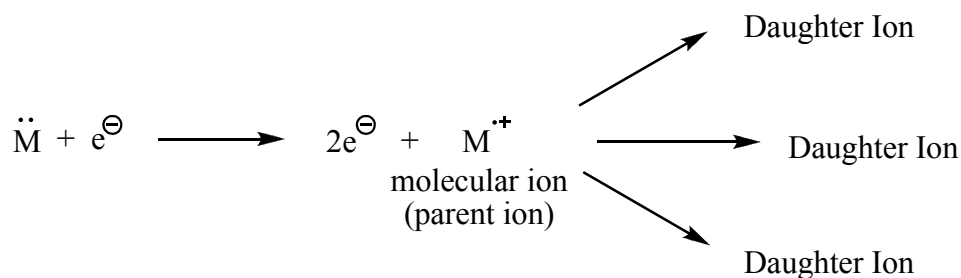
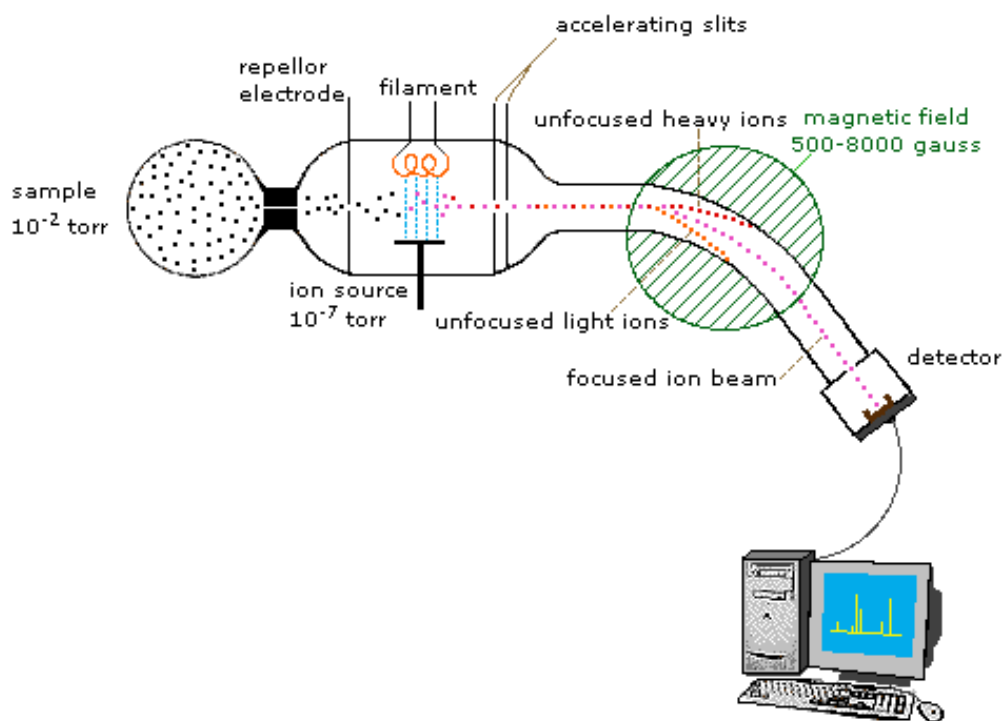


