Mass Spectroscopy

- Isotope effects
- What to look for for different functional groups
- Heterolytic & fragmentation
- Examples

Isotope effects - Halogens

^{19}F 100%

$^{35}Cl/^{37}Cl$ — ^{35}Cl 75%, ^{37}Cl 25%

$^{79}Br/^{81}Br$ — ^{79}Br 50%, ^{81}Br 50%

^{127}I 100%

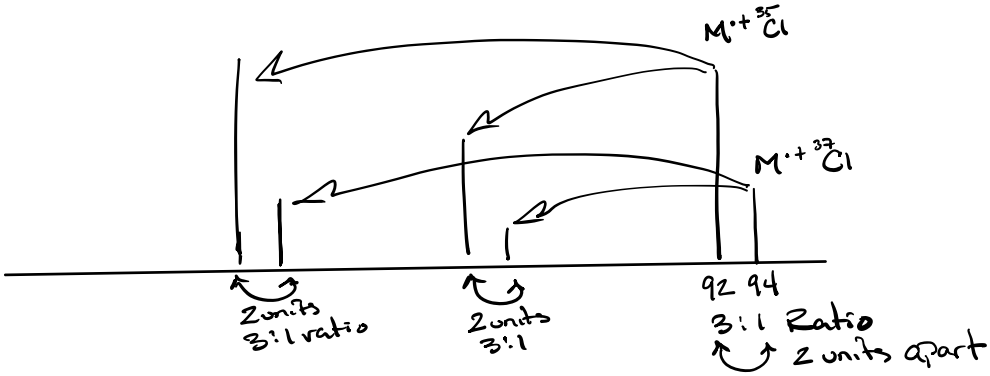
Can tell the type of halogen from spectrum

When a molecule Contains Chlorine

C_4H_9Cl M^{+} = 92

$C_4H_9{}^{35}Cl$ 92 75%

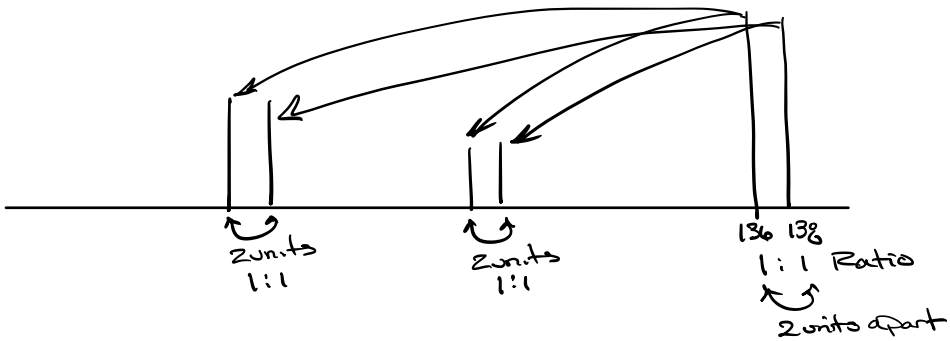
$C_4H_9{}^{37}Cl$ 94 25%



C_4H_9Br $M^{+\cdot} = 136$

$C_4H_9{}^{79}Br$ 136 50%

$C_4H_9{}^{81}Br$ 138 50%

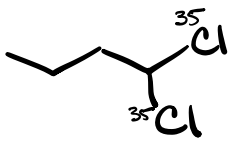


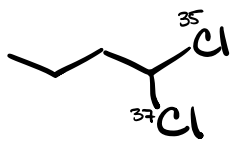
What happens w/ 2 Chlorines?

