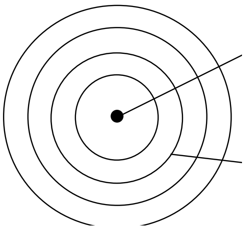
# SECTION 1 – Basics from GCSE

Atoms consist of a central **NUCLEUS** containing protons and **NEUTRONS**. The nucleus is **TINY** compared to the size of the whole atom. The nucleus is surrounded by **ELECTRONS** in energy levels (also called **SHELLS**). Atoms have no electric charge because they contain the same number of protons and **ELECTRONS**.

| sub-atomic particle | relative mass | relative charge |
|---|---|---|
| proton | **1** | **+1** |
| neutron | **1** | **0** |
| electron | **0.0005 or $\frac{1}{1836}$** | **-1** |



**Atomic number** = number of **PROTONS**

**Mass number** = number of **PROTONS** + number of **NEUTRONS**

The number of protons, neutrons and electrons in an atom can be worked out using the atomic number and mass number.

Number of protons = **ATOMIC NUMBER**

Number of neutrons = **MASS NUMBER - ATOMIC NUMBER**

Number of electrons = **ATOMIC NUMBER**

Atoms can be represented as follows:

${}^{\text{mass number}}_{\text{atomic number}}\text{Symbol}$ e.g. ${}^{19}_{9}\text{F}$ protons = **9** neutrons = **10** electrons = **9**

Atoms of the same element have the same number of **PROTONS.** In fact, it is the number of **PROTONS** that determines what type of atom it is (e.g. all atoms with 6 protons are carbon atoms). Atoms of different elements have different numbers of **PROTONS**.

**Isotopes** are atoms with the same number of **PROTONS** but a different number of **NEUTRONS** . This means they are atoms of the same **ELEMENT** with the same **ATOMIC** number but a different **MASS** number.

| | ${}^{35}_{17}\text{Cl}$ | ${}^{37}_{17}\text{Cl}$ |
|---|---|---|
| protons | **17** | **17** |
| neutrons | **18** | **20** |
| electrons | **17** | **17** |

Ions are charged particles with an unequal number of **PROTONS** and **ELECTRONS**.

Most ions have stable electron structures with the same electron structure as the elements in Group **0/8/18**.

Negative ions have **MORE** electrons than protons.

Positive ions have **FEWER** electrons than protons.

## TASK 1 – Atoms and ions

| Species | Atom / ion | Atomic number | Mass number | Number of protons | Number of neutrons | Number of electrons |
|---|---|---|---|---|---|---|
| $^{14}_{7}\text{N}$ | atom | **7** | **14** | **7** | **7** | **7** |
| $^{31}_{15}\text{P}$ | atom | **15** | **31** | **15** | **16** | **15** |
| $^{7}_{3}\text{Li}$ | atom | 3 | 7 | **3** | **4** | **3** |
| $^{20}_{10}\text{Ne}$ | atom | 10 | **20** | **10** | 10 | **10** |
| $^{40}_{20}\text{Ca}$ | atom | **20** | 40 | 20 | **20** | **20** |
| $^{40}_{18}\text{Ar}$ | atom | **18** | 40 | **18** | 22 | **18** |
| $^{9}_{4}\text{Be}$ | atom | **4** | **9** | 4 | 5 | **4** |
| $^{208}_{82}\text{Pb}$ | atom | 82 | **208** | **82** | 126 | **82** |
| $^{79}_{35}\text{Br}$ | atom | 35 | **79** | **35** | 44 | **35** |
| $^{81}_{35}\text{Br}$ | atom | 35 | **81** | **35** | 46 | **35** |
| $^{23}_{11}\text{Na}^{+}$ | **ion** | **11** | **23** | **11** | **12** | **10** |
| $^{16}_{8}\text{O}$ | **atom** | **8** | **16** | **8** | **8** | **8** |
| $^{16}_{8}\text{O}^{2-}$ | **ion** | **8** | **16** | **8** | **8** | **10** |
| $^{35}_{17}\text{Cl}^{-}$ | **ion** | 17 | 35 | **17** | **18** | 18 |
| $^{39}_{19}\text{K}$ | **atom** | 19 | **39** | **19** | 20 | 19 |
| $^{39}_{19}\text{K}^{+}$ | **ion** | 19 | **39** | **19** | 20 | 18 |
| $^{40}_{20}\text{Ca}^{2+}$ | **ion** | **20** | **40** | 20 | 20 | 18 |
| $^{1}_{1}\text{H}^{+}$ | **ion** | 1 | **1** | **1** | 0 | 0 |
| $^{127}_{53}\text{I}^{-}$ | **ion** | 53 | **127** | **53** | 74 | 54 |
| $^{14}_{7}\text{N}^{3-}$ | **ion** | **7** | 14 | **7** | 7 | 10 |