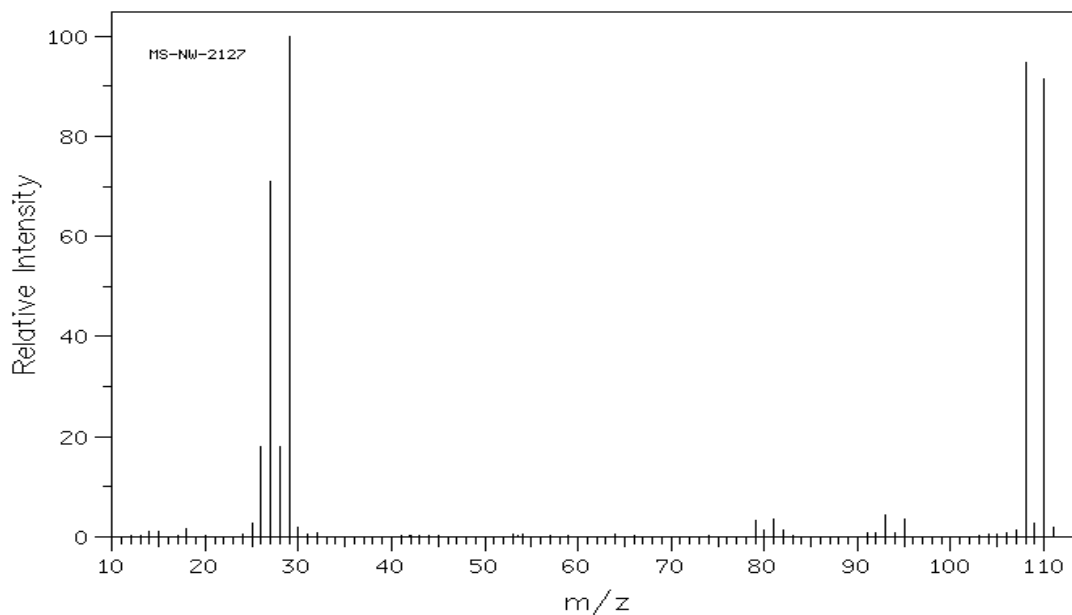
# Mass Spectrometry in Organic Chemistry Fragmentation Patterns



The mass spectrometry pictured above is courtesy of the Department of Chemistry, Michigan State University. The mass spectra in this document were extracted from SDBSWeb : <http://riodb01.ibase.aist.go.jp/sdbs/> (National Institute of Advanced Industrial Science and Technology, 9-20 to 9-28-2008)

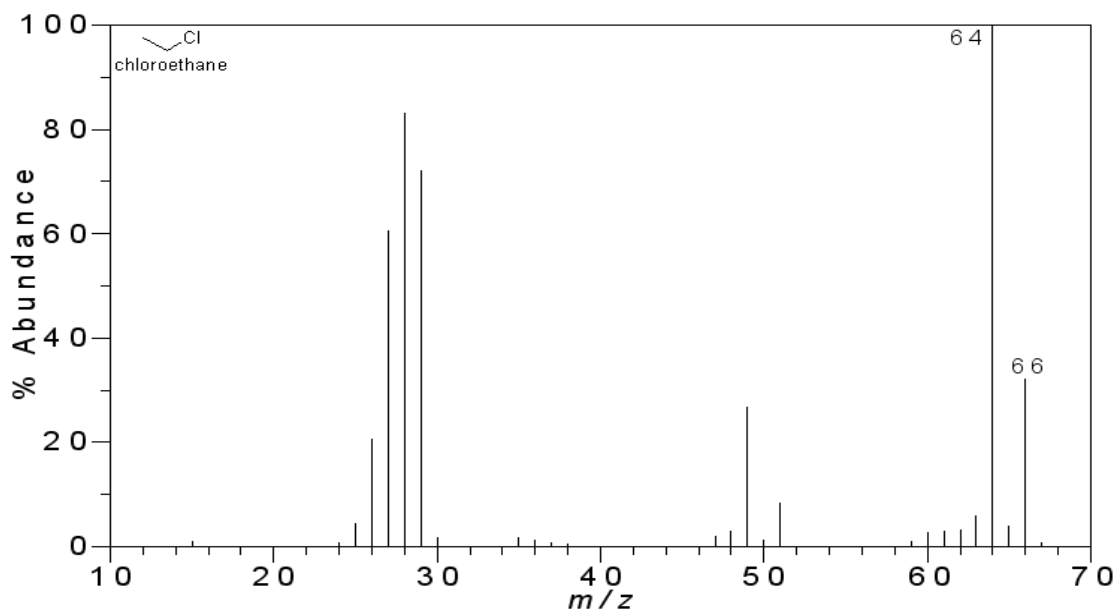
**Mass spectrum of bromoethane (C<sub>2</sub>H<sub>5</sub>Br).** The presence of molecular ion peaks that are nearly equal in intensity is usually suggestive of the presence of bromine which has two isotopes.

