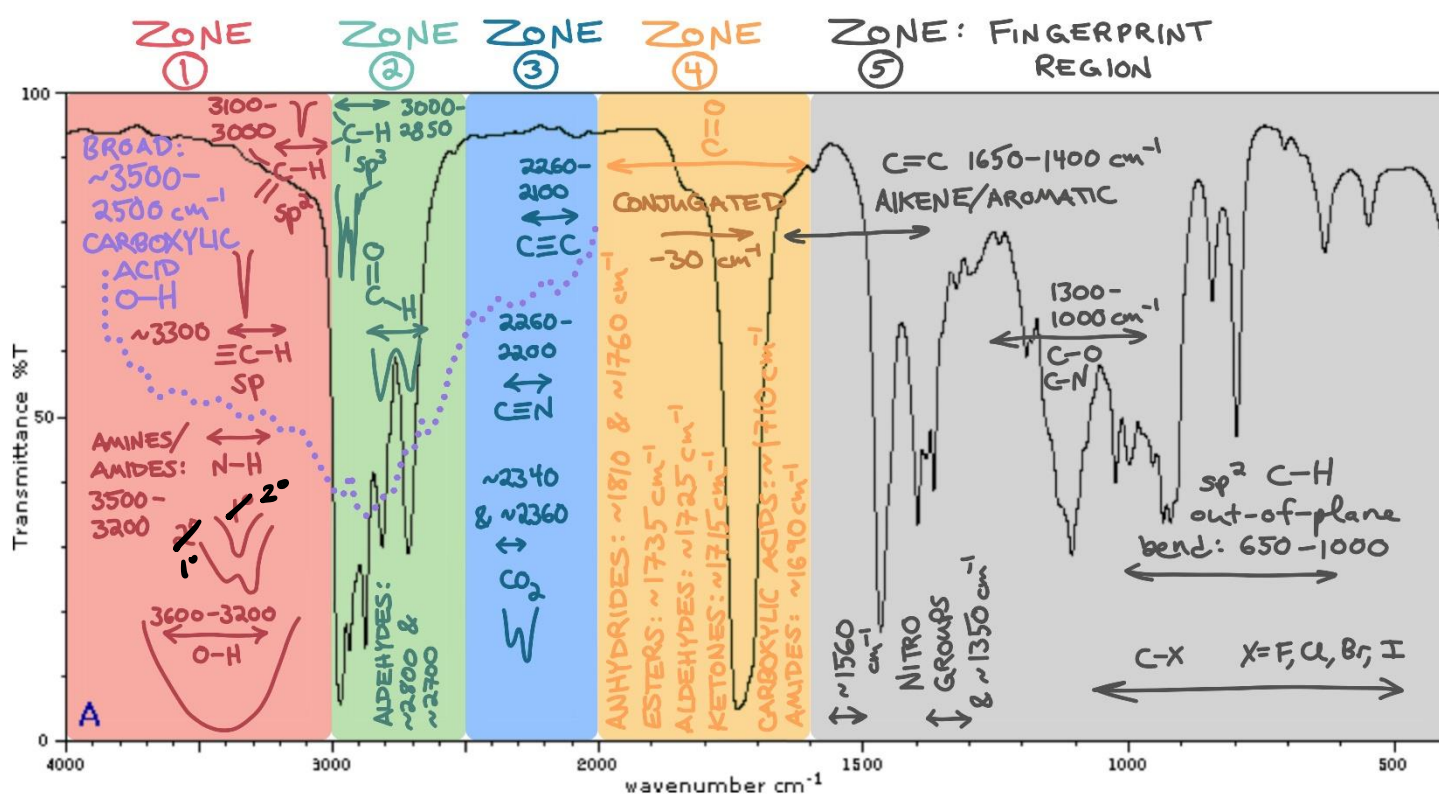


IDENTIFYING the MAJOR FUNCTIONAL GROUP:

