Structure 1.2 HL

IB CHEMISTRY HL

25	16		6	2	25
Mn	S	J	C	He	Mn
Manganese	Sulfur		Carbon	Helium	Manganese
54.938045	32.065		12.0107	4.002602	54.938045

Structure 1.2.3

Understandings:

- Mass spectra are used to determine the relative atomic masses of elements from their isotopic composition.

Learning outcomes:

- Interpret mass spectra in terms of identity and relative abundance of isotopes.

Additional notes:

- Relative masses and charges of the subatomic particles should be known; actual values are given in the data booklet. The mass of the electron can be considered negligible.

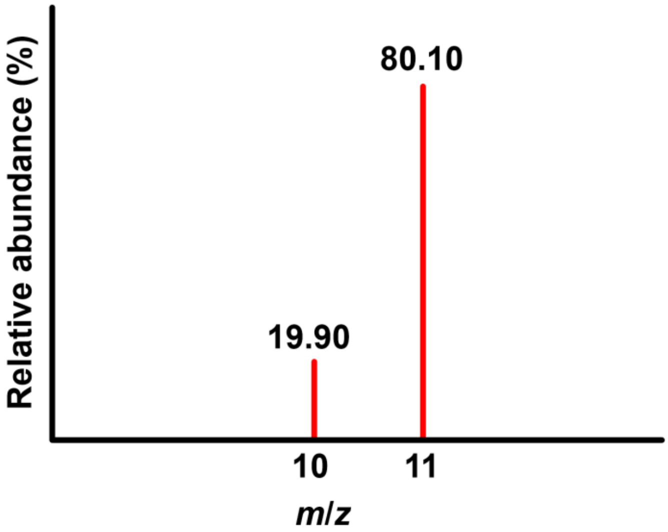
Linking questions:

- Structure 3.2—How does the fragmentation pattern of a compound in the mass spectrometer help in the determination of its structure?

Mass spectra of elements

- A mass spectrum shows relative abundance (or relative intensity) on the *y*-axis and mass to charge ratio (*m*/*z*) on the *x*-axis.
- Relative abundance is the percentage of an isotope in a naturally occurring sample of the element.
- Mass to charge ratio (*m*/*z*) is the relative mass of an ion divided by its charge – it tells us the mass of the ion and therefore the mass of the isotope.

Mass spectrum of boron showing relative abundance (%)



- The mass spectrum shows two peaks at *m*/*z* 10 and *m*/*z* 11 with abundances of 80.10 % and 19.90 % respectively.
- These correspond to the two isotopes of boron, ^{10}B and ^{11}B.

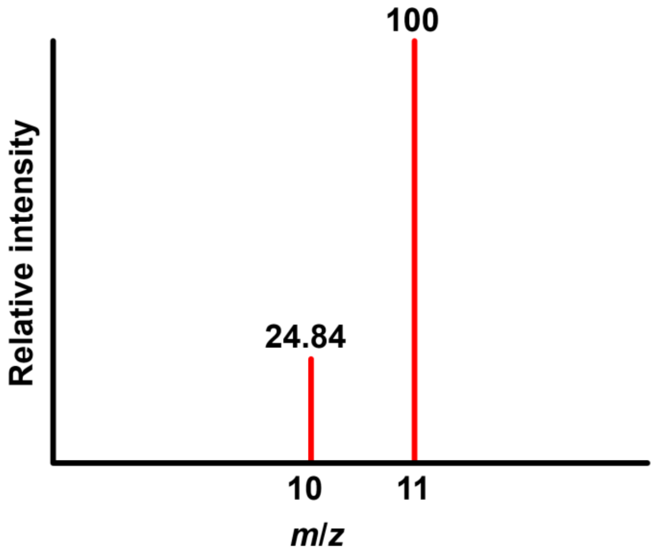
Isotope	*m*/*z*	Relative abundance (%)
^{10}B	10	19.90
^{11}B	11	80.10

- The relative atomic mass, A_r, can be calculated as follows:

$$A_r = \frac{(10\times19.90)+(11\times80.10)}{100} = 10.80$$

Mass spectrum of boron showing relative intensities

- Relative intensity is the amount of an ion produced in relation to the most abundant ion (the base peak) which is assigned a relative intensity of 100.