**Bromine isotopes:** 50.50% <sup>79</sup>Br and 49.50% <sup>81</sup>Br

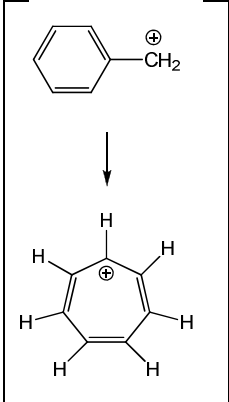
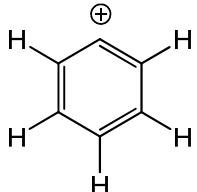
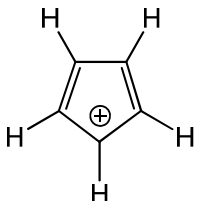
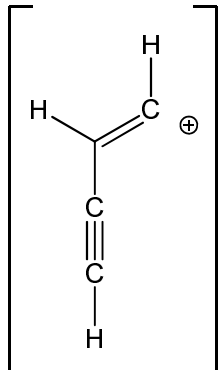


**Mass spectrum of chloroethane (C<sub>2</sub>H<sub>5</sub>Cl).** The presence of molecular ion peaks that are in a 3:1 ratio is usually suggestive of the presence of chlorine which has two isotopes.

**Chlorine:** 75.77% <sup>35</sup>Cl and 24.23% <sup>37</sup>Cl

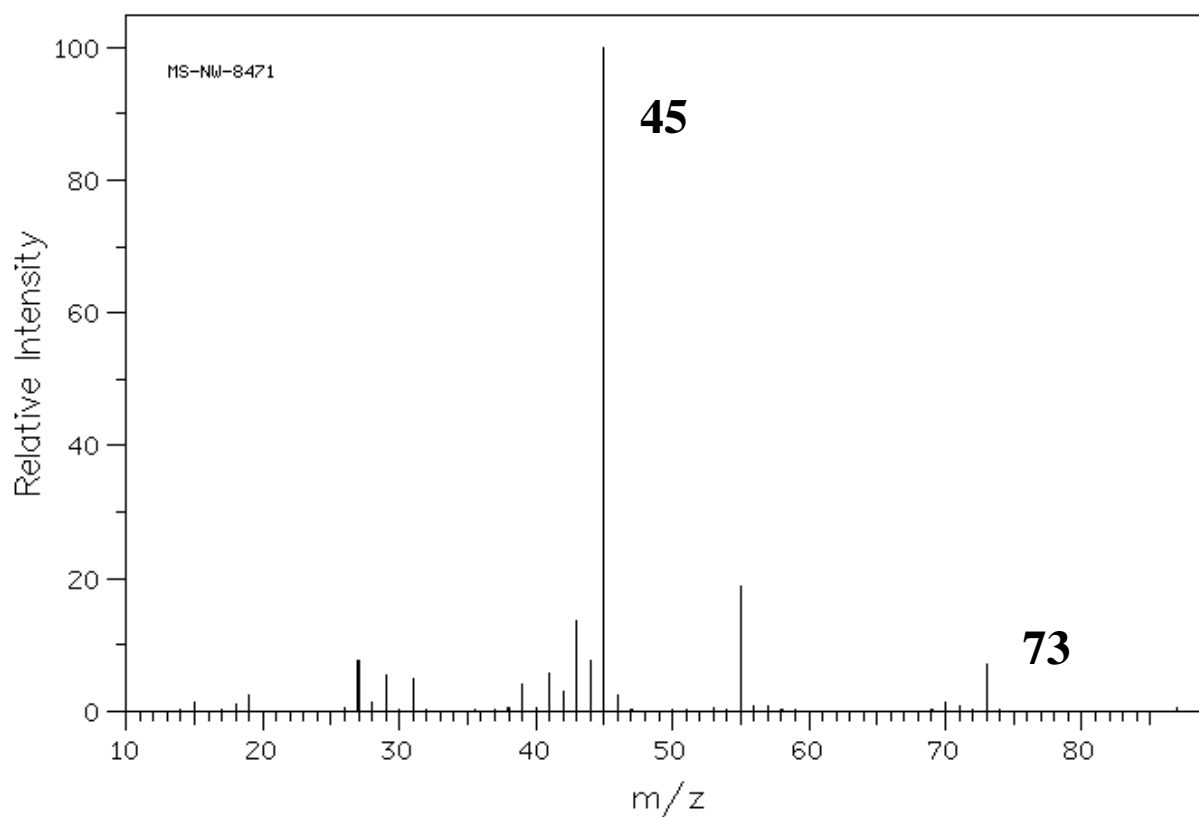
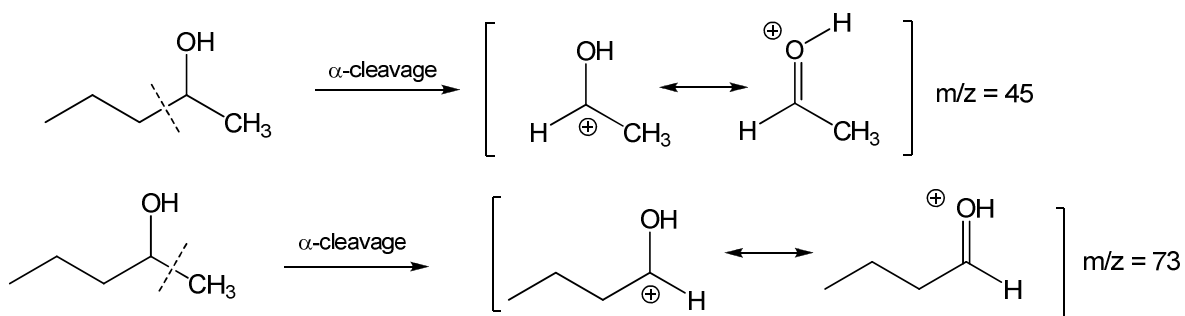