1. Is a carbonyl present? **Check ZONE 4.** If no carbonyl is present, go to step 3.
 - **The C=O double bond gives rise to a strong absorption in ZONE 4: 2000-1600 cm^{-1} . This peak is often the strongest in the spectrum, and characteristic of the type of carbonyl present (see spectrum below).**
2. If C=O is present, check for additional peaks to confirm the following types of carbonyls:
 - **Anhydrides have two C=O absorptions near 1810 & 1760 cm^{-1}**
 - Esters should also have C-O stretches in ZONE 5 around 1300-1100 cm^{-1} with medium intensity
 - **Aldehydes should also have two signals in ZONE 2: ~ 2800 & ~ 2700 cm^{-1}**
 - **Carboxylic acids should have a broad signal that extends from ZONE 1 through ZONE 2: 3500-2500 cm^{-1}**
 - **Amides (primary & secondary) should have a signal in ZONE 1: 3500-3200 cm^{-1}**
3. If C=O is absent, check for:
 - **Alcohols/Phenols have a broad signal in ZONE 1: 3600-3200 cm^{-1}**
 - **Signals for amines also show up in ZONE 1: 3500-3200 cm^{-1}**
 - i. **Primary amines (RNH_2) display 2 signals**
 - ii. **Secondary amines (R_2NH) display 1 signal**
 - Ethers have signals in ZONE 5 due to C-O stretch: 1300-1000 cm^{-1}
4. Double bonds and/or aromatic rings:
 - **Phenyl and vinyl sp^2 C-H stretches occur in ZONE 1 to the left of 3000 cm^{-1}**
 - **Alkenes display weak C=C stretching signals near 1650 cm^{-1}**
 - Medium to strong signals from 1650-1400 cm^{-1} imply an aromatic ring
5. sp Hybridized Triple bonds:
 - **Nitrile $\text{C}\equiv\text{N}$ bonds display in ZONE 3 around 2250 cm^{-1}**
 - **Alkyne $\text{C}\equiv\text{C}$ bonds display in ZONE 3 around 2150 cm^{-1}**
 - i. **Terminal alkynes also have a sharp signal in ZONE 1 around 3300 cm^{-1}**
6. Nitro groups, NO_2 :
 - N=O stretches observed as two signals in ZONE 5 around 1560 & 1350 cm^{-1}
7. Alkanes:
 - **Main signals for sp^3 hybridized C-H bonds are in ZONE 2 just below 3000 cm^{-1}**



OBSERVATION
PUDDLES AND WORMS...
IT MUST HAVE RAINED.
INFERENCE

OBSERVATION
AN IR BAND OF THIS SIZE AND SHAPE...
INFERENCE
PROBABLY THAT FUNCTIONAL GROUP.

ALL IR BANDS ARE EQUAL, BUT SOME ARE MORE EQUAL THAN OTHERS.

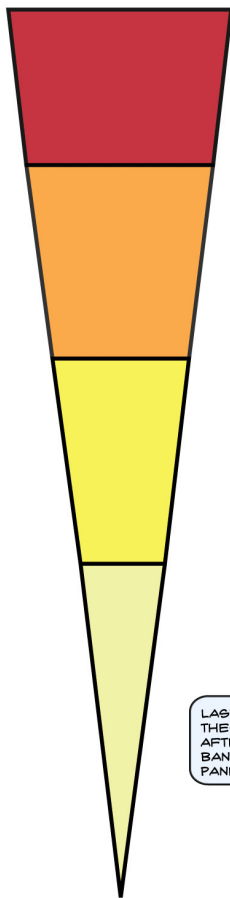
Alkyne (stretch)	ca. 3300	ca. 3.5
Aldehyde	2900-2800	3.4
	2800-2700	3.5
Alkane	not interpretatively useful	
Alkene	1600-1650	5.9
Aromatic	1600 and 1475	6.2
Alkyne	2250-2100	4.4
Aldehyde	1740-1720	5.7
Ketone	1725-1705	5.8
Carboxylic Acid	1725-1700	5.8
Ester	1750-1730	5.7
Amide	1670-1640	6.0
Anhydride	1810 and 1760	5.5
Acid Chloride	1800	5.6
Alcohols, Ethers, Esters, Carboxylic Acids, Anhydrides	1300-1000	7.6
Alcohol, Phenols		

MOVING DOWN THE CHART ONE AT A TIME, MATCHING BANDS AS YOU GO, IS NOT A USEFUL STRATEGY.

INSTEAD, LET'S ARRANGE THEM BY THEIR INTERPRETIVE POWER.