## TASK 2 – Identify the particle

In each case identify the particle. The first one has been done for you.

| | |
|---|---|
| 1 An atom with 6 protons and the same number of neutrons as a $^{14}N$ atom | ${}^{13}_{6}\mathrm{C}$ |
| 2 An atom with one more proton and the same number of neutrons than an atom of $^{39}K$ | ${}^{40}_{20}\mathrm{Ca}$ |
| 3 An atom with 10 protons and the same number of neutrons as an atom of $^{24}Mg$ | ${}^{22}_{10}\mathrm{Ne}$ |
| 4 An atom with one fewer proton and the same number of neutrons as an atom of $^{66}Zn$ | ${}^{65}_{29}\mathrm{Cu}$ |
| 5 An atom with the same number of protons and two more neutrons as an atom of $^{79}Br$ | ${}^{81}_{35}\mathrm{Br}$ |
| 6 An atom with two fewer protons and the same number of neutrons as an atom of $^{50}Cr$ | ${}^{48}_{22}\mathrm{Ti}$ |
| 7 An ion with one more proton and two more neutrons as an atom of $^{20}Ne$ but the same number of electrons | ${}^{23}_{11}\mathrm{Na}^{+}$ |
| 8 An ion with two fewer protons and two fewer neutrons as an atom of $^{40}Ar$ but the same number of electrons | ${}^{36}_{16}\mathrm{S}^{2-}$ |
| 9 An ion with two more protons and two more neutrons as an atom of $^{60}Ni$ but the same number of electrons | ${}^{64}_{30}\mathrm{Zn}^{2+}$ |
| 10 An ion with two more protons and three more neutrons as an atom of $^{20}Ne$ but the same number of electrons | ${}^{25}_{12}\mathrm{Mg}^{2+}$ |
| 11 An ion with one fewer proton, one fewer neutron and the same number of electrons as an atom of $^{129}Xe$. | ${}^{127}_{53}\mathrm{I}^{-}$ |
| 12 An ion with one more proton, two more neutrons, but the same number of electrons as an ion of $^{85}Rb^{+}$ | ${}^{88}_{38}\mathrm{Sr}^{2+}$ |
| 13 A particle with two fewer protons, two fewer neutrons and the same number of electrons as an atom of $^{20}Ne$ | ${}^{16}_{8}\mathrm{O}^{2-}$ |
| 14 A particle with one fewer proton, two fewer neutrons and one more electron as a $^{48}Ti^{2+}$ ion | ${}^{45}_{21}\mathrm{Sc}$ |
| 15 A particle with one fewer proton, two more neutrons and the same number of electrons as a $^{127}I^{-}$ ion | ${}^{128}_{52}\mathrm{Te}^{2-}$ |

# SECTION 2 – Development of atomic structure models

| | Atoms | Plum-pudding model | Nuclear model | | |
|---|---|---|---|---|---|
| lead scientist | John Dalton | JJ Thompson | Ernest Rutherford | Neils Bohr | James Chadwick |
| when | early 1800s | 1897 | 1911 | 1913 | 1932 |
| description of model | **atom was the smallest particle** | **a ball of solid positive charge with negative electrons spread throughout** | **atom has a tiny positive nucleus surrounded by mainly empty space in which electrons are moving** | **atom has a tiny positive nucleus surrounded by mainly empty space in which electrons are moving in energy levels (shells)** | **atom has a tiny positive nucleus containing protons and neutrons, surrounded by mainly empty space in which electrons are moving in energy levels (shells)** |
| what they discovered | | **electrons** | **the nucleus** | **electrons move in shells** | **neutrons in the nucleus** |
| what they did | | | **fired electrons at the thin piece of gold foil; a small proportion of alpha particles were deflected / bounced back** | | |

# SECTION 3 – Time of flight mass spectrometry

## TASK 3 – Relative atomic mass calculations

1) Find the relative atomic mass of the lithium using the data from mass spectrometry (give answer to 2 dp).

$^{6}$Li (7.4%) $^{7}$Li (92.6%) $$\frac{6(7.4)+7(92.6)}{7.4+92.6} = 6.93$$

2) The relative atomic mass of gallium is 69.72. It consists of two isotopes, $^{69}$Ga and $^{71}$Ga. Find the percentage composition by mass of these two isotopes in gallium.

