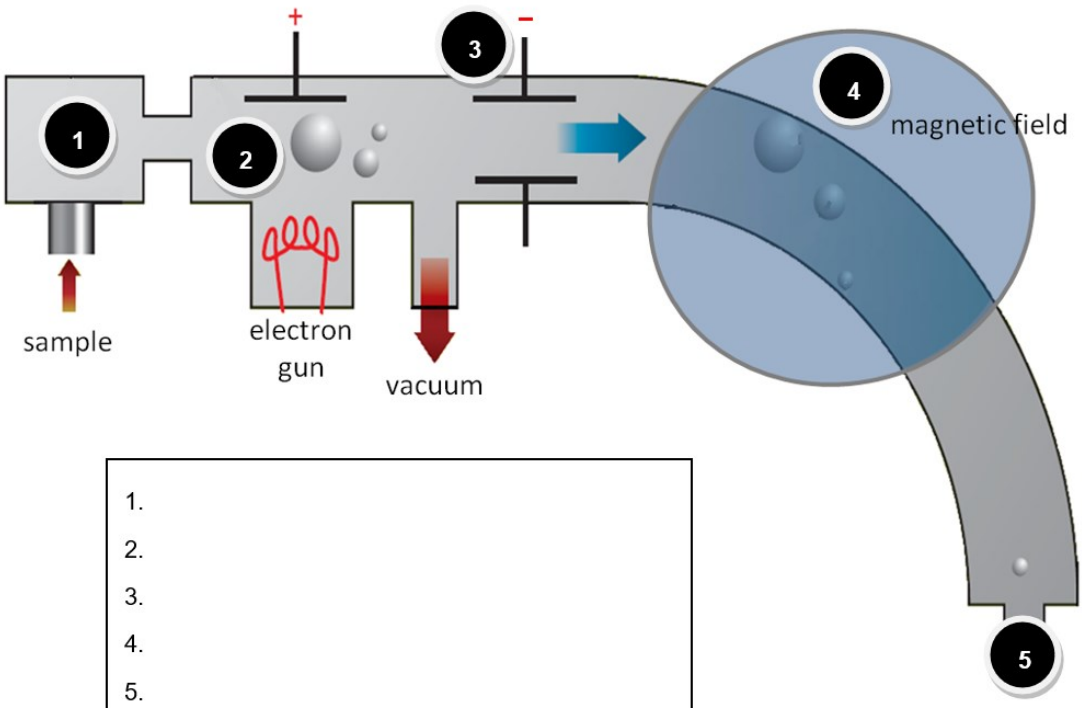
Analysis

Mass spectrometry

The mass spectrometer

1. The diagram below shows a simple mass spectrometer. Name the processes that occur at each of the points 1 - 5 highlighted;

(5 marks)



1.
2.
3.
4.
5.

2. For each of the statements below, indicate with the appropriate number, the stage in the mass spectrometer at which that process occurs. The first one has been done for you.

(5 marks)

Statement	Stage
The atoms are turned into ions	*2*
The ions are deflected. The size of the deflection depends upon the ratio of the ion's mass to its charge.	
A current is generated the size of which is proportional to the abundance of each ion	
$X(l) \rightarrow X(g)$	
The positive ions are attracted towards negatively charged plates	
$X(g) \rightarrow X^{+}(g)$	