Alkyne (stretch)	ca. 3300	
Aldehyde	2900-2800	
	2800-2700	
Alkane	not interpretatively useful	
Alkene	1600-1650	
Aromatic	1600 and 1475	
Alkyne	2250-2100	
Aldehyde	1740-1720	
Ketone	1725-1705	
Carboxylic Acid	1725-1700	
Ester	1750-1730	
Amide	1670-1640	
Anhydride	1810 and 1760	
Acid Chloride	1800	
Alcohols, Ethers, Esters, Carboxylic Acids, Anhydrides	1300-1000	
Alcohol, Phenols		

GREAT INTERPRETIVE POWER



THIS IS THE FIRST REGION YOU SHOULD LOOK AT, AND THERE ARE 4 DIFFERENT SHAPES OF BANDS THAT YOU MAY SEE HERE.

...AND IF YOU DON'T SEE ANY BAND HERE, YOU MOST LIKELY DON'T HAVE ANY OF THESE FUNCTIONAL GROUPS (FG)

A SMOOTH TONGUE MEANS AN ALCOHOL. -O-H

VAMPIRE FANGS MEANS A PRIMARY AMINE... -N-H

ONE KNOCK-OUT FANG MEANS A 2° AMINE OR A TERMINAL ALKYNE. -C≡C-H

HAIRY BEARD IS A SIGN FOR A CARBOXYLIC ACID. -COO-H

IN THE C=O REGION, IT'S NOT THE SHAPE, BUT THE EXACT LOCATION THAT REVEALS THE IDENTITY OF THE FG.

ACID CHLORIDES	1810
ANHYDRIDES	1800
ESTERS	1760
ALDEHYDES	1735
KETONES	1725
AMIDES	1710
	1690

NOTE THAT THE EXACT POSITION DEPENDS ON THE SURROUNDING ENVIRONMENT:

← +30CM⁻¹ STRAIN, OR CONJUGATED AT -O- →

← -30CM⁻¹ CONJUGATED AT C=O →

AT ~2200CM⁻¹, WE FIND TRIPLE BONDS: C≡C, AND C≡N

USUALLY SHARP (CAN BE SMALLISH)

HINT: USE 3300CM⁻¹ TO DISTINGUISH TERMINAL AND INTERNAL ALKYNES.

Interpreting IR spectra

JON - JKWCHUI@UVC.CA

LASTLY, YOU SHOULD LOOK AT THESE FEATURES (BUT ONLY AFTER ANALYSING THE MAJOR BANDS IN THE PREVIOUS PAGES)

UNSATURATED C-H STRETCH

SATURATED C-H STRETCH

MONO

ORTHO

META

PARA

ALKENE/AROMATIC SUBSTITUTION PATTERN CAN BE SEEN IN THE C-H BEND REGIONS.

STRONG 990, 910

~900 (STRONG)

~700 (WEAK)

~910 (STRONG)

MONO

GEM (1,1-) DI-SUBSTITUTED

CIS-

TRANS-

LASTLY, A PEAK AT 2700CM⁻¹, TOGETHER WITH A C=O, IS INDICATIVE OF AN ALDEHYDE.

C-H STRETCH

2700CM⁻¹

C=O STRETCH

KETONES HAVE NO C-H IN THEM AND CAN HAVE NO 2700 C-H STRETCH PEAKS.

NOTES

** IF YOU'RE NOT SURE WHAT THE DIFFERENCE BETWEEN AN ACID AND AN ALCOHOL IS, DO THE QUICK "FUNCTIONAL GROUP IDENTIFICATION" EXERCISE.