$\text{let \% of } {}^{69}_{31}\text{Ga} = a$

$$69.72 = \frac{69a + 71(100 - a)}{100}$$

$6972 = 69a + 7100 - 71a$

$2a = 128$

$a = 64$ $\quad {}^{69}_{31}\text{Ga} = 64\% \quad {}^{71}_{31}\text{Ga} = 36\%$

3) The relative atomic mass of neon is 20.18. It consists of three isotopes, $^{20}$Ne, $^{21}$Ne and $^{22}$Ne. It contains 90.5% $^{20}$Ne. Find the percentage composition by mass of the other two isotopes in neon.

$let\ \%\ of\ {}^{21}_{10}\text{Ne} = b$

$therefore\ \%\ of\ {}^{22}_{10}\text{Ne} = (100 - 90.5) - b = 9.5 - b$

$$20.18 = \frac{20(90.5) + 21b + 22(9.5 - b)}{100}$$

$2018 = 1810 + 21b + 209 - 22b$

$b = 1.0$ $\quad {}^{21}_{10}\text{Ne} = 1.0\% \quad {}^{22}_{10}\text{Ne} = 8.5\%$

4) a) Calculate the relative atomic mass of lead given the mass spectroscopy data below. Give your answer to 2dp.

| m/z | 204 | 206 | 207 | 208 |
|---|---|---|---|---|
| relative intensity | 0.287 | 4.51 | 4.32 | 10.00 |

$$\frac{204(0.287) + 206(4.51) + 207(4.32) + 208(10.00)}{0.287 + 4.51 + 4.32 + 10.00} = 207.24$$

b) Identify the species responsible for the peak at *m/z* 208. ${}^{208}_{82}\text{Pb}^{+}$

c) Which ion will have the shortest time of flight and reach the detector fastest? ${}^{204}_{82}\text{Pb}^{+}$

5) Find the relative atomic mass of the following elements using the data from mass spectrometry (give answers to 2 dp).

a) gallium $^{69}$Ga (1.00) $^{71}$Ga (0.66) $$\frac{69(1.00)+71(0.66)}{1.00+0.66} = 69.80$$

b) iron $^{54}$Fe (5.8%) $^{56}$Fe (91.6%) $^{57}$Fe (2.2%) $^{58}$Fe (0.3%) $$\frac{54(5.8)+56(91.6)+57(2.2)+58(0.3)}{5.8+91.6+2.2+0.3} = 55.91$$

## Some ToF MS calculations examples

1) Calculate the time it takes an ion of ${}^{12}_{6}C^{+}$ to travel along a time of flight tube of length 80 cm given kinetic energy of 4.60 x $10^{-15}$ J

$$KE = \frac{mv^2}{2} = \frac{md^2}{2t^2}$$

$$t^2 = \frac{m\,d^2}{2\,KE}$$

$$t = \sqrt{\frac{m\,d^2}{2\,KE}} = \sqrt{\frac{\frac{0.012}{6.022\,x\,10^{23}}\;(0.80)^2}{2\,(4.60\,x\,10^{-15})}} = 1.2\text{ x }10^{-6}\text{ s (2sf)}$$

2) It takes the ${}^{16}_{8}O^{+}$ ion 1.37 x $10^{-5}$ s to travel along the flight tube in a time of flight mass spectrometer. How long would it take the ${}^{18}_{8}O^{+}$ ion to travel down the same flight tube under the same conditions?

$$KE = \frac{mv^2}{2} = \frac{md^2}{2t^2}$$

$$\text{isotope 16 } \frac{md^2}{2t^2} = \text{ isotope 18 } \frac{md^2}{2t^2}$$

$$\frac{mass(16)x\,d^2}{2\,time(16)^2} = \frac{mass(18)x\,d^2}{2\,time(18)^2}$$

we can cancel out the d$^2$ and the 2 $\frac{mass(16)}{time(16)^2} = \frac{mass(18)}{time(18)^2}$

$$time(18)^2 = \frac{mass(18)\;x\;time(16)^2}{mass(16)}$$

$$time(18) = time(16)\sqrt{\frac{mass(18)}{mass(16)}} = 1.37\,x\,10^{-5}\;x\;\sqrt{\frac{18}{16}} = 1.45\,x\,10^{-5}\;s$$

# TASK 4a – ToF MS calculations

1 It takes the ${}^{12}_{6}\mathrm{C}^{+}$ ion 1.23 x $10^{-5}$ s to travel along the flight tube in a time of flight mass spectrometer having been given 5.94 x $10^{-17}$ J of kinetic energy. Calculate the length of the flight tube.

$$KE = \frac{mv^2}{2} = \frac{md^2}{2t^2}$$

$$d^2 = \frac{2\ KE\ t^2}{m}$$

$$d = \sqrt{\frac{2\ KE\ t^2}{m}} = \sqrt{\frac{2\left(5.94\ x\ 10^{-17}\right)\left(1.23\ x\ 10^{-5}\right)^2}{\frac{0.012}{6.022\ x\ 10^{23}}}} = 0.95\ \mathrm{m}\ \ (2\mathrm{sf})$$

