

1 Atoms, molecules and stoichiometry

This topic illustrates how quantitative relationships can be established when different substances react. (The term relative formula mass or Mr will be used for all compounds including ionic.)

- 1.1 Relative masses of atoms and molecules
- 1.3 The determination of relative atomic masses, Ar

2 Atomic structure

- 2.1 Particles in the atom
- 2.2 The nucleus of the atom

ATOMIC STRUCTURE

Physical chemistry

1 Atoms, molecules and stoichiometry

This topic illustrates how quantitative relationships can be established when different substances react.
(The term *relative formula mass* or M_r will be used for all compounds including ionic.)

Learning outcomes

Candidates should be able to:

1.1 Relative masses of atoms and molecules

- a) define and use the terms *relative atomic*, *isotopic*, *molecular* and *formula masses*, based on the ^{12}C scale

1.2 The mole and the Avogadro constant

- a) define and use the term *mole* in terms of the Avogadro constant

1.3 The determination of relative atomic masses, A_r

- a) analyse mass spectra in terms of isotopic abundances
(knowledge of the working of the mass spectrometer is not required)
- b) calculate the relative atomic mass of an element given the relative abundances of its isotopes, or its mass spectrum

1.4 The calculation of empirical and molecular formulae

- a) define and use the terms *empirical* and *molecular formula*
- b) calculate empirical and molecular formulae, using combustion data or composition by mass

1.5 Reacting masses and volumes (of solutions and gases)

- a) write and construct balanced equations
- b) perform calculations, including use of the mole concept, involving:
 - (i) reacting masses (from formulae and equations)
 - (ii) volumes of gases (e.g. in the burning of hydrocarbons)
 - (iii) volumes and concentrations of solutions

When performing calculations, candidates' answers should reflect the number of significant figures given or asked for in the question. When rounding up or down, candidates should ensure that significant figures are neither lost unnecessarily nor used beyond what is justified (see also Practical Assessment, Paper 3, Display of calculation and reasoning on page 52)

- c) deduce stoichiometric relationships from calculations such as those in 1.5(b)

2 Atomic structure

This topic describes the type, number and distribution of the fundamental particles which make up an atom and the impact of this on some atomic properties.

Learning outcomes

Candidates should be able to:

2.1 Particles in the atom

- a) identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses
- b) deduce the behaviour of beams of protons, neutrons and electrons in electric fields
- c) describe the distribution of mass and charge within an atom
- d) deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers and charge

2.2 The nucleus of the atom

- a) describe the contribution of protons and neutrons to atomic nuclei in terms of proton number and nucleon number
- b) distinguish between isotopes on the basis of different numbers of neutrons present
- c) recognise and use the symbolism x_yA for isotopes, where x is the nucleon number and ${}_y$ is the proton number

WHAT WE KNOW ABOUT ATOMS

Atoms are mostly empty space!

Atoms have 2 **charged** particles:

- Positively charged **protons**.
- Negatively charged **electrons**.

Atoms have 1 **uncharged** particle called a **neutron**.

The total number of protons, neutrons and electrons in any one atom determines its properties.

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WHAT WE KNOW ABOUT ATOMS

the **nucleus** is very small;
it contains the **protons**
and the **neutrons**

most of the volume
of the atom is occupied
by the **electrons**

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THE STRUCTURE OF ATOMS

| | Mass / g | Charge / C | Relative mass | Relative charge |
|-----------------|-------------------------|-------------------------|------------------|-----------------|
| PROTON | 1.672×10^{-24} | 1.602×10^{-19} | 1 | +1 |
| NEUTRON | 1.675×10^{-24} | 0 | 1 | 0 |
| ELECTRON | 9.109×10^{-28} | 1.602×10^{-19} | $\frac{1}{1836}$ | -1 |

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EXAMPLE

Calculate the mass of a carbon-12 atom.