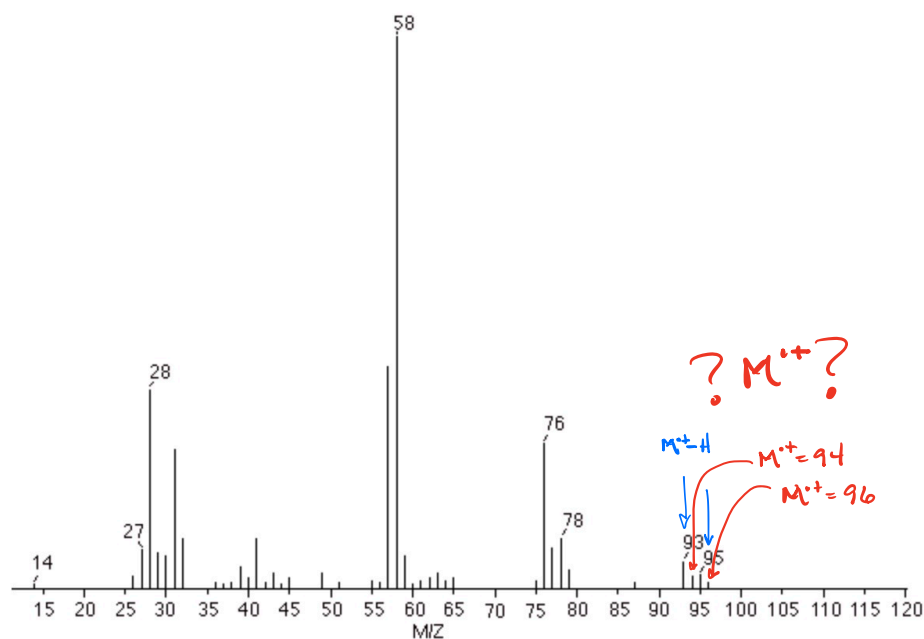
** ...IF YOU HAVE ONE FG. TWO 2° AMINE WOULD LOOK LIKE A 1 AMINE.

WE LOOKED AT THESE LAST BECAUSE THEY CAN BE AMBIGUOUS TO INTERPRET, OR THEY HAVE ONLY A NARROW NICHE OF USEFULNESS.

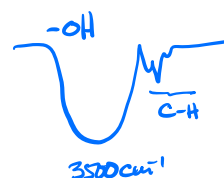
CoOP #3, Problem 3

Mass Spec

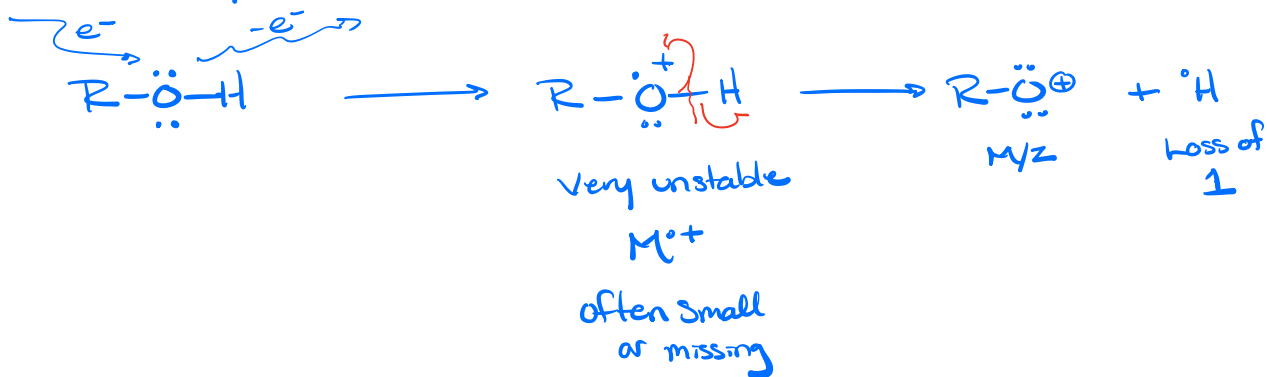
Problem 3: Positive EI Mass Spectrum



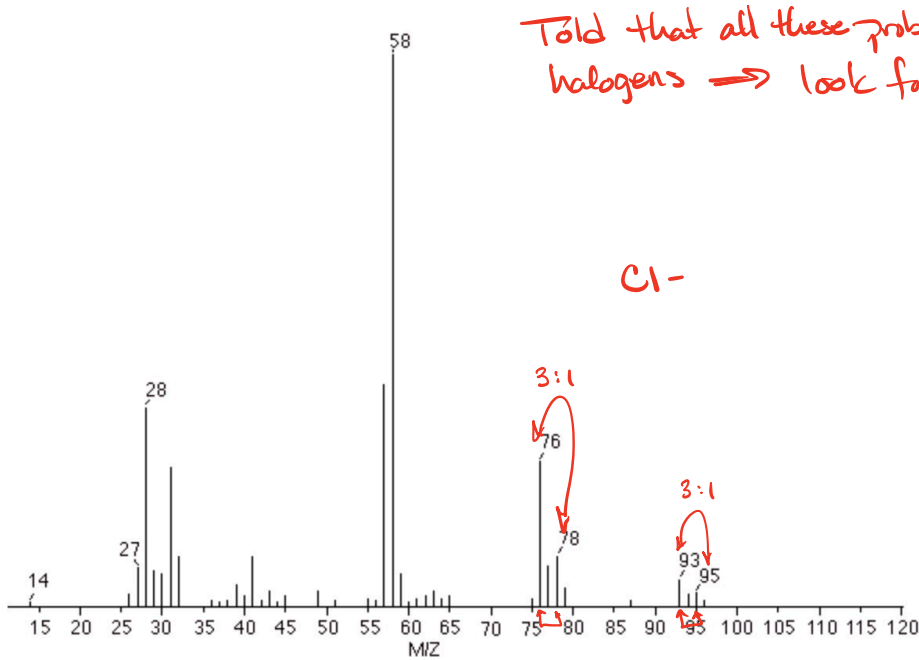
IR - shows strong Alcohol @ 3500 cm^{-1}



