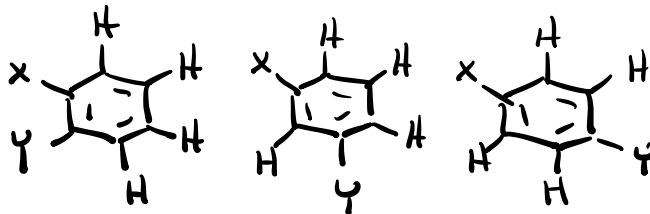


quartet  
1:3:3:1



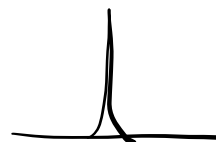
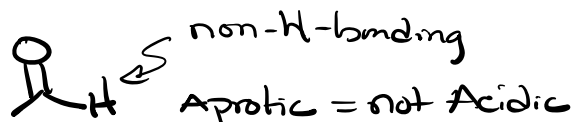
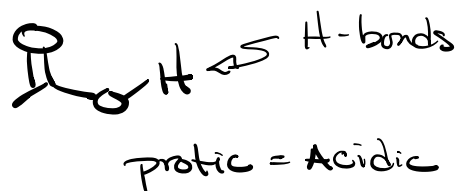
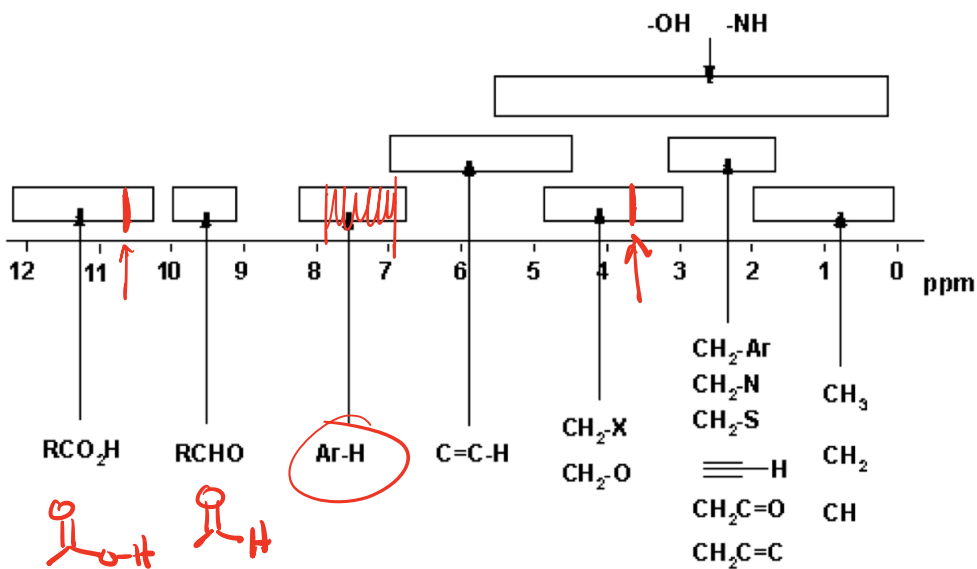
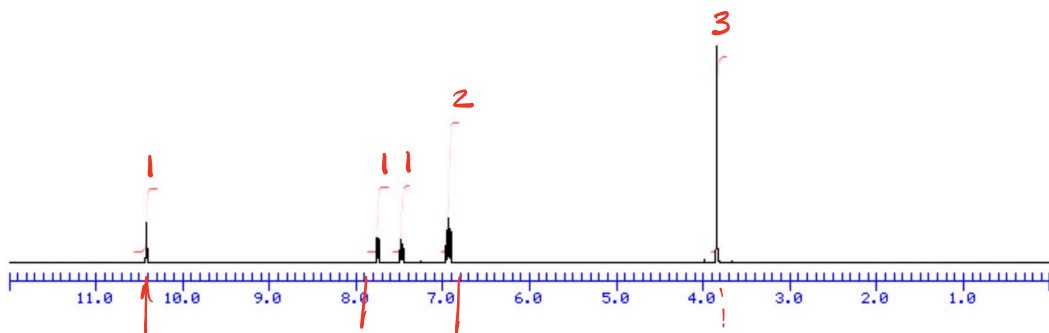
5 Chemical Environments

ppm	Int	mult	neighbors	Assignment
3.8	3	Singlet	∅	EWG-CH <sub>3</sub>
7.0	2	multiplet	?	Ar-H } 4 H's
7.5	1	t	2	
7.8	1	d	1	

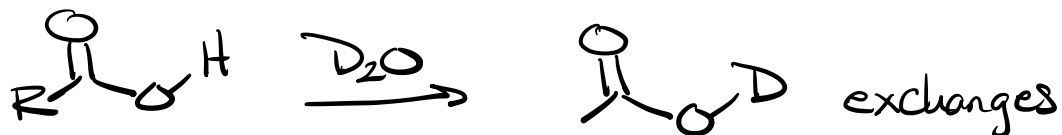


10.4 1 S ∅

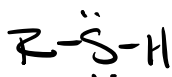
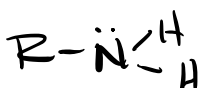




# Exchange experiment



Signal disappears  
("exchanges")



→ exchange



does not exchange