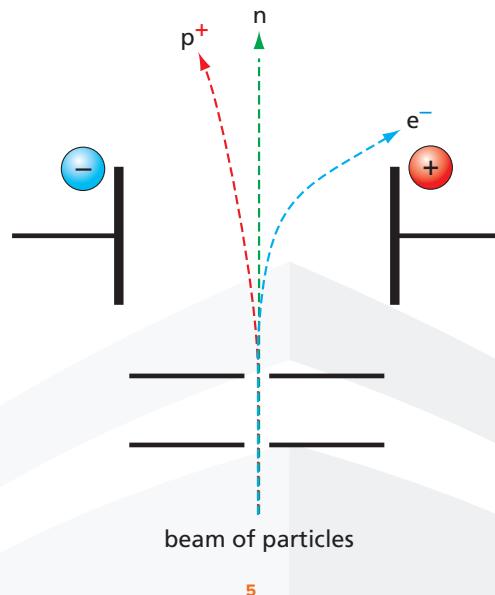
A neutral ^{12}C atom has 6 protons, 6 neutrons, and 6 electrons.

Therefore, its mass is:

$$(6 \times 1.672 \times 10^{-24}) + (6 \times 1.675 \times 10^{-24}) + (6 \times 9.109 \times 10^{-28}) \\ = 2.0089 \times 10^{-23} \text{ g}$$

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BEHAVIOUR OF SUB ATOMIC PARTICLES

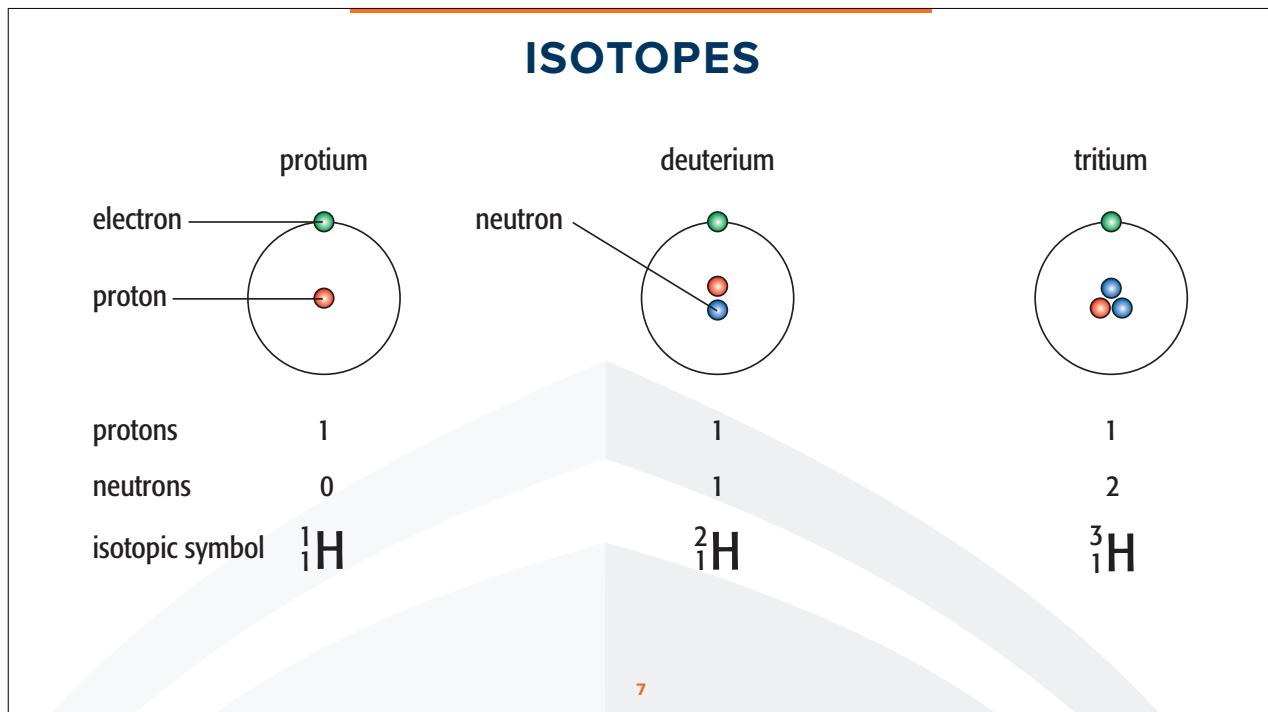


ISOTOPES

Isotopes are atoms with:

- the same number of protons and electrons but different number of neutrons.
- the same atomic number but different mass number

Chemical properties of isotopes are identical, whereas, physical properties (such as density) can differ.