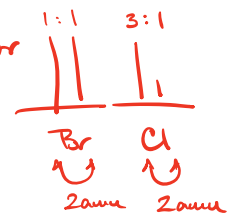
Mass Spec R-OH



Problem 3: Positive EI Mass Spectrum

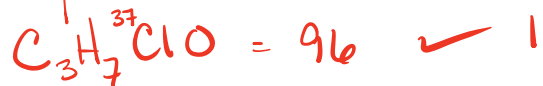
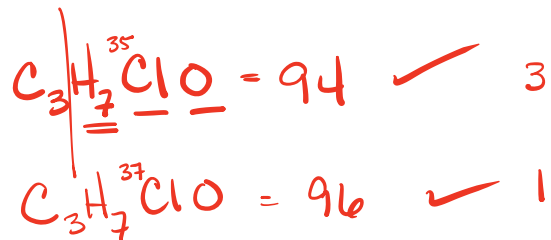


Told that all these problems have halogens → look for



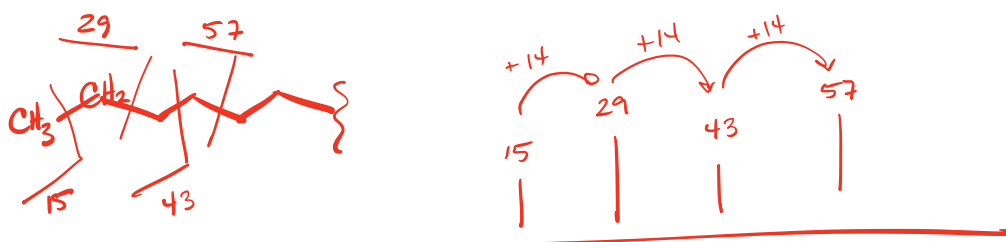
Cl-

HNMR H_7 }
 CNMR C_3 }
 min #
 Could be more

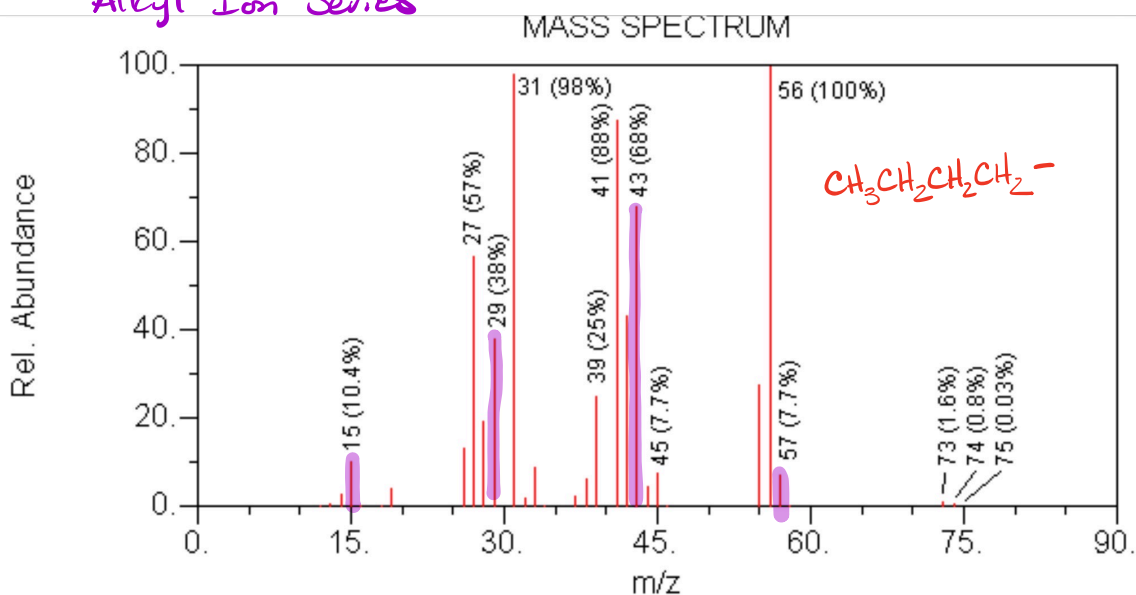