## COMMON AROMATIC FRAGMENTS

Alkyl Fragment	Name	Molecular formula	Mass/charge ratio (m/z)
	benzyl cation rearranges to form the tropylium ion.	$C_7H_7^+$	91
	phenyl cation	$C_6H_5^+$	77
	cyclopentadienyl cation	$C_5H_5^+$	65
	Unstable cation	$C_4H_3^+$	51

# FRAGMENTATIONS OF ALCOHOLS

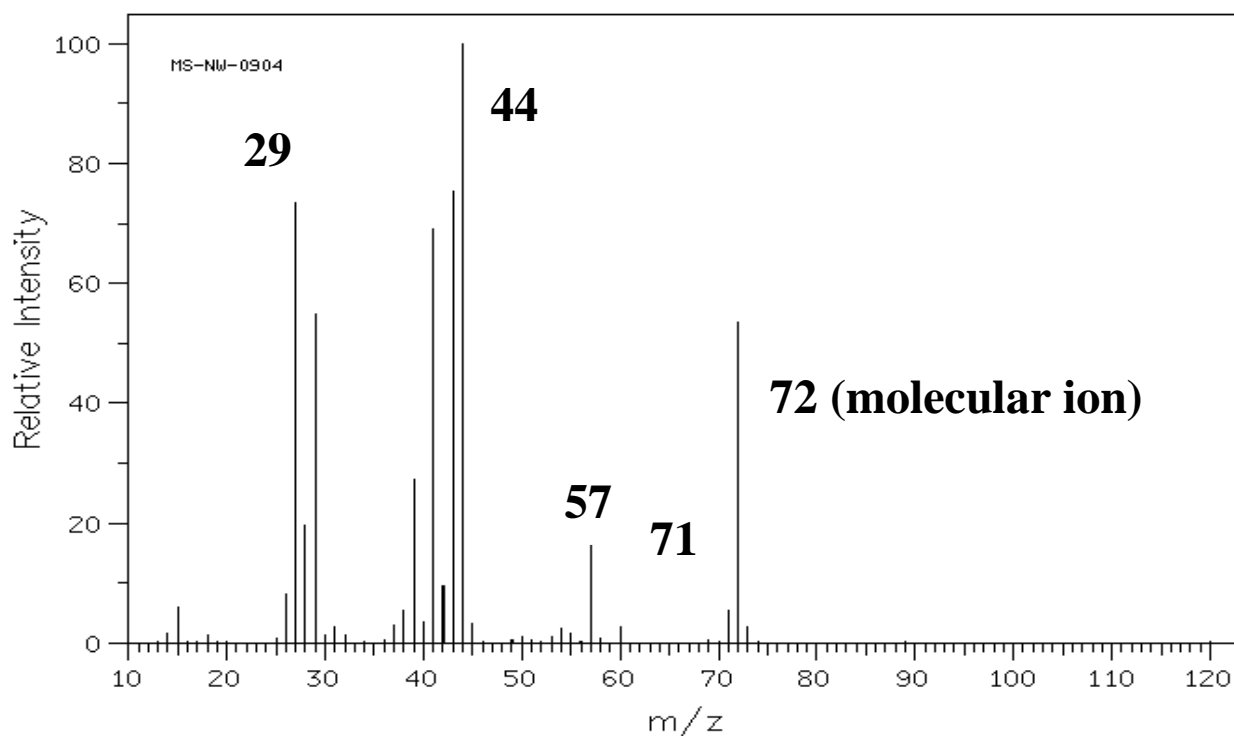