2 Find the time it takes the ${}^{7}_{3}\mathrm{Li}^{+}$ ion to travel down a 78 cm time of flight tube given 1.52 x $10^{-18}$ J of kinetic energy.

$$KE = \frac{mv^2}{2} = \frac{md^2}{2t^2}$$

$$t^2 = \frac{m\ d^2}{2\ KE}$$

$$t = \sqrt{\frac{m\ d^2}{2\ KE}} = \sqrt{\frac{\frac{0.007}{6.022\ x\ 10^{23}}\ (0.78)^2}{2\ (1.52\ x\ 10^{-18})}} = 4.8\ \mathrm{x}\ 10^{-5}\ \mathrm{s}\ (2\mathrm{sf})$$

3 It takes the ${}^{81}_{35}\mathrm{Br}^{+}$ ion 2.83 x $10^{-5}$ s to travel along the flight tube in a time of flight mass spectrometer. How long would it take the ${}^{79}_{35}\mathrm{Br}^{+}$ ion to travel down the same flight tube under the same conditions?

$$KE = \frac{mv^2}{2} = \frac{md^2}{2t^2}$$

$$\text{isotope 81}\ \frac{md^2}{2t^2} = \text{isotope 79}\ \frac{md^2}{2t^2}$$

$$\frac{mass(81) x\ d^2}{2\ time(81)^2} = \frac{mass(79) x\ d^2}{2\ time(79)^2}$$

**we can cancel out the d$^2$ and the 2** $\quad \dfrac{mass(81)}{time(81)^2} = \dfrac{mass(79)}{time(79)^2}$

$$time(79)^2 = \frac{mass(79)\ x\ \ time(81)^2}{mass(81)}$$

$$time(79) = time(81)\sqrt{\frac{mass(79)}{mass(81)}} = 2.83\ x\ 10^{-5}\ x\ \sqrt{\frac{79}{81}} = 2.79\ x\ 10^{-5}\ s$$

4 An ion takes 3.81 x $10^{-5}$ s to travel along the 85 cm flight tube in a time of flight mass spectrometer having been given 1.6 x $10^{-17}$ J of kinetic energy. Calculate the mass number of this ion.

$$KE = \frac{mv^2}{2} = \frac{md^2}{2t^2}$$

$$m = \frac{2\,KE\,t^2}{d^2}$$

$$m = \frac{2\left(1.6 \text{ x } 10^{-17}\right)\left(3.81 \text{ x } 10^{-5}\right)^2}{0.85^2} = 6.48 \text{ x } 10^{-26}\text{ kg}$$

$$mass\ of\ 1\ mole = 6.48 \text{ x } 10^{-26} \text{ x } 6.022 \text{ x } 10^{23} = 0.039\ kg$$

$$mass\ number = 39$$

5 The relative atomic mass of lithium is 6.924. It consists of two isotopes, $^{6}_{3}\text{Li}$ and $^{7}_{3}\text{Li}$. Find the percentage composition by mass of $^{6}_{3}\text{Li}$ in lithium.

$$let\ \%\ of\ ^{6}_{3}\text{Li} = a$$

$$6.924 = \frac{6a + 7(100 - a)}{100}$$

$$692.4 = 6a + 7(100 - a)$$

$$692.4 = 6a + 700 - 7a$$

$$a = 7.6$$

6 The relative atomic mass of silicon is 28.109. It consists of three isotopes, $^{28}_{14}\text{Si}$, $^{29}_{14}\text{Si}$ and $^{30}_{14}\text{Si}$. It contains 92.2% $^{28}_{14}\text{Si}$. Find the percentage composition by mass of $^{29}_{14}\text{Si}$ in silicon.

$$let\ \%\ of\ ^{29}_{14}\text{Si} = b$$

$$therefore\ \%\ of\ ^{30}_{14}\text{Si} = (100 - 92.2) - b = 7.8 - b$$

$$28.109 = \frac{28(92.2) + 29b + 30(7.8 - b)}{100}$$

$$2810.9 = 2581.6 + 29b + 234 - 30b$$

$$b = 4.7$$

# TASK 4b – ToF MS calculations

1) a) The mass of one mole of $^{18}O^+$ ions is 18.0 g. The Avogadro constant is 6.022 x $10^{23}$ mol$^{-1}$
Find the mass of a single ion of $^{18}O^+$ in kg.