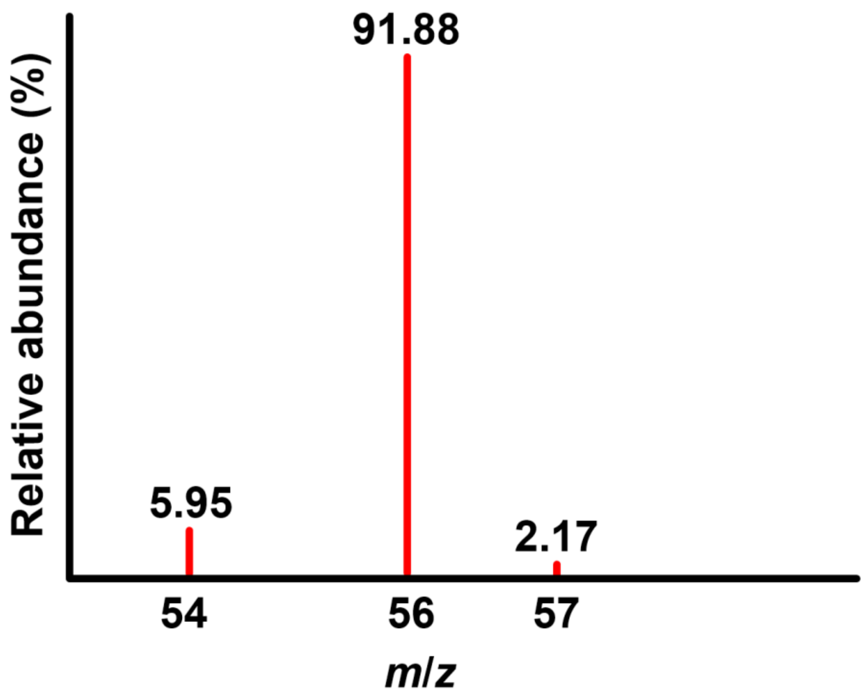
- The base peak is for the ion $^{11}B^{+}$ as it has the highest abundance and the highest intensity.
- To calculate the intensity of the $^{10}B^{+}$ ion, divide 100 by 80.10 and multiply by the % abundance (100 / 80.10 × 19.90 = 24.84).

Isotope	*m*/*z*	Relative intensity
^{10}B	10	24.84
^{11}B	11	100

- The relative atomic mass, A_r, can be calculated as follows:

$$A_r = \frac{(10 \times 24.84) + (11 \times 100)}{(24.84 + 100)} = 10.80$$

Exercise: The mass spectrum for iron, Fe, is shown. Complete the table below and calculate the relative atomic mass, A_r, of iron.