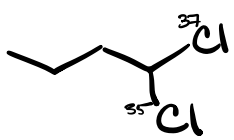
$C_4H_{10}Cl_2$

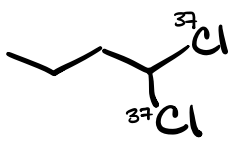
^{35}Cl 75%

^{37}Cl 25%





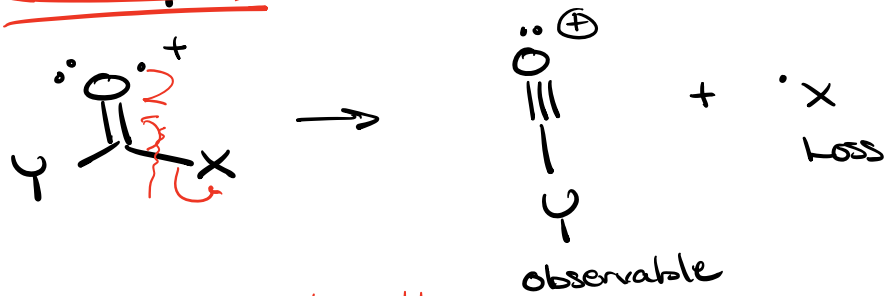


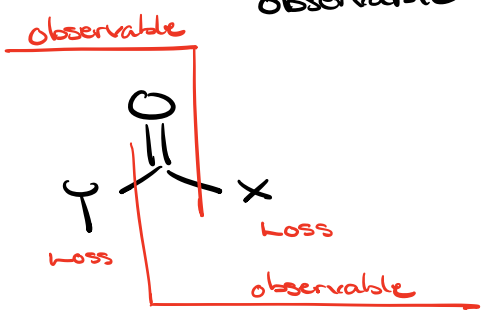


most likely

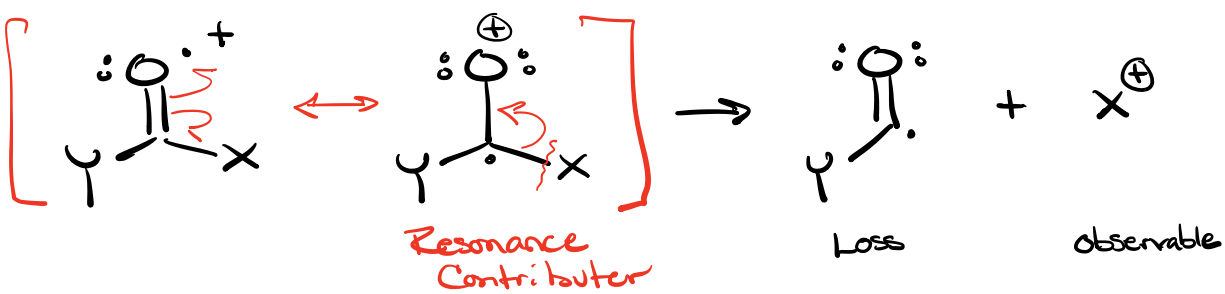
α - Cleavages

Homolytic