**mass of one $^{18}O^+$ ion =** $\frac{0.018}{6.022\ x\ 10^{23}}$ **= 2.99 x $10^{-26}$ kg**

b) Find the time it takes an ion of $^{18}O^+$ to travel along a flight tube of 75.0 cm length if given 2.50 x $10^{-15}$ J of energy.

$$t = d\sqrt{\frac{m}{2KE}} = 0.75\sqrt{\frac{2.99?\ x\ 10^{-26}}{2\ x\ 2.50\ x\ 10^{-15}}} = 1.84 \text{ x } 10^{-6} \text{ s}$$

2) a) Calculate the relative atomic mass of chromium given the mass spectroscopy data below.

| m/z | 50 | 52 | 53 | 54 |
|---|---|---|---|---|
| relative abundance (%) | 4.3 | 83.8 | 9.5 | 2.4 |

$$\frac{50(4.3) + 52(83.8) + 53(9.5) + 54(2.4)}{4.3 + 83.8 + 9.5 + 2.4} = 52.06$$

b) Identify the species responsible for the peak at *m/z* 52. $^{52}_{24}Cr^+$

c) Which ion will have the shortest time of flight and reach the detector fastest? $^{50}_{24}Cr^+$

d) All the particles have the same kinetic energy (= ½ mv$^2$, where m = mass of particle and v = velocity) and the velocity of the particles is given by v = d/t (where d = distance travelled and t = time taken). If the time of flight of a $^{54}Cr^+$ ion is 1.486 x $10^{-5}$ s, calculate the time of flight of a $^{50}Cr^+$ ion. Give your answer to the appropriate number of significant figures.

$$\frac{mass(50)}{time(50)^2} = \frac{mass(54)}{time(54)^2}$$

$$time(50) = time(54)\sqrt{\frac{mass(50)}{mass(54)}} = 1.486\ x\ 10^{-5}\ x\sqrt{\frac{50}{54}} = 1.430\ x\ 10^{-5}\ s$$

3) It takes an ion 2.34 x $10^{-6}$ s to travel along a flight tube of length 50 cm having been given 8.35 x $10^{-16}$ J of kinetic energy. Find the mass number of this ion.

$$KE = \frac{mv^2}{2} = \frac{md^2}{2t^2}$$

$$m = \frac{2\ KE\ t^2}{d^2}$$

$$m = \frac{2\ (8.35 \text{ x } 10^{-16})\ (2.34 \text{ x } 10^{-6})^2}{0.50^2} = 3.66 \text{ x } 10^{-26} \text{ kg}$$

$$mass\ of\ 1\ mole = 3.66 \text{ x } 10^{-26} \text{ x } 6.022 \text{ x } 10^{23} = 0.022\ kg$$

$$mass\ number = 22$$

4) The mass spectrum of butanone shows its main peak at m/z 72. It also has a small signal at m/z 73.

a) Which ionisation technique is likely to have been used? **electron impact**

b) What is the relative formula mass of this compound? **72**

c) Give two reasons for the peak at m/z 73. **due to presence of $^{2}$H or $^{13}$C**

d) There would also be tiny peaks at m/z 74, 75, etc. Explain why some ions with these m/z values may be formed but why their signals may be too small to be seen.

**due to presence of more than one atom of $^{2}$H or $^{13}$C**

5) The mass spectrum of chloromethane ($CH_3Cl$) shows two main peaks at m/z 50 and m/z 52. (the main two isotopes of chlorine are $^{35}$Cl and $^{37}$Cl in the ratio 3:1)

a) Explain why these two peaks are produced. **due to $CH_3{}^{35}Cl^+$ and $CH_3{}^{37}Cl^+$**

b) Predict the relative intensity of these two signals. Explain your answer.

**3:1 as relative abundance of $^{35}$Cl : $^{37}$Cl = 3:1**

6) The element bromine is made of diatomic molecules. There are two isotopes of bromine, namely $^{79}$Br and $^{81}$Br of roughly equal abundance. Sketch what the time of flight mass spectrum of the element bromine will look like. (the main two isotopes of bromine are $^{79}$Br and $^{81}$Br in the ratio 1:1)

**3 peaks at 158, 160 and 162 in ratio 1:2:1**

7) Calculate the relative atomic mass of krypton given the mass spectroscopy data below.

| m/z | 78 | 80 | 82 | 83 | 84 | 86 |
|---|---|---|---|---|---|---|
| relative abundance (%) | 0.3 | 2.3 | 11.6 | 11.5 | 56.9 | 17.4 |

$$\frac{78(0.3)+80(2.3)+82(11.6)+83(11.5)+84(56.9)+86(17.4)}{0.3+2.3+11.6+11.5+56.9+17.4} = 83.89$$

