

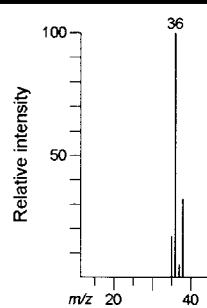
Chemistry 212, Dr. Glaser

Exercise Assignment: Applications of Mass Spectroscopy

The effects of isotopes are illustrated in Unknowns 2.1 to 2.3. The characteristic ratio of 3:1 for Unknown 2.1 makes the element easily recognizable. Note that the interpretation of m/z 36 as a fragment ion would be totally misleading! It is important that you become familiar with the isotope ratios of the common elements.

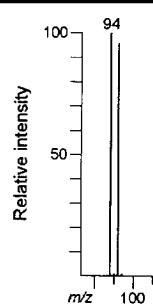
Unknown 2.1

m/z	Int.
35	12.
36	100.
37	4.1
38	33.



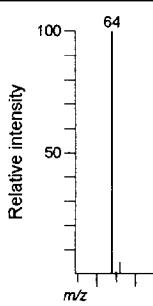
Unknown 2.2

m/z	Int.
94	100.
95	1.1
96	96.
97	1.1



Unknown 2.3

m/z	Int.
64	100.
65	0.9
66	5.0

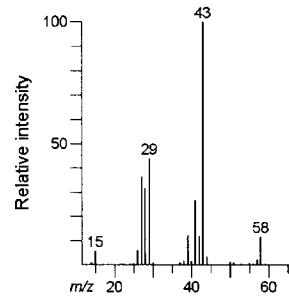


Chemistry 212, Dr. Glaser**Exercise Assignment: Applications of Mass Spectroscopy**

In Unknown 2.4, calculate (after checking for $(M+2)$ elements) the maximum number of carbon atoms in the ions m/z 43 and 58. The results indicate that m/z 43 is formed from m/z 58 by the loss of what group?

Unknown 2.4

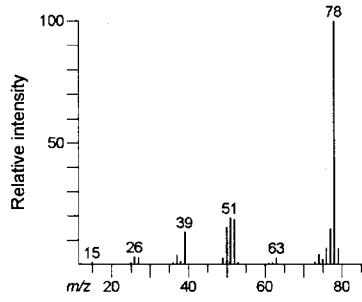
m/z	Int.	m/z	Int.
12	0.1	40	1.6
13	0.3	41	27.
14	1.0	42	12.
15	5.3	43	100.
25	0.5	44	3.3
25.5	0.4	48	0.1
26	6.1	49	0.4
26.5	0.1	50	1.2
27	37.	51	1.0
27.5	0.1	52	0.3
28	32.	53	0.7
29	44.	54	0.2
30	1.0	55	0.9
36	0.1	56	0.7
37	1.0	57	2.4
38	1.8	58	12.
39	12.	59	0.5



The Unknown 2.5 has a small but important peak at m/z 80. The m/z 79 peak could not be consistently explained if the m/z 80 would be taken as indicative of ^{18}O . Why not. What is this compound?

Unknown 2.5

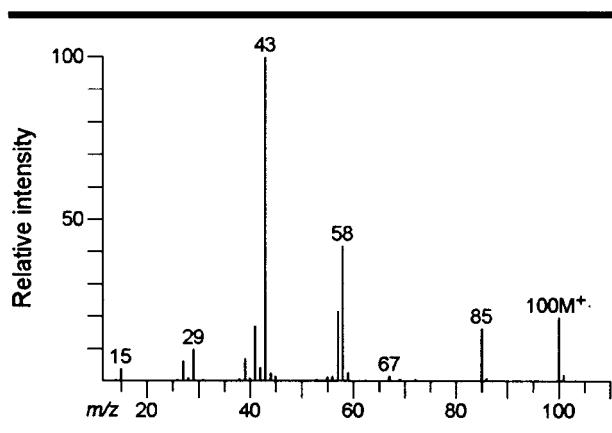
m/z	Int.	m/z	Int.
12	0.2	53	0.8
13	0.4	60	0.2
14	0.4	61	0.4
15	1.0	62	0.8
24	0.4	63	2.9
25	0.8	64	0.2
26	3.2	72	0.4
27	2.6	73	1.0
36	0.9	74	3.9
37	3.8	75	2.2
39	13.	76	7.0
40	0.4	77	15.
50	16.	78	100.
51	19.	79	6.8
52	20.	80	0.2



