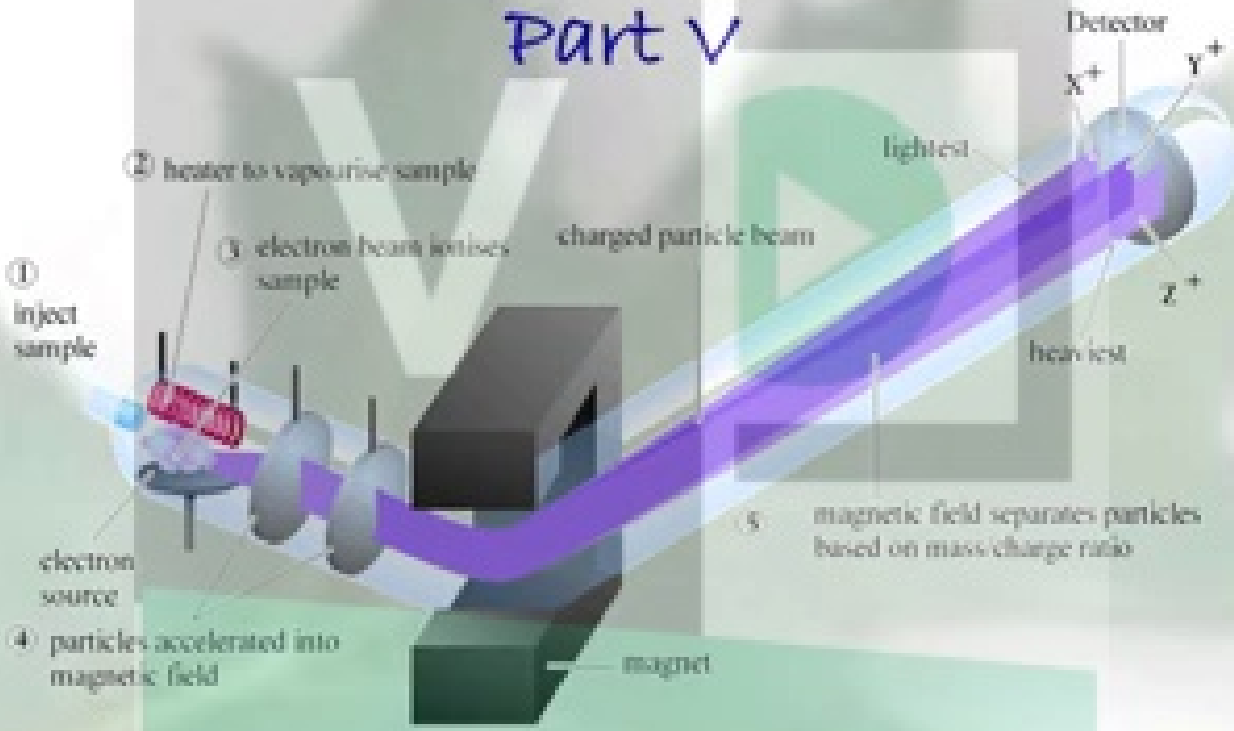
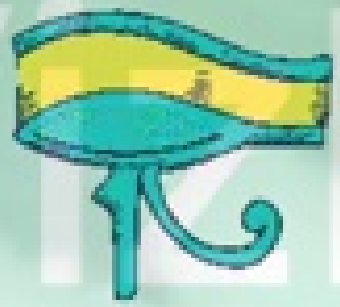
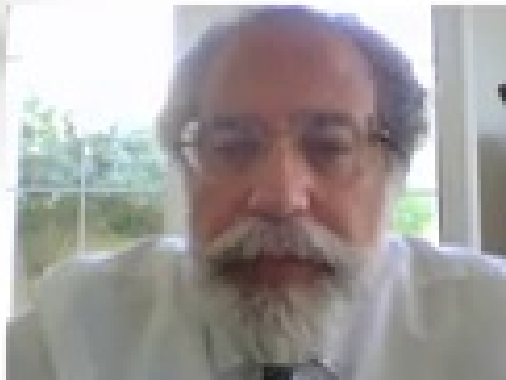
Mass spectrometry