Ratio

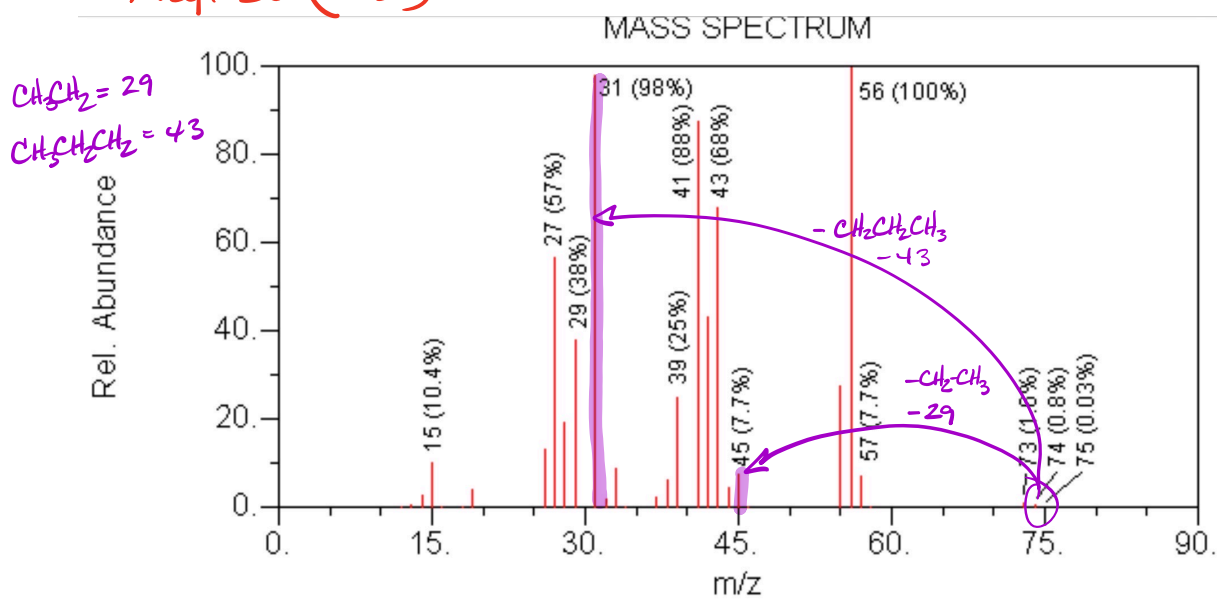
Mass Spec Alkyl Ion Series



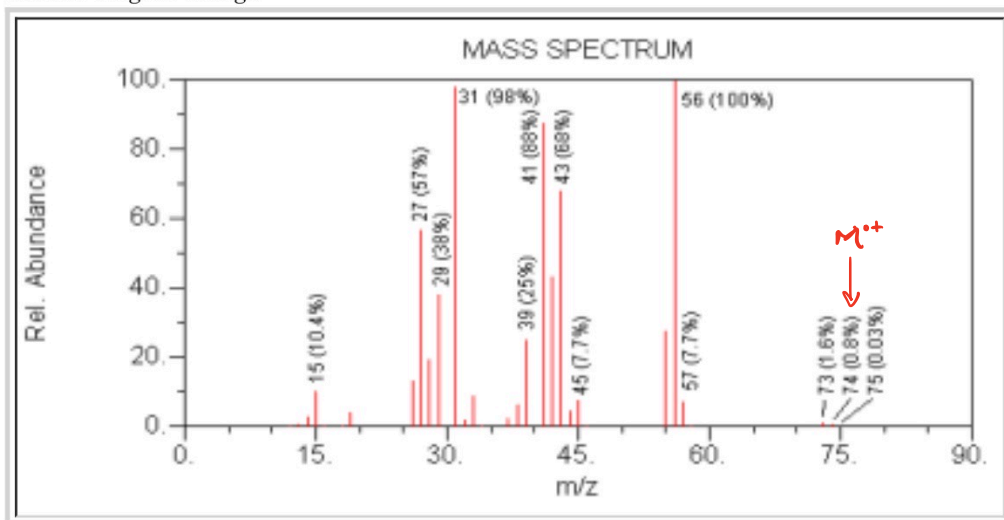
Alkyl Ion Series



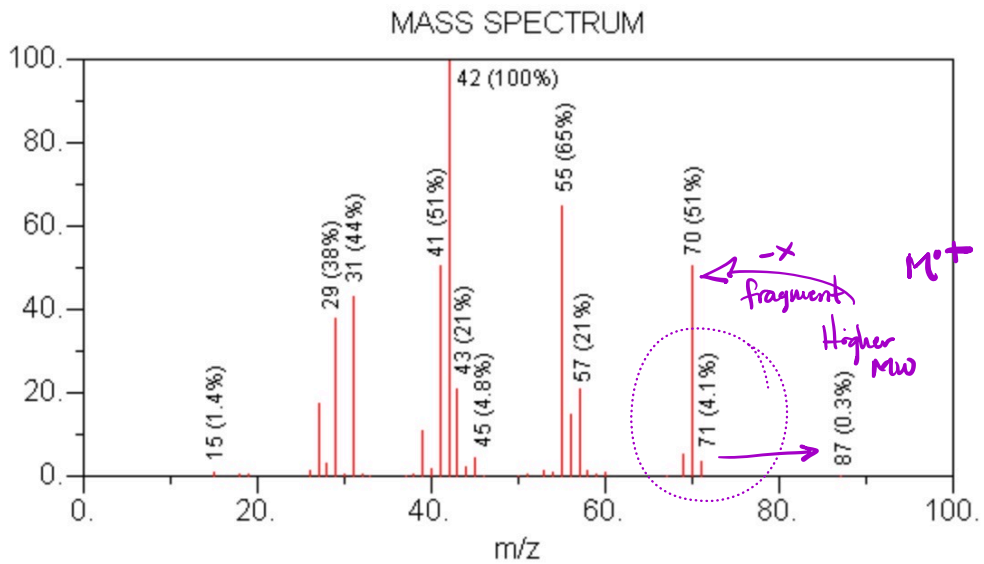
Alkyl Ion(Loss) Series



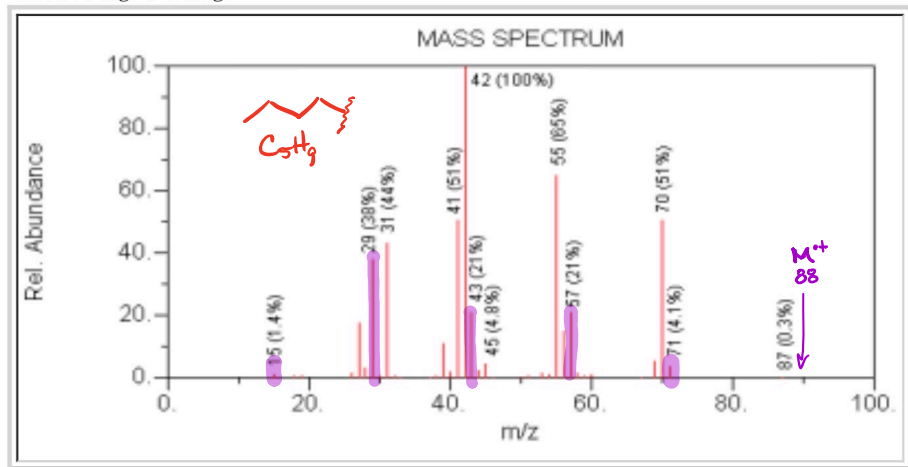
Click on image to enlarge



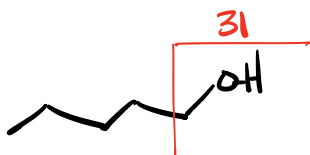
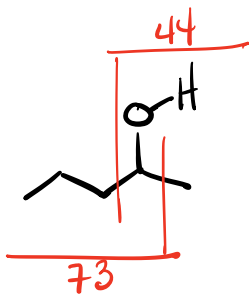