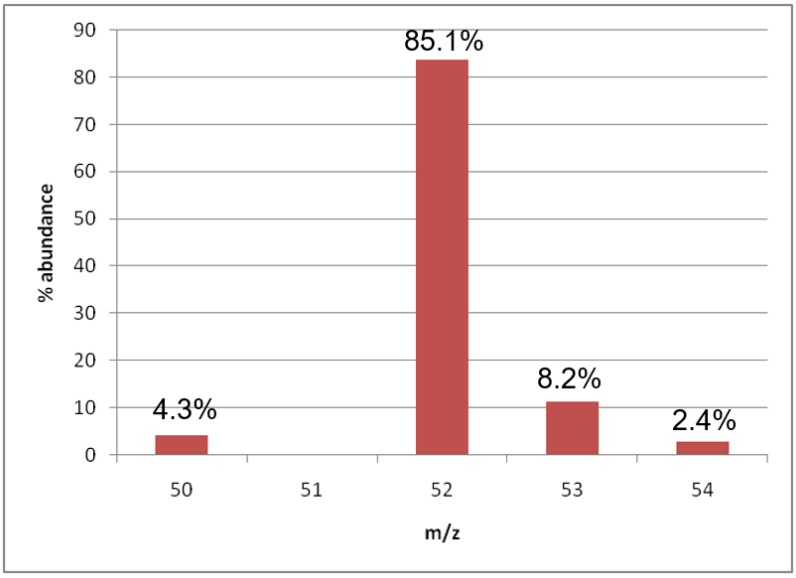
Isotopic abundance

1. The ratio of the different isotopes of certain elements can be used to identify objects from outer space. By comparing the isotope patterns with samples known to originate on earth the scientists can determine the origins of unknown objects.

The mass spectrum opposite is of a sample of chromium extracted from a rock recently found in the Nevada desert. Scientists believe it may be from a meteor.

Use the mass spectrum to determine the relative atomic mass of the chromium in the rock. Based on your result, make a recommendation as to the origin of the rock sample.

(3 marks)



2. The data below gives the *m/z* ratio and relative abundance of different isotopes of an element X. Determine the relative atomic mass of the element X to 1 d.p. Suggest an identity for X.

(4 marks)

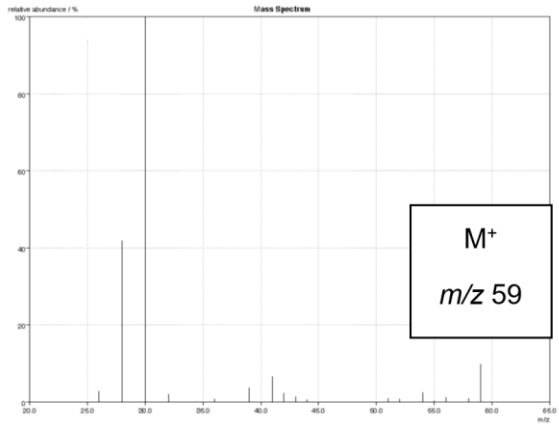
3. The element magnesium (relative atomic mass 24.3) has three naturally occurring isotopes, $^{24.0}$Mg, $^{25.0}$Mg and $^{26.0}$Mg. If the percentage of the heaviest isotope is 11.0%, what is the percentage of the lightest isotope present?

(3 marks)

Molecular mass spectrometry

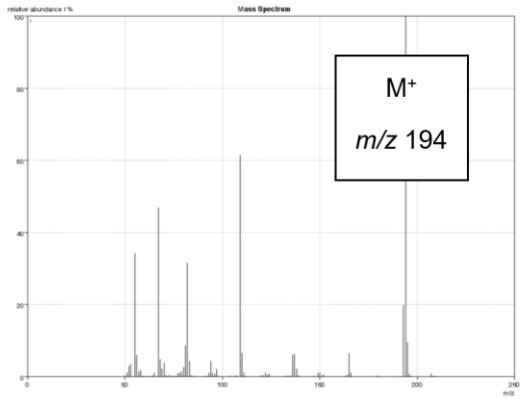
Use the elemental analysis data together with the mass spectrum to propose a molecular formula for the unknowns A to C. Easy!

(3 marks for each)