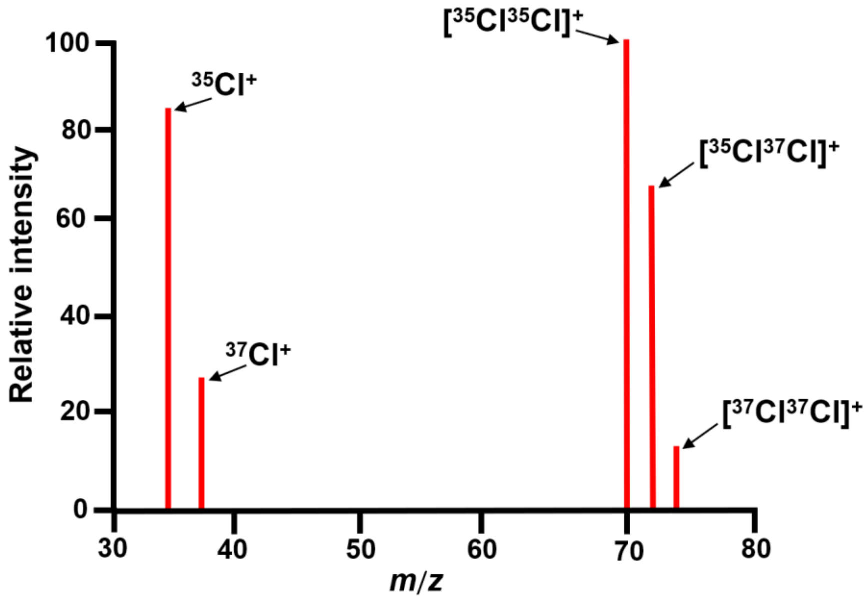


Isotope	Relative abundance (%)
^{54}Fe	5.95
^{56}Fe	91.88
^{57}Fe	2.17

$$A_r = \frac{(54 \times 5.95) + (56 \times 91.88) + (57 \times 2.17)}{100} = 55.90$$

Mass spectra of diatomic elements

Mass spectrum of chlorine, Cl_2



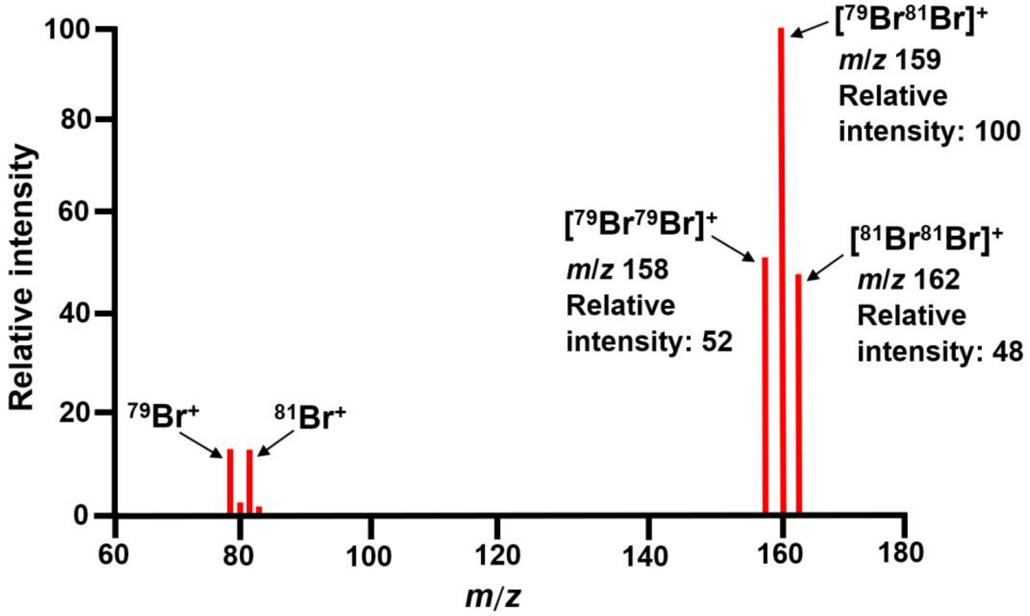
- Chlorine has two isotopes, ^{35}Cl and ^{37}Cl, with abundances of 75 % and 25 % respectively (3:1 ratio).
- The $^{35}Cl^+$ and $^{37}Cl^+$ ions occur in a 3:1 ratio.
- The molecular ions are shown in the table together with their relative intensities and ratios.

Molecular ions	m/z	Relative intensities (%)	Ratio
$[^{35}Cl^{35}Cl]^+$ *or* $[^{35}Cl_2]^+$	70	100	9
$[^{37}Cl^{35}Cl]^+$	72	66.67	6
$[^{37}Cl^{37}Cl]^+$ *or* $[^{37}Cl_2]^+$	74	11.11	1

- Using the relative intensities, the relative formula mass of chlorine, Cl_2, can be calculated.

$$M_{\mathrm{r}} = \frac{(70\times100) + (72\times66.67) + (74\times11.11)}{(100 + 66.67 + 11.11)} = 71.00$$

Exercise: Using the mass spectrum shown, calculate the relative formula mass of bromine, Br_2.



$$M_r = \frac{(158\times52) + (159\times100) + (162\times48)}{(52 + 100 + 48)} = 159.46$$