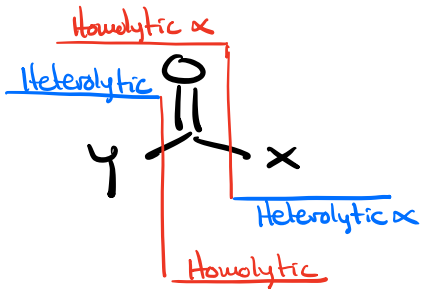
Heterolytic α- Cleavage



For every Carbonyl there are 4 possible α

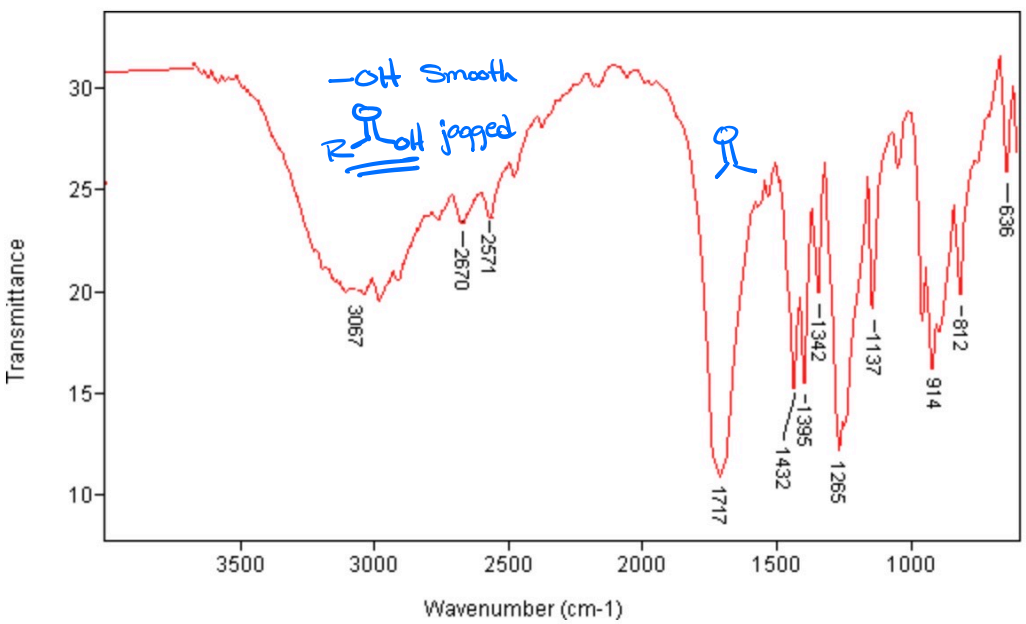
2 Homolytic

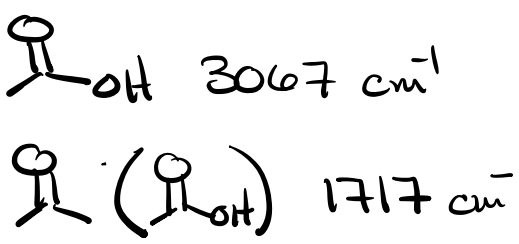
2 Heterolytic



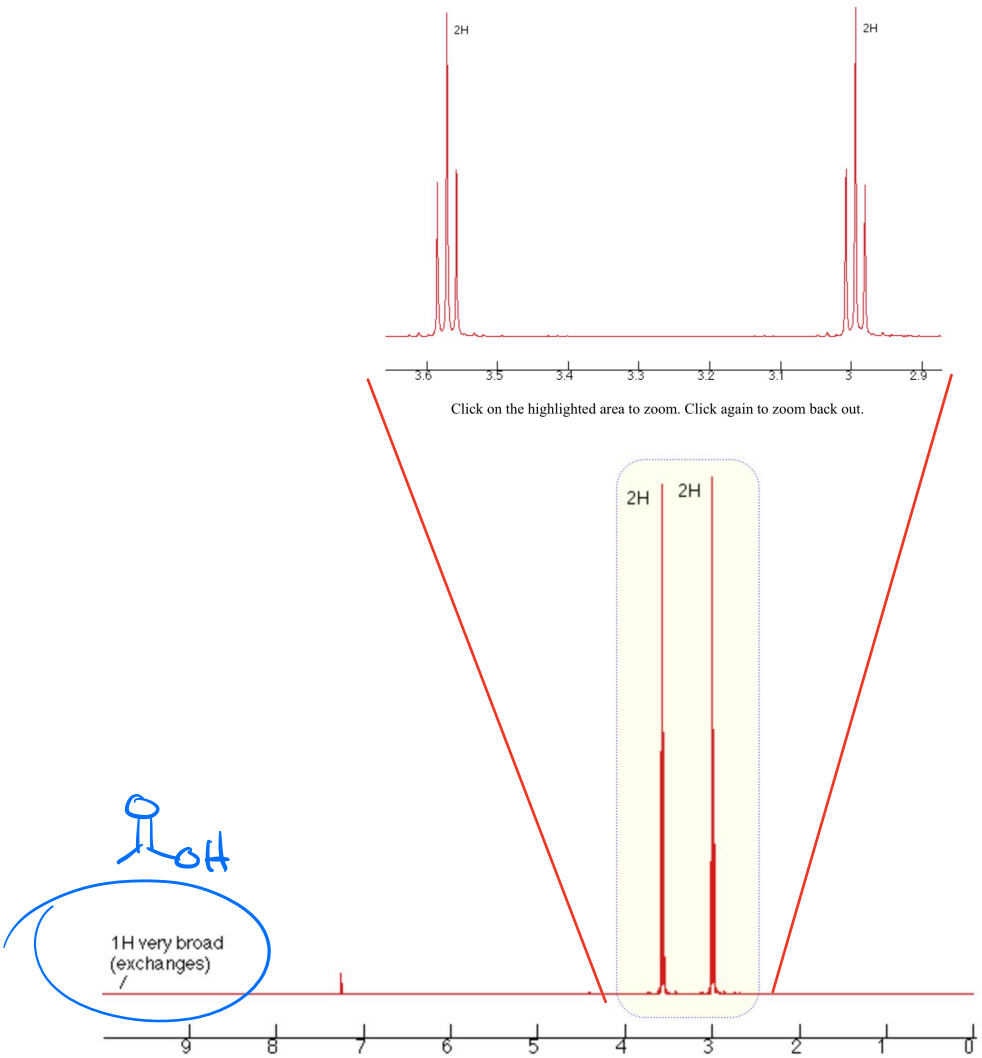
How many are actually observed depends on stability of fragments.