Part V





Prof. Adel Amer



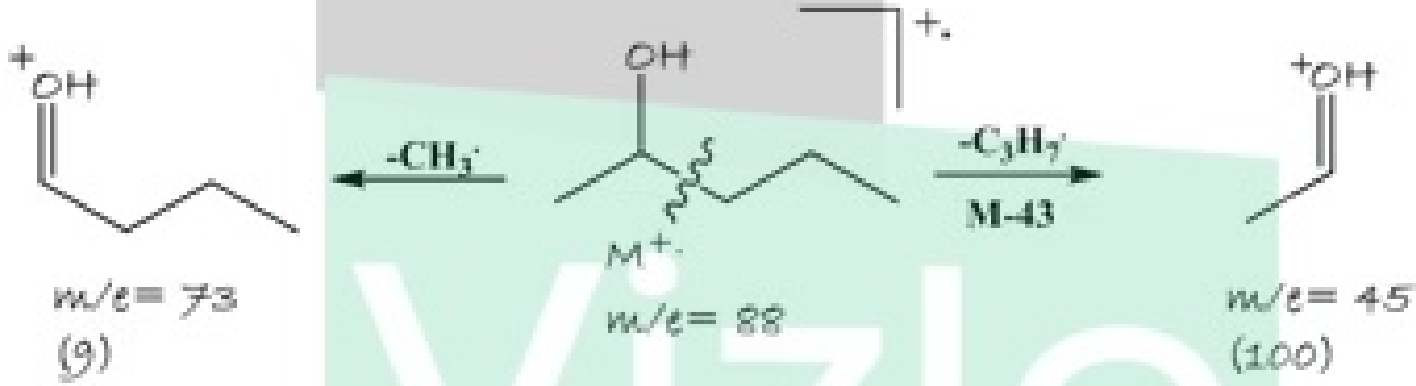
Typical fragmentation of functional groups

- ✓ Alkanes [Straight Chain, Branched, Cyclic]
- ✓ Alkenes [Straight Chain, Cyclic]
- ✓ Alkynes
- ✓ Aromatics

Fragmentation - Alcohols

The molecular ion peak is usually very weak or absent for alcohols.

The most important fragmentation process for alcohols involves the loss of an alkyl group (α-cleavage). The largest alkyl group is preferentially lost as shown