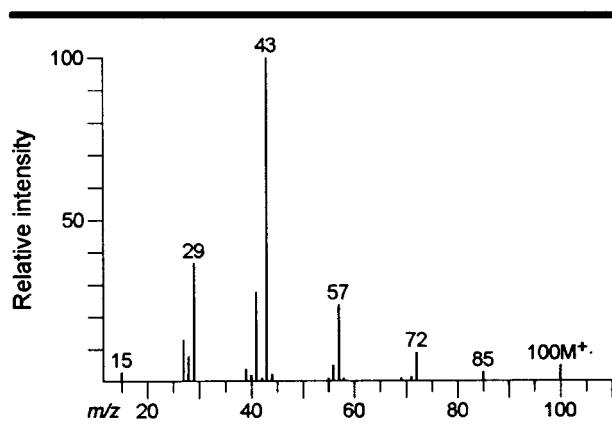
McLafferty Rearrangement of Ketones

These are the spectra of 3- and 4-methyl-2-pentanone. Which one is which?

Unknown 4.16

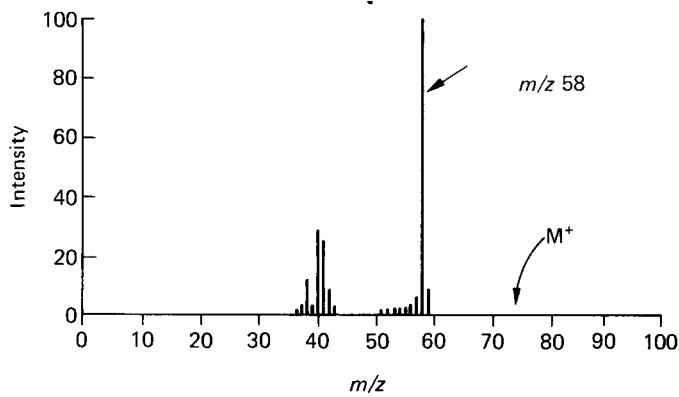
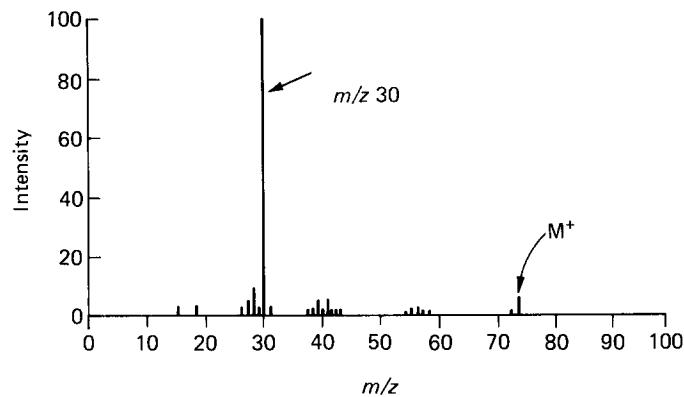


Unknown 4.17



Mass Spectra of Isomeric Amines

These are the spectra of isobutylamine and of t-butylamine. Which one is which?
Discuss the fragmentation paths for the isomers.



Mass Spectra of Oxygen Containing Compounds

These are the spectra of an alcohol and of an aldehyde. Which one is which? Give the structures of the compounds and explain the fragmentation patterns observed.