you may observe 1, 2, 3, or all 4.





Problem 1 - ^{1}H NMR spectrum ($CDCl_3$, 500 MHz)



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

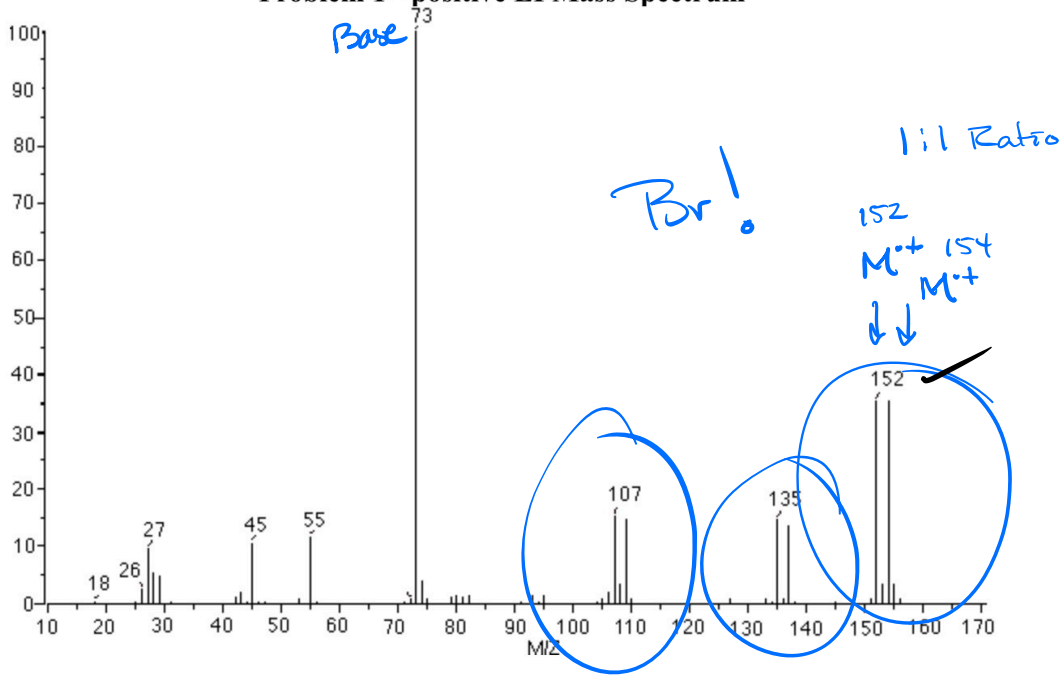
Environments = 3

PPm	Int	Mult	# neighbors	Assignment
3.0	2	t	2	$-CH_2-$
3.7	2	t	2	$-CH_2-$
10	1	S exchanges ø		OH