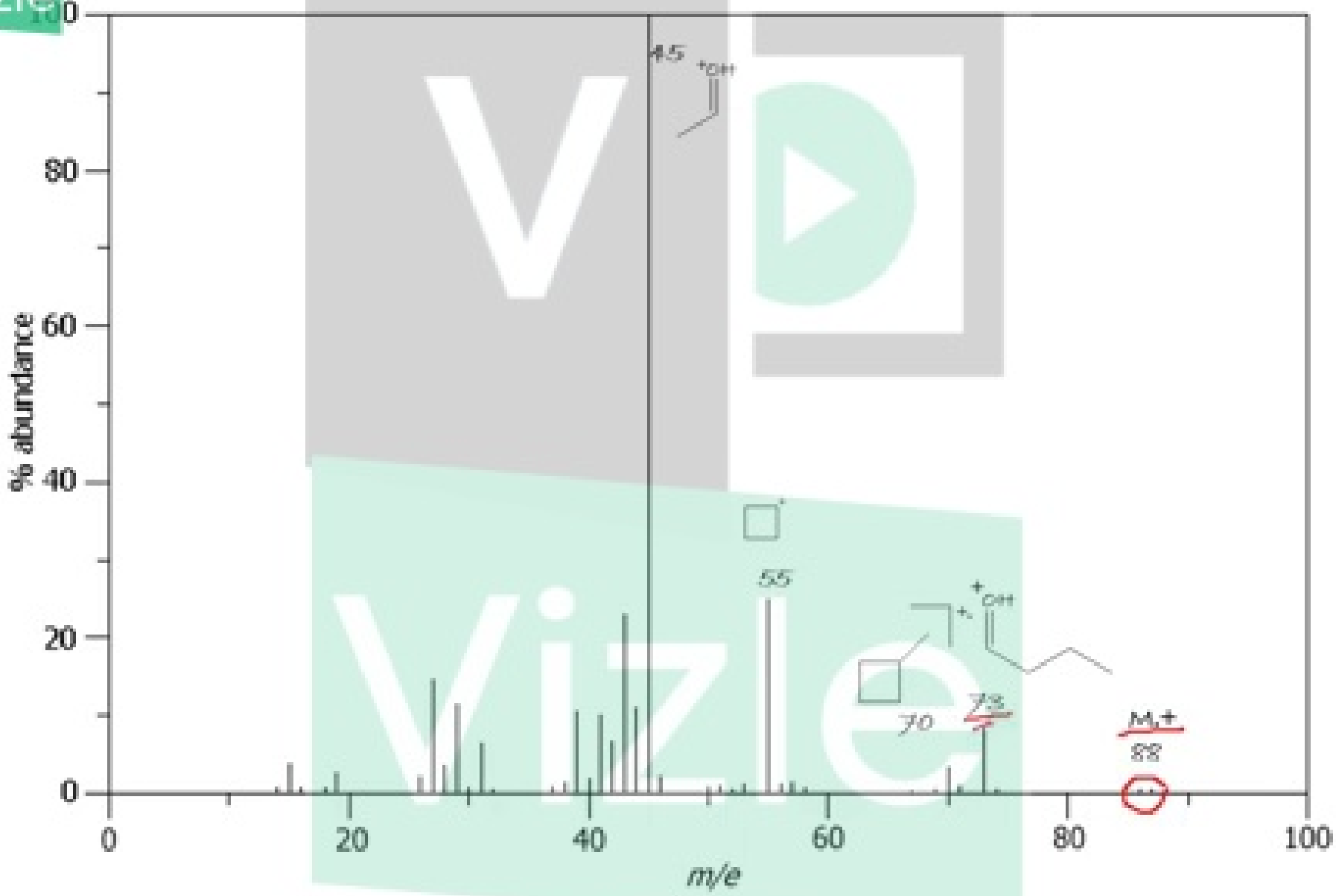


second common mode of fragmentation involves dehydration. The importance of this fragmentation process increases with increasing chain length. Loss of water (M - 18) is very indicative of an alcohol functionality