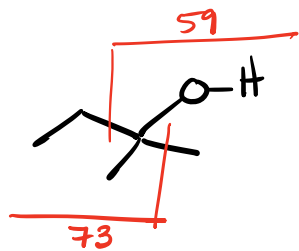
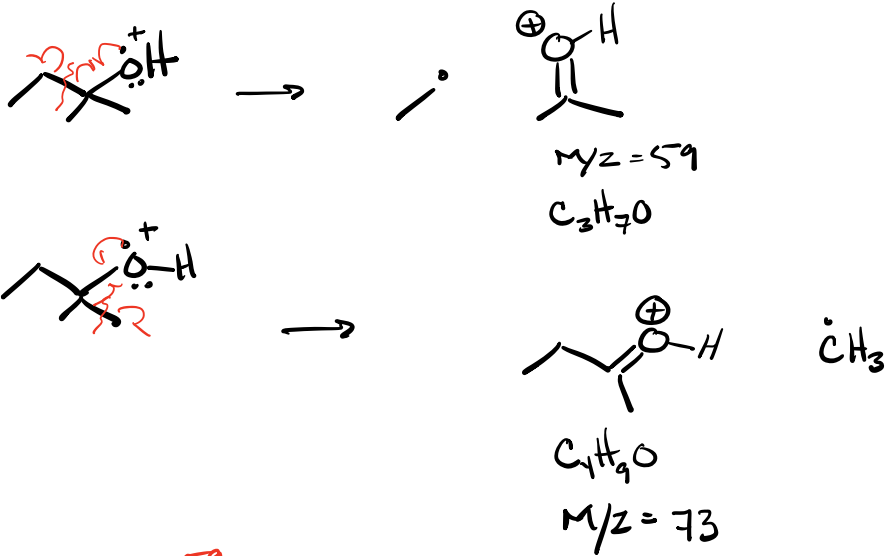
- a) 2-methyl-2-propanol CC(C)(C)O $C_4H_{10}O$ 74 *No straight chain*
- b) 1-butanol CCCCO $C_4H_{10}O$ 74 *straight chain*
- c) 2-butanol CCC(O)C $C_4H_{10}O$ 74
- d) 1-pentanol CCCCCO $C_5H_{12}O$ 78
- e) 2-methyl-1-propanol CC(C)CO $C_4H_{10}O$ 74 *No straight chain*



