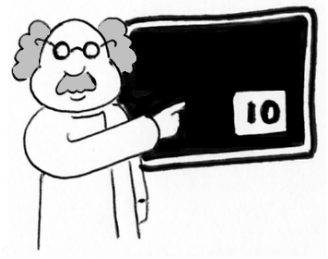
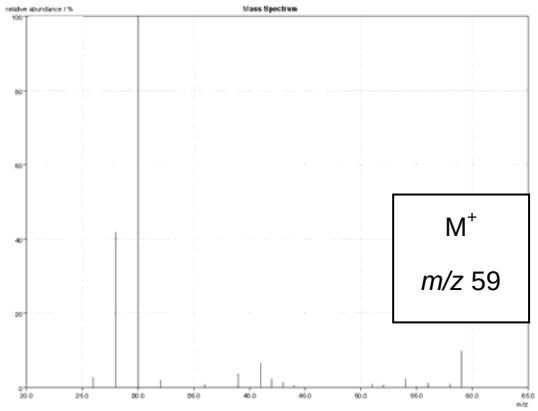


STARTER FOR 10...

10.1.3. Molecular mass spectrometry

Use the elemental analysis data together with the mass spectrum to propose a molecular formula for the unknowns A to C. Easy! (3 marks for each)

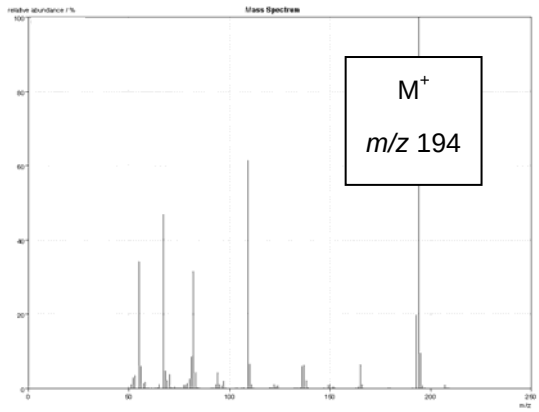


M^+

m/z 59

Unknown A

C 61.02%; H 15.25%; N 23.73%

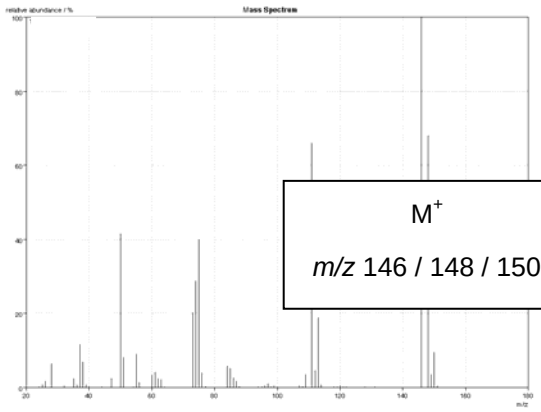


M^+

m/z 194

Unknown B

C 49.48%; H 5.15%; O 16.49%; N 28.87%



M^+

m/z 146 / 148 / 150

Unknown C

C 49.02%; H 2.74%; Cl 48.23%

BONUS MARK Why does unknown C appear to have three molecular ions each differing in mass by 2? (1 mark)

81 = y% (1 mark)

Therefore the percentage of the lightest isotope present is **81%**

10.1.3. Molecular mass spectrometry

(1 mark for calculations, 1 mark for empirical formula, 1 mark for molecular formula of each unknown)

Unknown A

(1-aminopropane)

	C	H	N
Mass in 100 g	61.02	15.25	23.73
Moles in 100 g	5.09	15.25	1.70
Ratio	3	9	1

Empirical formula = $\mathbf{C_3H_9N}$

Molecular weight of empirical formula = 59 = M^+, therefore molecular formula = $\mathbf{C_3H_9N}$

Unknown B

(caffeine)

	C	H	N	O
Mass in 100 g	49.48	5.15	28.87	16.49
Moles in 100 g	4.12	5.15	2.06	1.03
Ratio	4	5	2	1

Empirical formula = $\mathbf{C_4H_5N_2O}$

Molecular weight of empirical formula = 97; M^+ = 194, therefore molecular formula = $\mathbf{C_8H_{10}N_4O_2}$

Unknown C

(1,4-dichlorobenzene)

	C	H	Cl
Mass in 100 g	49.02	2.74	48.23
Moles in 100 g	4.09	2.74	1.36
Ratio	3	2	1

Empirical formula = $\mathbf{C_3H_2Cl}$

Molecular weight of empirical formula = 73.5; M^+ = 146/148/150, therefore molecular formula = $\mathbf{C_6H_4Cl_2}$

BONUS MARK – The mass spectrum of unknown C appears to have three molecular ion peaks owing to the common isotopes of Cl, ^{35}Cl and ^{37}Cl which are found naturally in a 3:1 ratio. As the unknown contains two chlorine atoms, this results in three possible combinations of these isotopes in the molecule.

Chlorine Isotopes in unknown C	Molecular weight of molecule containing these isotopes	Probability
^{35}Cl : ^{35}Cl	146	3 × 3 = 9
^{35}Cl : ^{37}Cl	148	3 × 1 = 3
^{37}Cl : ^{35}Cl	148	1 × 3 = 3
^{37}Cl : ^{37}Cl	150	1 × 1 = 1

(3 + 3 = 6)