5 H's total

$-CH_2-CH_2-$

Problem 1 - positive EI Mass Spectrum



^{79}Br $M^{\cdot+}$ 152

^{81}Br $M^{\cdot+}$ 154

$$13\overline{)152}\quad 11$$
$$13$$
$$22$$
$$13$$
$$9$$

Mass Spec Br

IR, HNMR, CMMR } R_{OH}

$$13\overline{)79}\quad 6$$
$$78$$

C_6H_7

$^{79}Br = C_6H_7$

$C_{11}H_{20}$

$+O$ $-CH_4$ → $C_{10}H_{16}O$

→ $C_9H_{12}O_2$

$+Br$ $-$ → $C_3H_5O_2Br = 152$ ✓

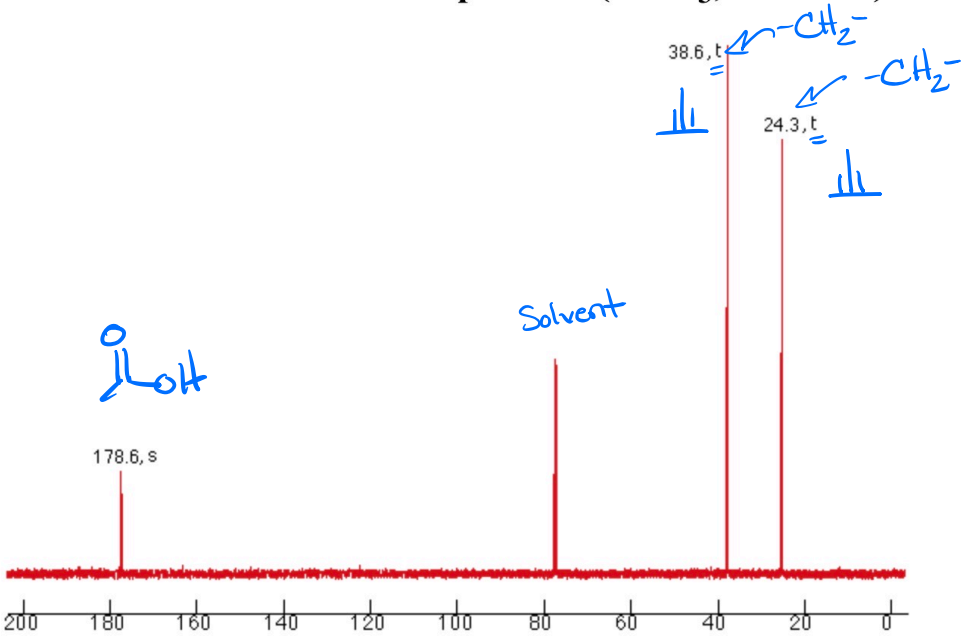
Units of unsaturation

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

$$7$$
$$-5$$
$$2\overline{)2}$$

1 unit unsat

Problem 1 - ^{13}C NMR spectrum ($CDCl_3$, 125 MHz)



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

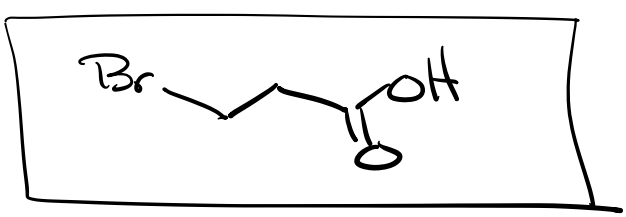
1 unit unsat

$C_3H_5O_2Br$

IR 

HNMR  $-CH_2-CH_2-$

CNMR  $-CH_2-CH_2-$



152 m/z