ISOTOPES

| Isotope | Mass relative to hydrogen | Relative abundance |
|--------------|---------------------------|--------------------|
| boron-10 | 10.0 | 20% |
| boron-11 | 11.0 | 80% |
| neon-20 | 20.0 | 91% |
| neon-22 | 22.0 | 9% |
| magnesium-24 | 24.0 | 79% |
| magnesium-25 | 25.0 | 10% |
| magnesium-26 | 26.0 | 11% |

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RELATIVE MASSES

The ^{12}C (carbon-12) isotope is chosen as a standard and given a relative mass of exactly 12.

Important relative masses measured against this standard are:

Relative Atomic Mass (A_r)

The relative atomic mass (A_r) of an element is the weighted average mass of the naturally occurring isotopes of the element relative to one-twelfth the mass of the Carbon-12 isotope.

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RELATIVE MASSES

Relative Isotopic Mass

The relative isotopic mass of an element is the mass of an atom of the isotope of the element relative to one twelfth of the mass of an atom of the isotope carbon-12.

Relative Molecular Mass (M_r)

The relative molecular mass (M_r) of a compound is the mass of a molecule of that compound relative to one-twelfth the mass of the Carbon-12 isotope.

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RELATIVE MASSES

Relative Formula Mass

Used for ionic compounds and any formula of a species or ion e.g. NaCl or OH⁻ etc...

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SKILL CHECK 1

A How many protons, electrons and neutrons are present in a sulphide ion, S²⁻? Sulphur has atomic number 16 and mass number 32.

B How many protons, neutrons and electrons are present in a potassium ion, K⁺? Potassium has atomic number 19 and mass number 39.

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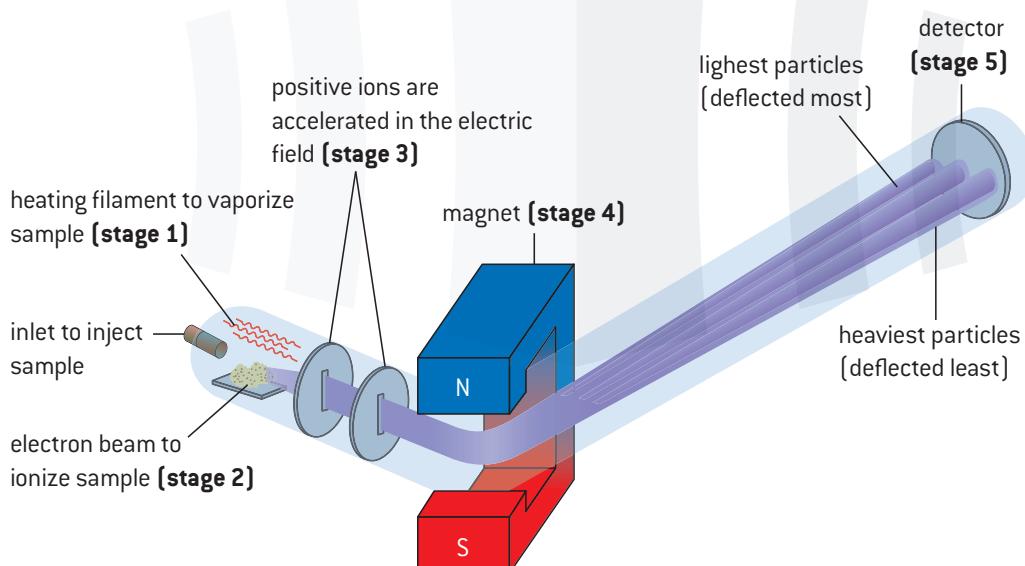
MASS SPECTROMETER

A **mass spectrometer** is used to calculate the **relative atomic mass** of an atom by comparing it with the mass of a ^{12}C atom.

You can also use a mass spectrometer to calculate the **relative abundance** of different **isotopes** of any element.