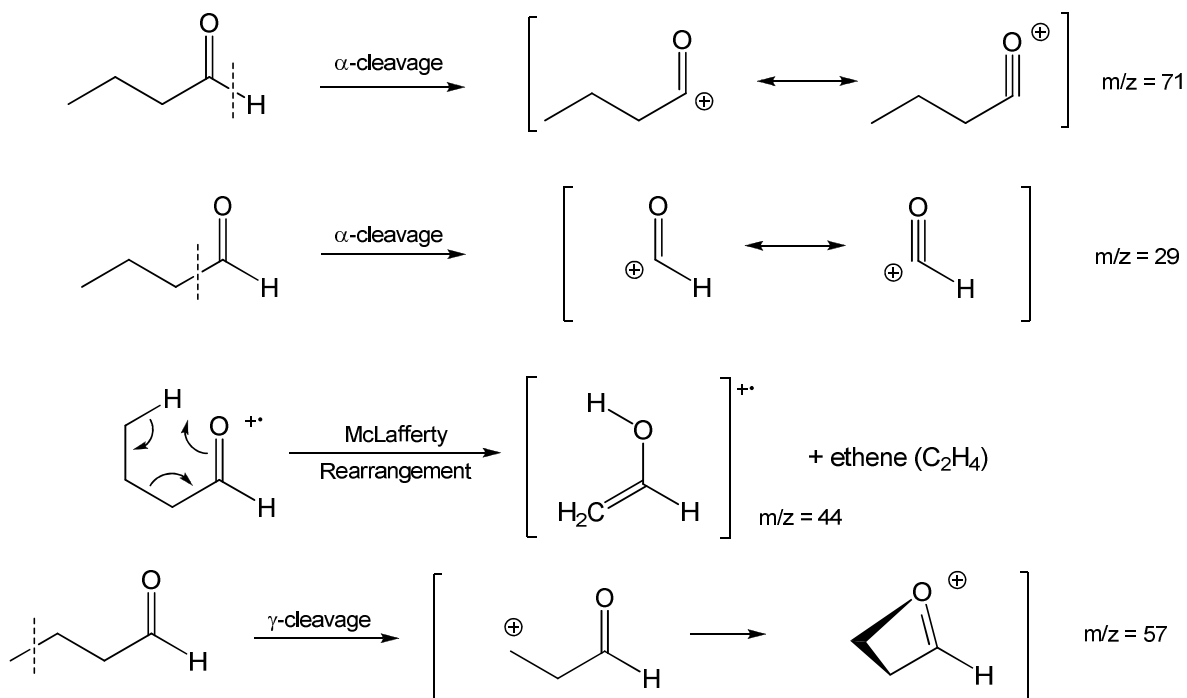
The parent molecular ion for alcohols is often very weak or not observed at all due to facile fragmentation pathways. The dominant pathway for fragmentation is  $\alpha$ -cleavage. There are other fragmentation patterns but they are beyond the scope of this work.