# TASK 5 – Electron structure

| | $e^-$'s | full structure | short structure | 1s | 2s | 2p | | | 3s | 3p | | | 4s | 3d | | | | | 4p | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Li | 3 | $1s^2\ 2s^1$ | [He] $2s^1$ | ↑↓ | ↑ | | | | | | | | | | | | | | | | |
| C | 6 | $1s^2\ 2s^2\ 2p^2$ | [He] $2s^2\ 2p^2$ | ↑↓ | ↑↓ | ↑ | ↑ | | | | | | | | | | | | | | |
| O | 8 | $1s^2\ 2s^2\ 2p^4$ | [He] $2s^2\ 2p^4$ | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑ | | | | | | | | | | | | | |
| F | 9 | $1s^2\ 2s^2\ 2p^5$ | [He] $2s^2\ 2p^5$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | | | | | | | | | | | | | |
| Mg | 12 | $1s^2\ 2s^2\ 2p^6\ 3s^2$ | [Ne] $3s^2$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | | | | | | | | | | | |
| S | 16 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$ | [Ne] $3s^2\ 3p^4$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑ | | | | | | | | | | |
| K | 19 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$ | [Ar] $4s^1$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | | | | | | | | |
| Ti | 22 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^2$ | [Ar] $4s^2\ 3d^2$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑ | | | | | | |
| Fe | 26 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$ | [Ar] $4s^2\ 3d^6$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑ | ↑ | ↑ | | | |
| Cr | 24 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^5$ | [Ar] $4s^1\ 3d^5$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑ | ↑ | ↑ | ↑ | ↑ | | | |
| Ni | 28 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^8$ | [Ar] $4s^2\ 3d^8$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑ | ↑ | | | |
| Cu | 29 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^{10}$ | [Ar] $4s^1\ 3d^{10}$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | | |
| Br | 35 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5$ | [Ar] $4s^2\ 3d^{10}\ 4p^5$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ |
| $Ca^{2+}$ | 18 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$ | [Ar] | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | | | | | | | | |
| $S^{2-}$ | 18 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$ | [Ar] | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | | | | | | | | |
| $V^{3+}$ | 20 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^2$ | [Ar] $3d^2$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | ↑ | ↑ | | | | | | |
| $Cu^{2+}$ | 27 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^9$ | [Ar] $3d^9$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ | | | |
| $Sc^{3+}$ | 18 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$ | [Ar] | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | | | | | | | | |
| $Fe^{3+}$ | 23 | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5$ | [Ar] $3d^5$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | ↑ | ↑ | ↑ | ↑ | ↑ | | | |

# SECTION 5 – Evidence for electron structure

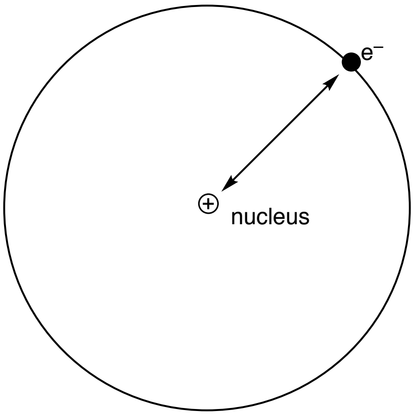
## What is ionisation energy?

- Evidence for how the electrons are arranged in atoms comes from ionisation energies.
- 1st ionisation energy is the energy required to remove one electron from each atom in a mole of gaseous atoms producing one mole of 1+ gaseous ions.
- Note that 2nd ionisation energy is the energy required to remove the second electron (not both electrons).

e.g. 1st ionisation energy of Na: **$Na(g) \rightarrow Na^+(g) + e^-$**

2nd ionisation energy of Na: **$Na^+(g) \rightarrow Na^{2+}(g) + e^-$**

## Factors affecting ionisation energy

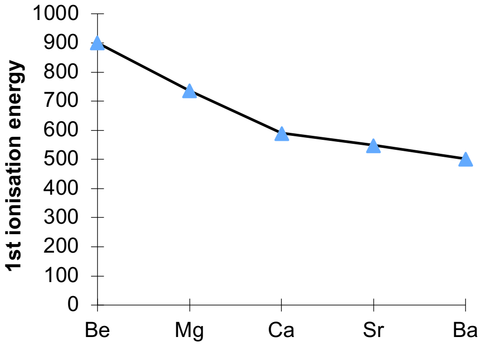


| Factor | Effect |
|---|---|
| 1) Atomic radius | **the smaller the radius, the stronger the attraction between the nucleus and the electron** |
| 2) Number of protons | **the more protons, the stronger the attraction between the nucleus and the electron** |
| 3) Shielding | shielding = repulsion by electrons in shells between the electron and the nucleus)<br>**the more shielding, the weaker the attraction between the nucleus and the electron** |