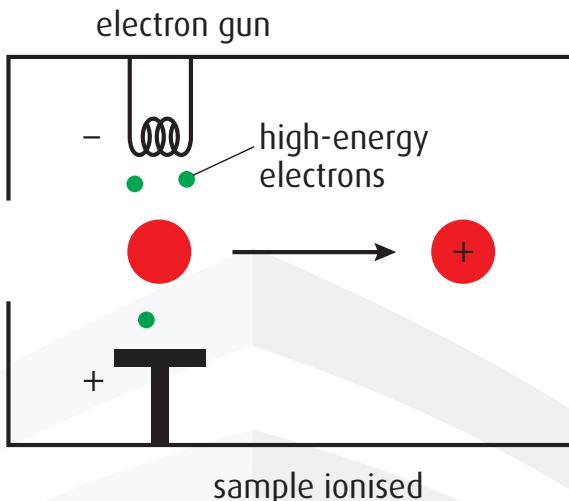
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HOW DOES A MASS SPECTROMETER WORK?



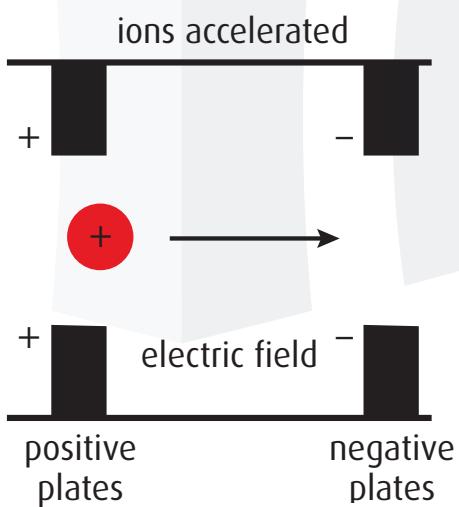
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HOW DOES A MASS SPECTROMETER WORK?



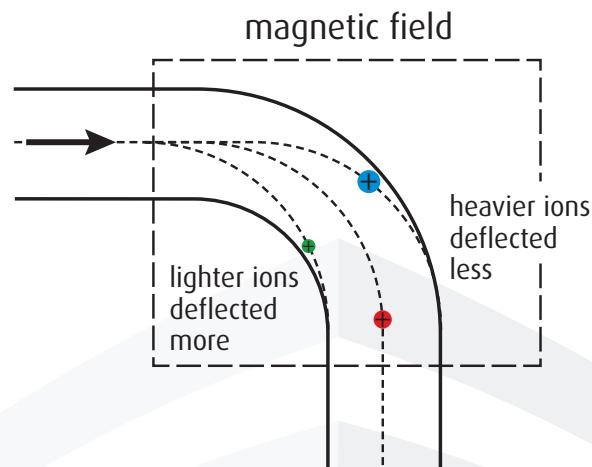
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HOW DOES A MASS SPECTROMETER WORK?



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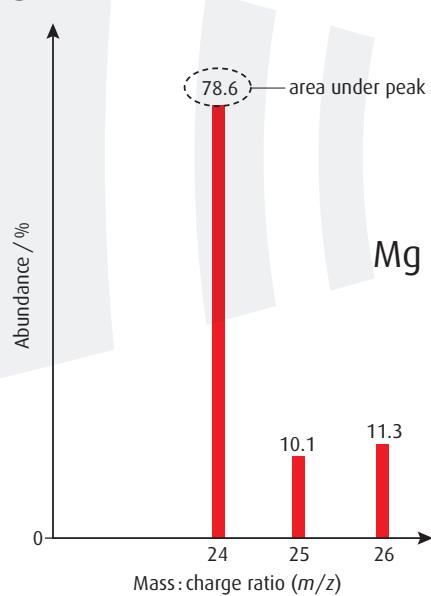
HOW DOES A MASS SPECTROMETER WORK?



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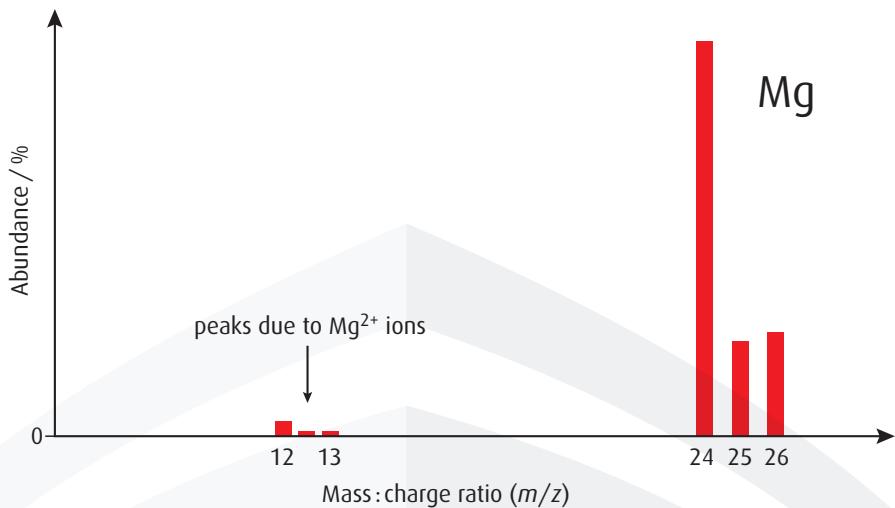
MASS SPECTRA