The peak at 55 m/z is the cyclobutyl cation that arises a series of fragmentation pathways. This peak is beyond the scope of our investigations at this stage.

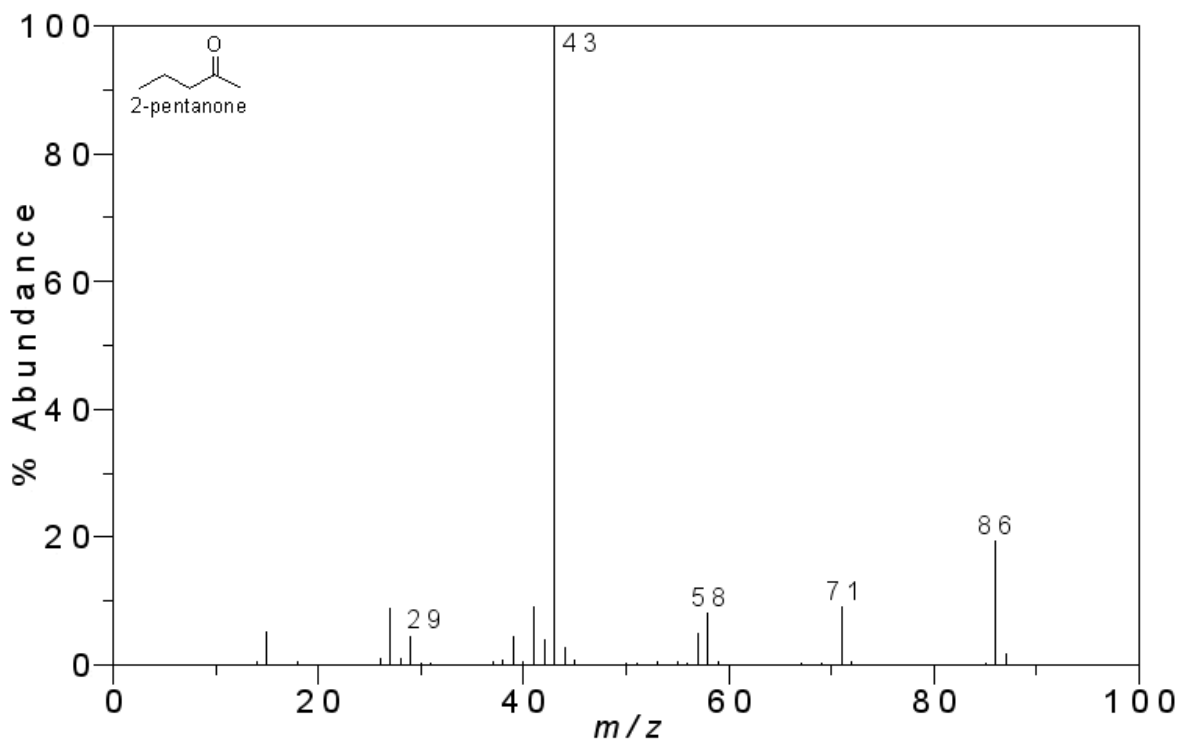
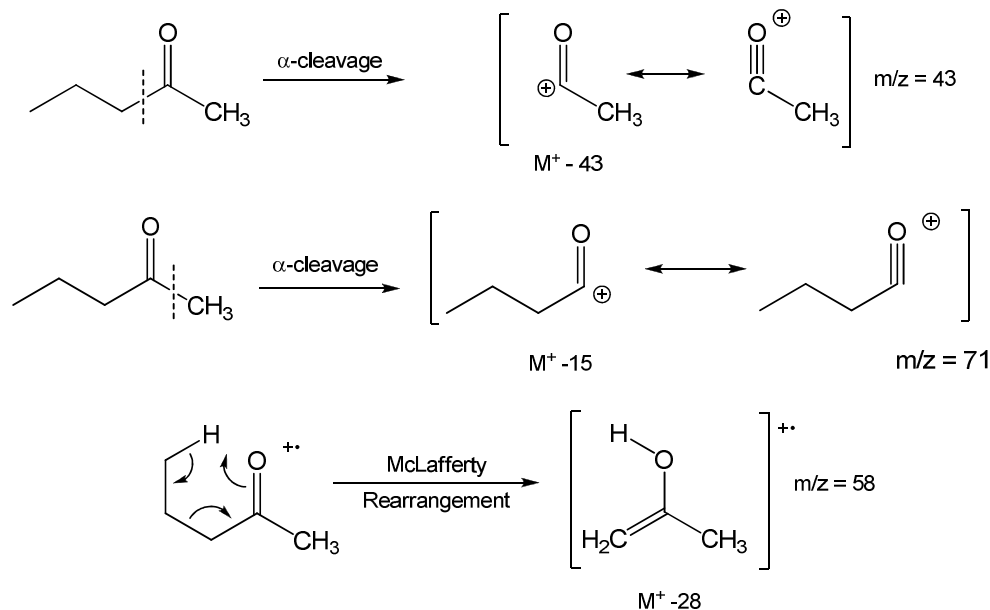
# FRAGMENTATIONS OF ALDEHYDES