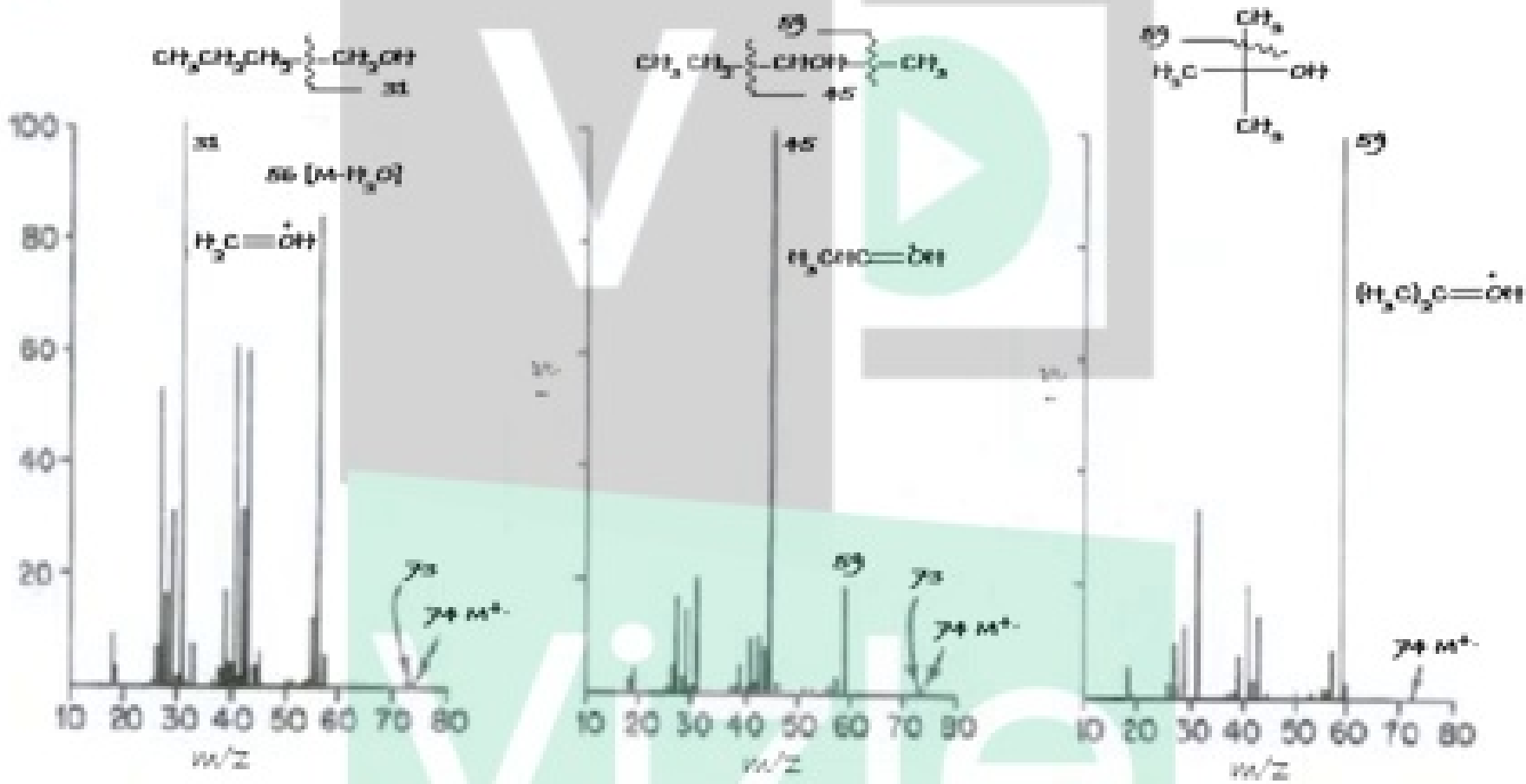
$M^{+\cdot}$

m/e= 88

Mass spectrum of 2-pentanol



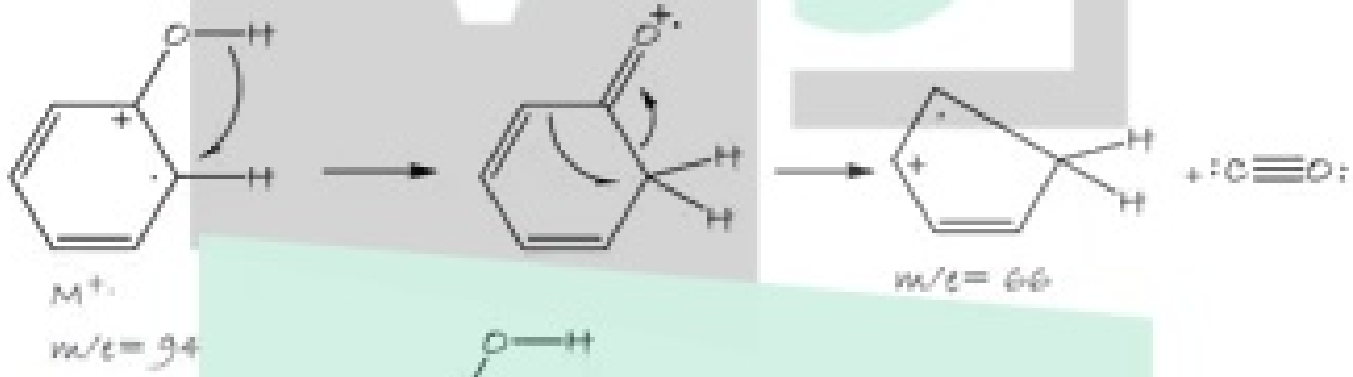
We can distinguish isomers e.g. butanol

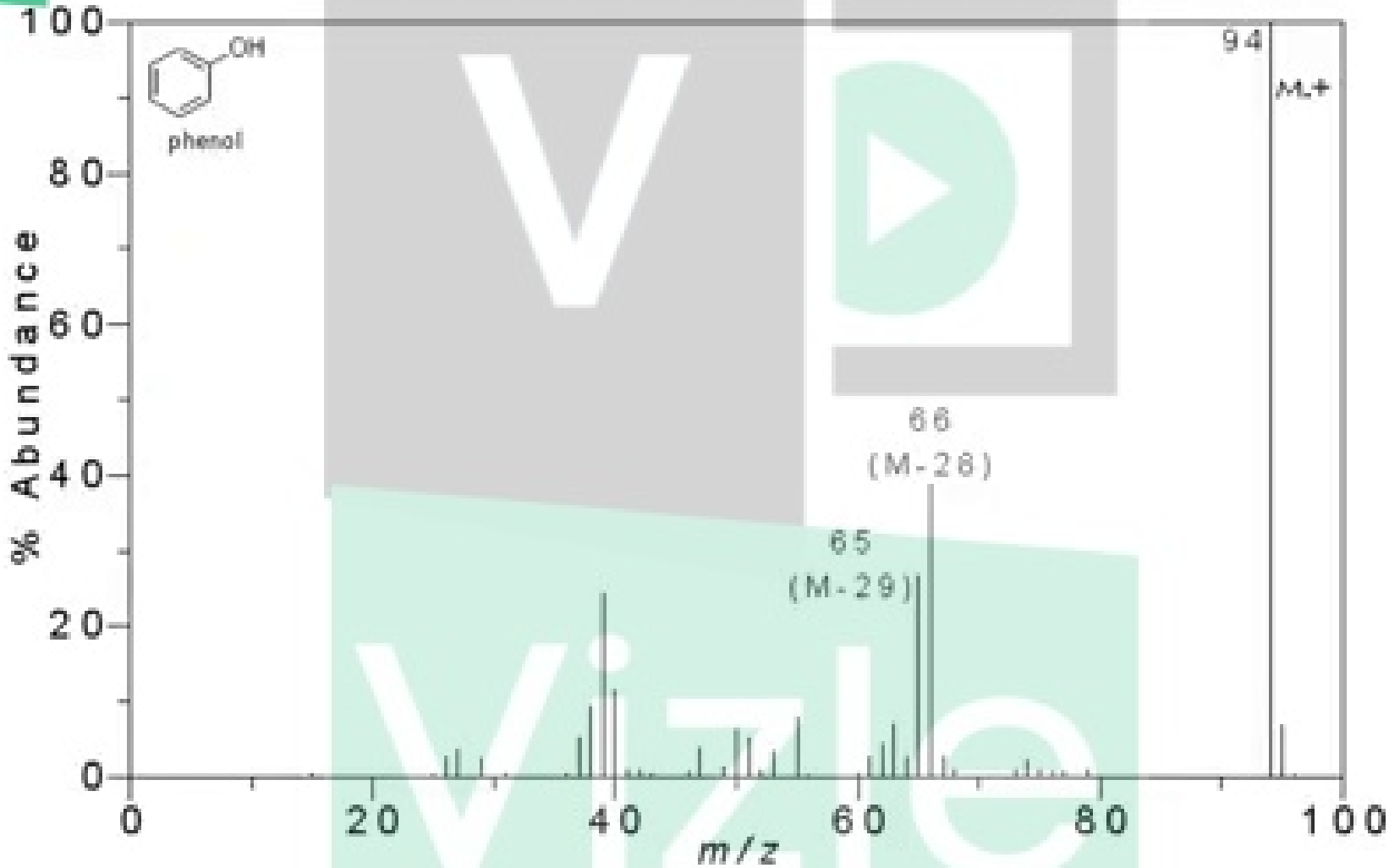


Mass spectra of the three isomers of butanol

Phenols can lose the elements of carbon monoxide to give strong peaks at M - 28.

Phenols can also lose the elements of the formyl radical (HCO·) to give strong peaks at M - 29.




100
80
60
40
20
0
% Abundance
OH
phenol
94
M+
66
(M-28)
65
(M-29)
0
20
40
60
80
100
m/z