The mass spectrum is a plot of **relative abundance** (of each isotope) versus **m/e** or the **mass number**. The height of each peak indicates the relative abundance of the respective isotope.



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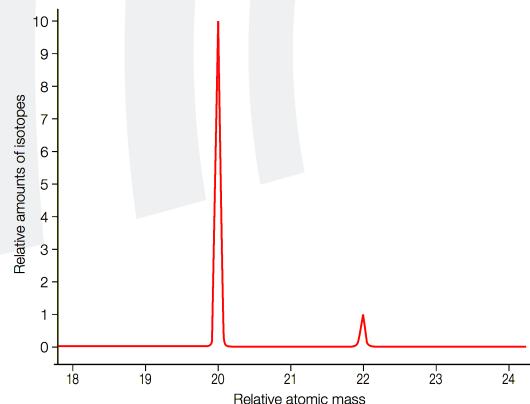
MASS SPECTRA



SKILL CHECK 2

The graph shows the mass spectrum of Neon.

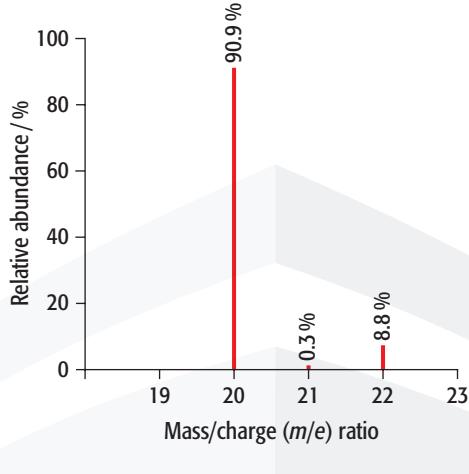
1. How many isotopes does Neon contain?
2. What are the relative isotopic masses of the isotopes of Neon?
3. What are the relative amounts of the isotopes of Neon?



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SKILL CHECK 3

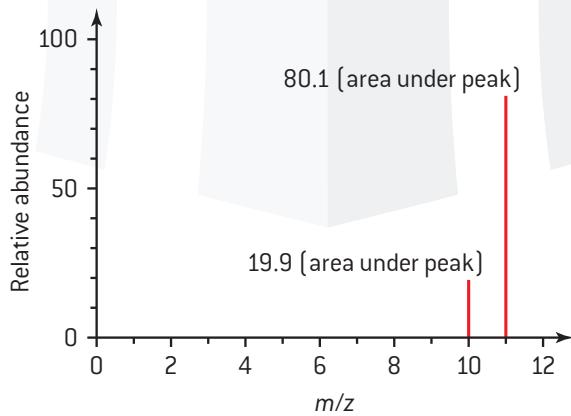
Calculate the average relative atomic mass of neon using the information below:



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SKILL CHECK 4

Calculate the average relative atomic mass of an element producing the following peaks in its mass spectrum:



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SKILL CHECK 5

Boron has two naturally occurring isotopes with the natural abundances shown. Calculate Boron's relative atomic mass.