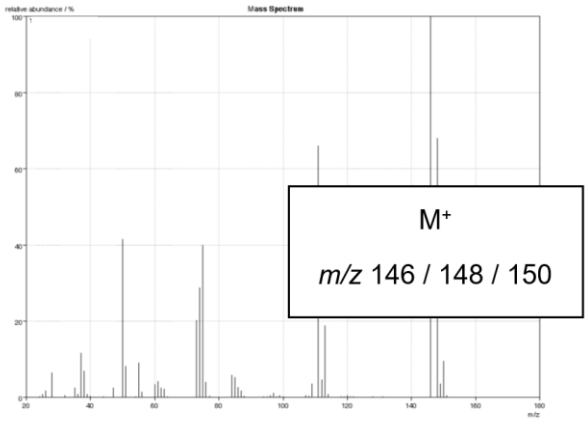
Unknown A

C 61.02%; H 15.25%; N 23.73%



Unknown B

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



Unknown C

C 49.02%; H 2.74%; Cl 48.23%

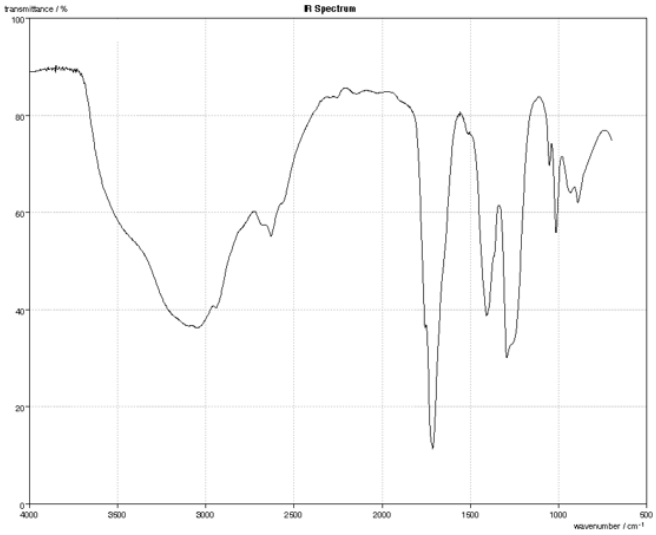
BONUS MARK Why does unknown C appear to have three molecular ions each differing in mass by 2?

(1 mark)

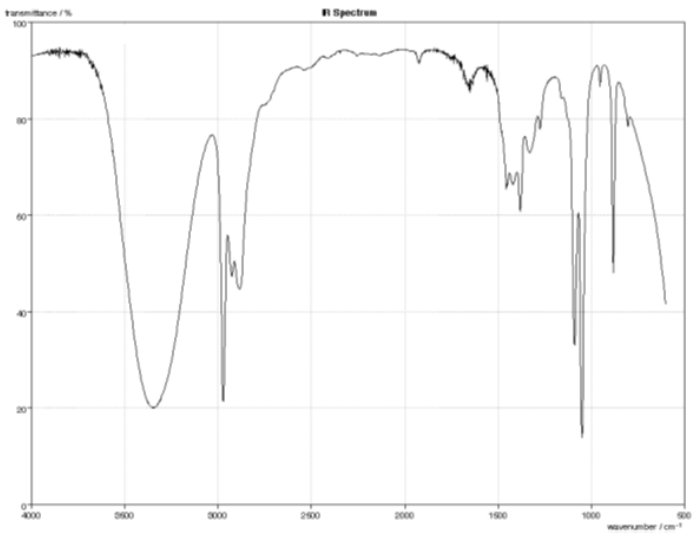
Infra-red spectroscopy

Help! The computer has gone crazy and mixed up all my spectra. Can you use the infra-red spectra together with the empirical formula to help me identify the compounds A - D below;