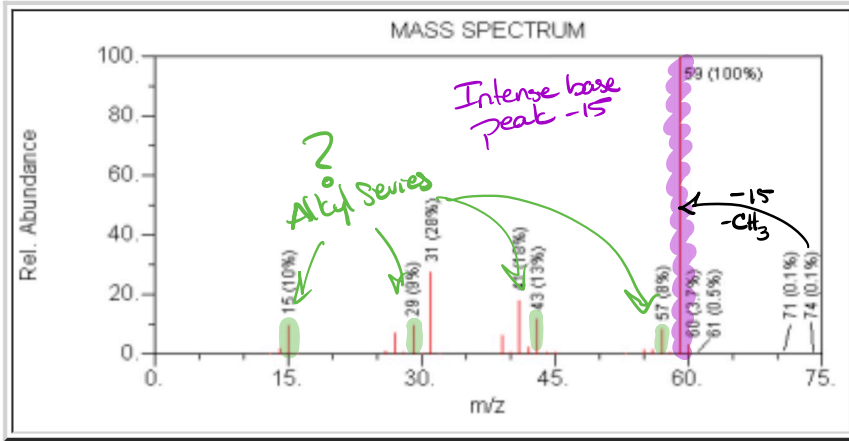
Click on image to enlarge



- a) 1-hexanol $C_6H_{14}O$ 102
- b) 1-pentanol $C_5H_{12}O$ 88
- c) 2-methyl-2-butanol $C_5H_{12}O$ 88
- d) 2-pentanol $C_5H_{12}O$ 88
- e) 1-butanol $C_4H_{10}O$ 74



Click on image to enlarge



- a) 2-methyl-2-butanol
- b) 2-methyl-2-propanol
- c) 2-butanol
- d) 1-butanol
- e) 2-methyl-1-propanol

