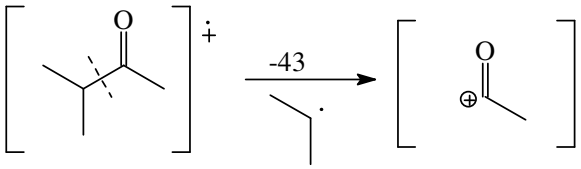
CHM 202 - Mass Spectrometry Problems (with some IR)

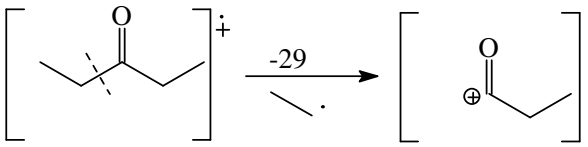
1. The two mass spectra below correspond to two isomers of $C_5H_{10}O$: 3-methyl-2-butanone and 3-pentanone. Draw the two structures. Match the spectrum with the compound and draw the fragment ion that corresponds to the base peak.

a) 3-methyl-2-butanone



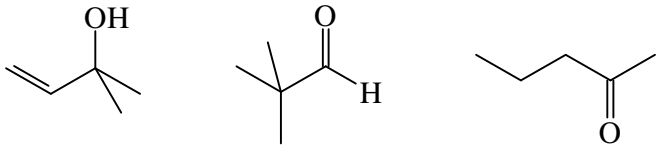
$m^+ = 86$ m/z = 43 base peak

b) 3-pentanone

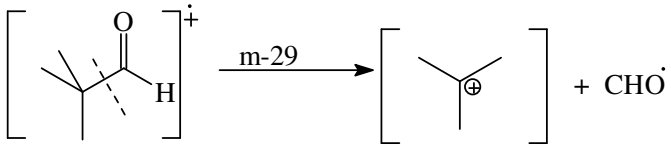


$m^+ = 86$ m/z = 57 base peak

2. The three compounds shown below are structural isomers of each other. Match each compound with its corresponding mass spectrum (a,b, and c) and draw the fragment ion corresponding to the base peak in each.

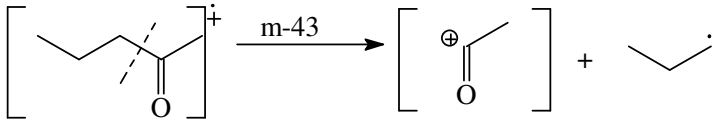


a)



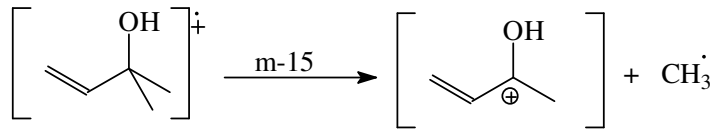
m/z = 57

b)



m/z = 43

c)



m/z = 71

3. An unknown compound gives rise to the following infrared and mass spectra. Propose a structure for the compound. Explain by citing features from both spectra.

Infrared spectrum

3600-3200 cm^{-1} O-H str

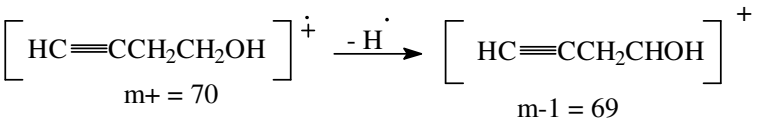
3300 cm^{-1} sp C-H str

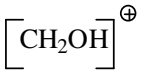
2900 cm^{-1} sp^3 CH str

2150 cm^{-1} CC triple bond str

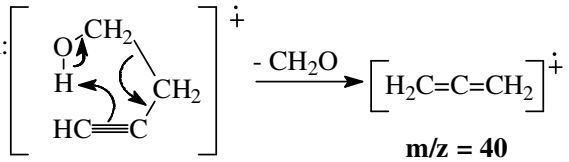
1050 cm^{-1} C-O str (1^o)

Mass spectrum



peak at 31 is 

base peak is very unusual: loss of formaldehyde (neutral molecule)



m+ = 70

m/z = 40