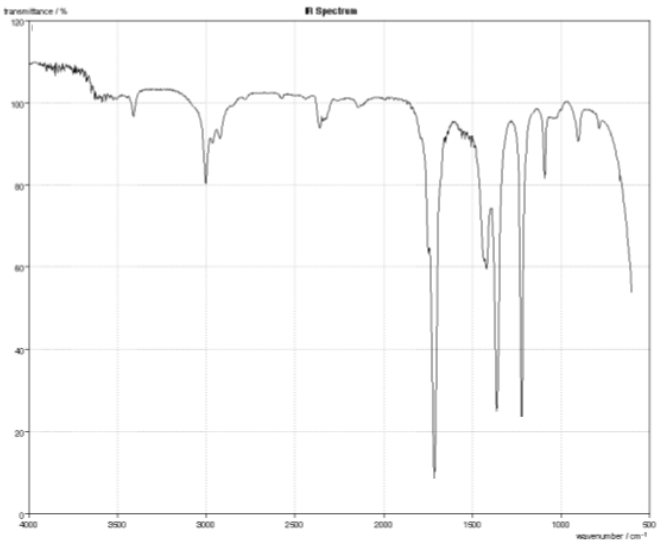
Compound A, $C_2H_4O_2$



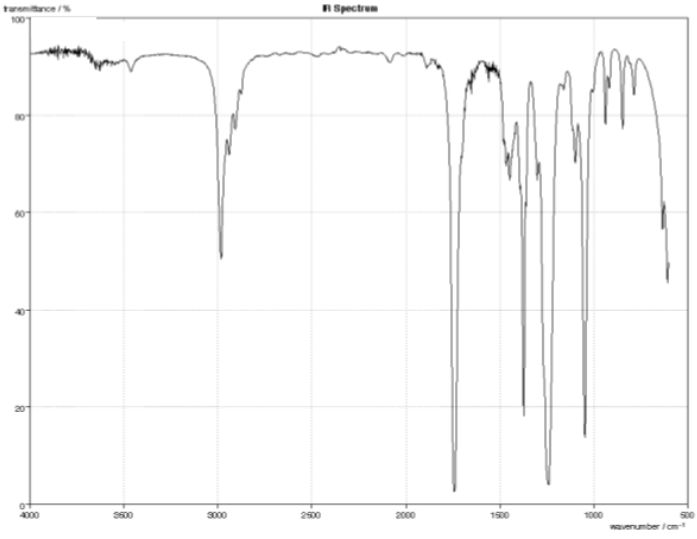
Compound B, C_2H_6O



Compound C, Empirical formula C_3H_6O



Compound D, Empirical formula $C_4H_8O_2$



BONUS MARKS

There is more than one possible structure for **compounds C** and **D**. Can you suggest an alternative structure for each which is still compatible with the infra-red spectrum provided?

Analysis – Answers

Mass spectrometry

The mass spectrometer

1.

1. vaporisation
2. ionisation
3. acceleration
4. deflection
5. detection

(5 marks)

2.

Statement	Stage
The atoms are turned into ions	*2*
The ions are deflected. The size of the deflection depends upon the ratio of the ion's mass to its charge.	**4**
A current is generated the size of which is proportional to the abundance of each ion	**5**
$X(l) \rightarrow X(g)$	**1**
The positive ions are attracted towards negatively charged plates	**3**
$X(g) \rightarrow X^{+}(g)$	**2**

(5 marks)

Isotopic abundance

1.

$$\frac{(4.3\% \times 50) + (85.1\% \times 52) + (8.2\% \times 53) + (2.4\% \times 54)}{100\ \%} = \mathbf{52.0}$$

(2 marks)

2.

$$\frac{(2.7 \times 204) + (46.0 \times 206) + (42.2 \times 207) + (100 \times 208)}{(2.7 + 46.0 + 42.2 + 100.0)} = \mathbf{207.2}$$

(2 marks)

(1 d.p. 1 mark)

Based on its atomic mass, X is likely to be **Pb, lead** (1 mark)

3.

If there is 11% of the heaviest isotope present we can say that the percentage of the lightest isotope present is 'y' and therefore the percentage of the remaining isotope present must be;

100% - 11% - y% = 89% - y

(1 mark)

Therefore substituting these numbers into our equation;

$$\frac{(26 \times 11\%) + (24 \times y\%) + [25 \times (89 - y)\%]}{100\ \%} = 24.3$$

286.0 + 24 y% + 2225 – 25 y% = 2430
2511 – y% = 2430
81 = y%

(1 mark each)

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

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 } = 6
^{37}Cl : ^{35}Cl	148	1 × 3 = 3 }
^{37}Cl : ^{37}Cl	150	1 × 1 = 1

Infra-red spectroscopy

Compound A = **ethanoic acid**

(1 mark for molecule with C-H, O-H and C=O, 1 mark for correct structure)

Compound B = **ethanol**

(1 mark for molecule with C-H and O-H, 1 mark for correct structure)

Compound C = **propanone**

(1 mark for molecule with C-H and C=O, 1 mark for correct structure)

Compound D = **ethyl ethanoate**

(1 mark for molecule with C-H and C=O, 1 mark for correct structure)

Possible alternative structures for;

Compound C = propanal

(1 mark)

Compound D = methyl propanoate, propyl methanoate or *iso*-propyl methanoate

(1 mark)