| ISOTOPE | NATURAL ABUNDANCE (%) |
|-----------------|-----------------------|
| ^{10}B | 19.9 |
| ^{11}B | 80.1 |

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SKILL CHECK 6

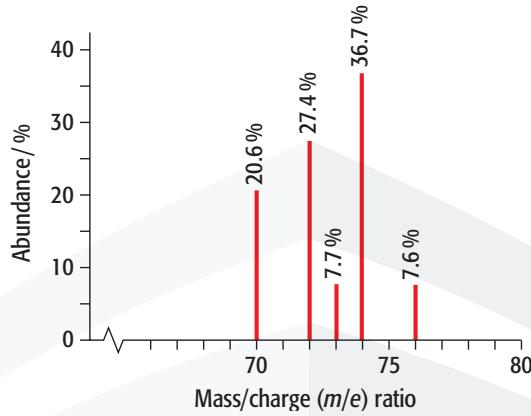
Calculate the average relative atomic mass of lead using the information below:

| Isotopic mass | Relative abundance/% |
|---------------|----------------------|
| 204 | 2 |
| 206 | 24 |
| 207 | 22 |
| 208 | 52 |

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SKILL CHECK 7

Calculate the average relative atomic mass of Germanium using the information below:



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MASS SPECTRA: CALCULATING ABUNDANCE

Naturally occurring potassium consists of potassium-39 and potassium-41. Calculate the percentage of each isotope present if the average is 39.1:

Assume there are x nuclei of ^{39}K in every 100, so there will be $(100 - x)$ of ^{41}K

This means that:

$$\frac{39x + 41(100 - x)}{100} = 39.1$$

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MASS SPECTRA: CALCULATING ABUNDANCE

$$\text{therefore } 39x + 4100 - 41x = 3910$$

$$\text{thus } -2x = -190$$

$$x = 95$$

There will be 95% ^{39}K and 5% ^{41}K !

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SKILL CHECK 8

Silver has two isotopes. 51.35% of the atoms are Silver-107 and 48.65% of the atoms are Silver-109. Calculate the relative atomic mass of Silver.

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SKILL CHECK 9

The relative atomic mass of copper is 63.5. Calculate the relative abundance of the two copper isotopes with relative isotopic masses of 63.0 and 65.0

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SKILL CHECK 10

Silver has two isotopes. 51.35% of the atoms are Silver-107 and 48.65% of the atoms are Silver-109. Calculate the relative atomic mass of Silver.

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SKILL CHECK 11

A sample of element X contains 69% of ^{63}X and 31% of ^{65}X . What is the relative atomic mass of X in this sample?

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SKILL CHECK 12

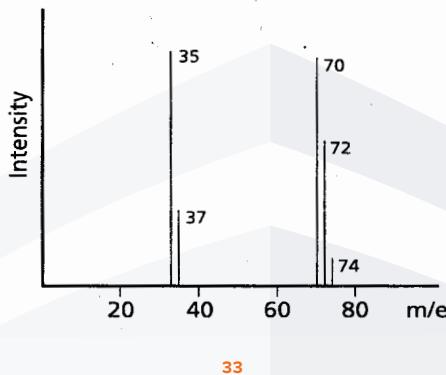
A sample of element X contains 69% of ^{63}X and 31% of ^{65}X . What is the relative atomic mass of X in this sample?

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MASS SPECTRA: MOLECULAR IONS

Molecules also give peaks in their mass spectrum.

For example the mass spectrum of chlorine gaseous molecule includes both peaks of its isotopes and peaks of its molecular form (molecular ions):



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MASS SPECTRA: MOLECULAR IONS

Cl_2^+ molecular ion produces three peaks:

peak at m/e @ 70: $^{35}\text{Cl} - ^{35}\text{Cl}$

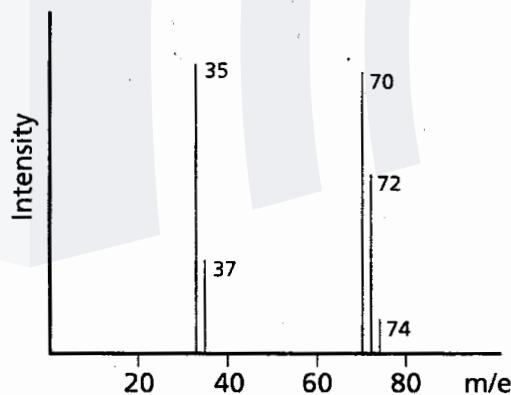
Species responsible: $^{70}\text{Cl}_2^+$

peak at m/e @ 72: $^{35}\text{Cl} - ^{37}\text{Cl}$

Species responsible: $^{72}\text{Cl}_2^+$

peak at m/e @ 74: $^{37}\text{Cl} - ^{37}\text{Cl}$

Species responsible: $^{74}\text{Cl}_2^+$



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