Aldehydes yield an even-numbered molecular ion with primarily odd-numbered fragments. The dominant fragmentation pathways involve  $\alpha$ -cleavage and the McLafferty rearrangement.



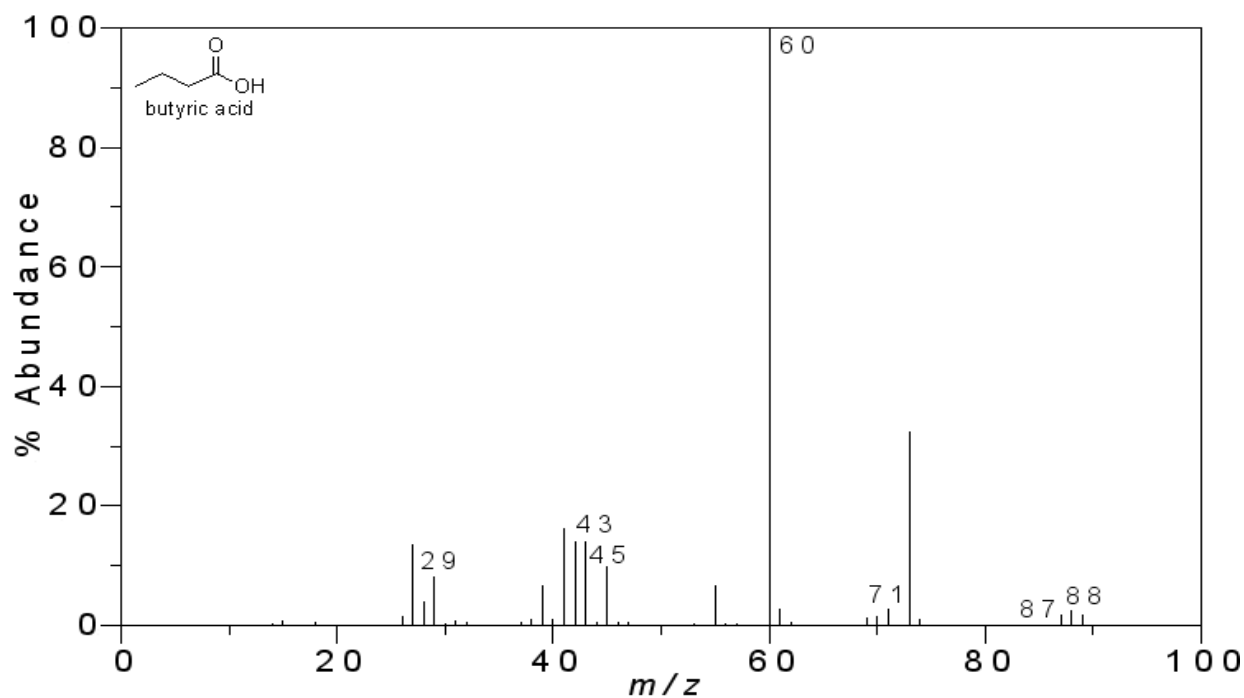
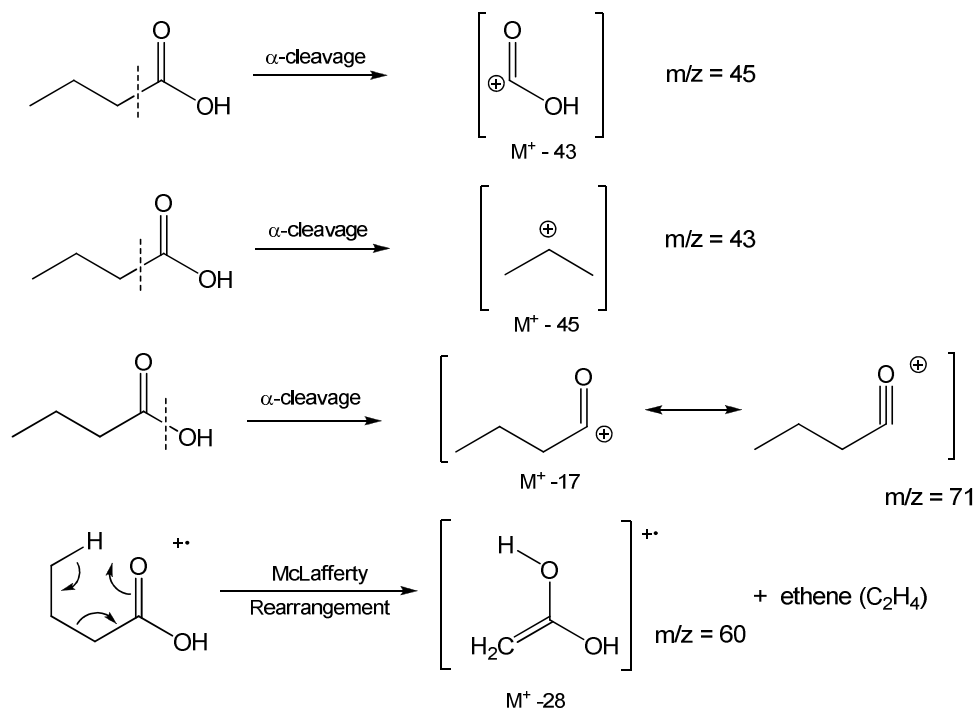
# FRAGMENTATIONS OF KETONES

Ketones yield an even-numbered molecular ion with primarily odd-numbered fragments. The dominant fragmentation pathways involve  $\alpha$ -cleavage and the McLafferty rearrangement.



# FRAGMENTATIONS OF CARBOXYLIC ACIDS

Carboxylic acids yield an even-numbered molecular ion with primarily odd-numbered fragments. The dominant fragmentation pathways involve  $\alpha$ -cleavage and the McLafferty rearrangement.



# FRAGMENTATIONS OF ESTERS

Esters yield an even-numbered molecular ion with primarily odd-numbered fragments. The dominant fragmentation pathways involve  $\alpha$ -cleavage and the McLafferty rearrangement.