## How and why ionisation varies:

### Down a group (e.g. Group 2)

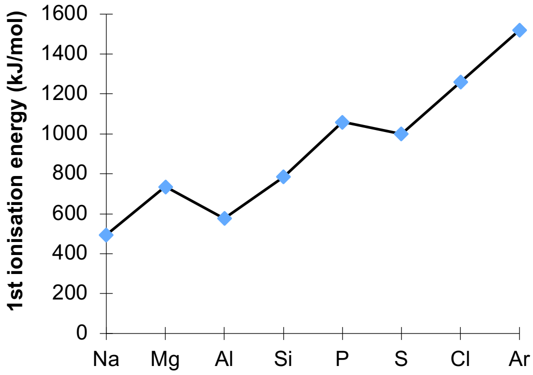
- **ionisation energy decreases**
- **smaller atomic radius**
- **more shielding**
- **so weaker attraction between nucleus and the electron**



## Across a period (e.g. period 3)

General increase across period:

- **ionisation energy increases**
- **smaller atomic radius**
- **more protons**
- **so stronger attraction between nucleus and the electron**



Group 2 to 3 dip:

- **group 2 from s orbital, group 3 from p orbital**
- **p orbital higher energy than s orbital**

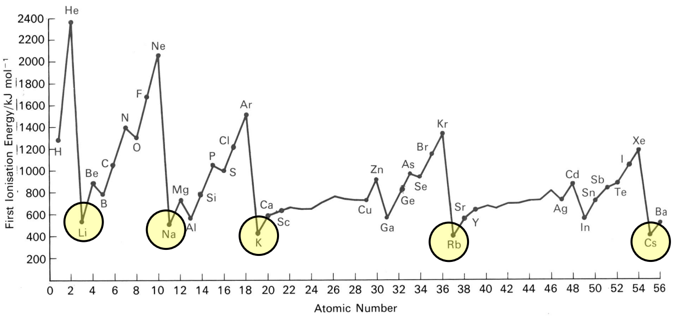
Group 5 to 6 dip:

- **group 5 from orbital with 1 electron, group 6 from orbital with 2 electrons**
- **more electron-electron repulsion in orbital with 2 electrons**

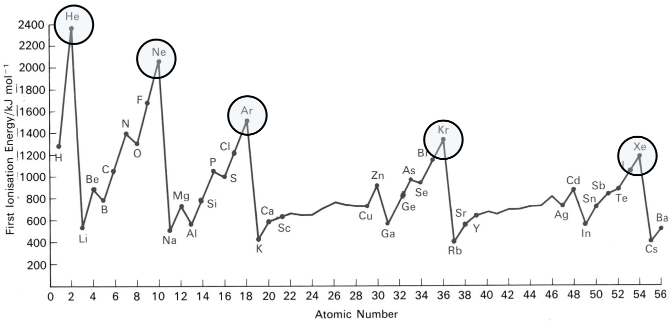
## First ionisation energy (up to element 56)

***highlight these trends***

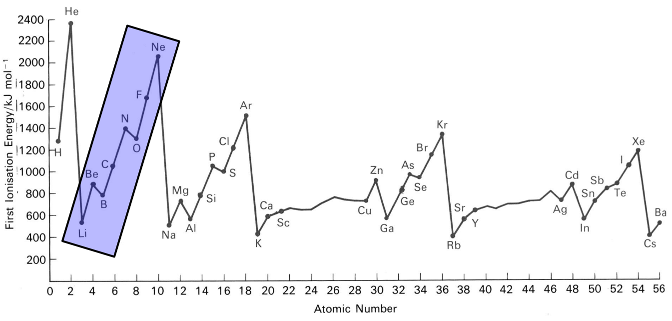
*down group 1*



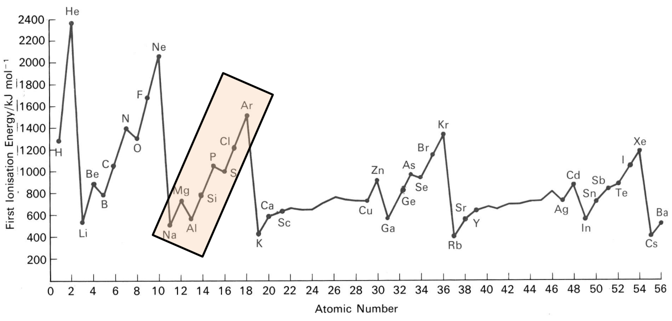
*down group 0*



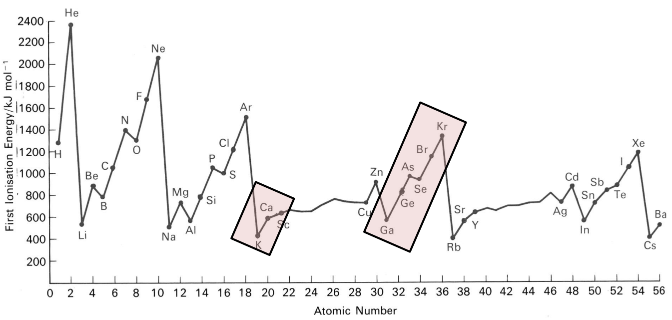
*across period 2*



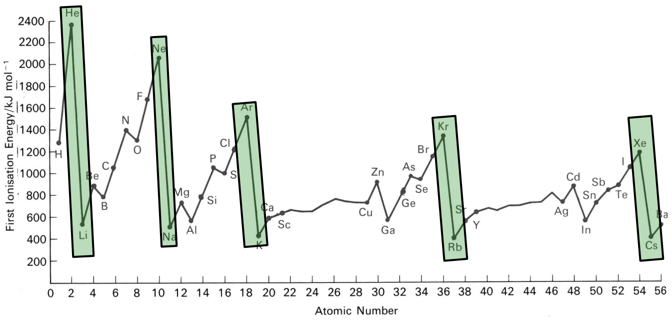
*across period 3*



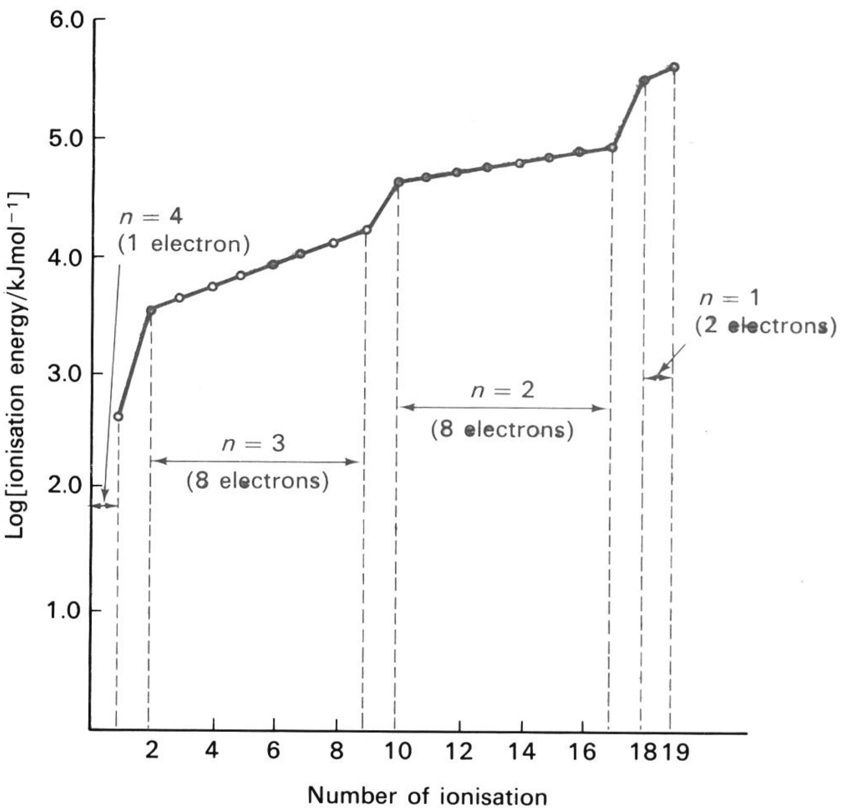
*across period 4*



*end of a period*



**Successive ionisation energies**



*Logarithmic plot of successive ionisation energies (of potassium)*

When an electron is taken from a different shell that is closer to the nucleus, there is a big jump in ionisation energy (as the electron is closer to the nucleus plus there is one fewer shell of shielding)

In this example, there is a big jump after the 1st IE suggesting the element is in Group 1.

As it is potassium with electron structure 2,8,8,1 in GCSE terms (or $1s^2\ 2s^2\ 2p^6\ 3s^3\ 3p^6\ 4s^1$ in A level terms), there are jumps after the

- 1st IE (shell 3 rather than 4)
- 9th IE (shell 2 rather than 3)
- 17th IE (shell 1 rather than 1)

## TASK 6 – Successive ionisation energies

In each case identify which the element belongs to by studying values of successive ionisation energies. They are all elements in Groups 0-7 and none of them are transition metals, lanthanides or actinides.

| | *1st* | *2nd* | *3rd* | *4th* | *5th* | *6th* | *7th* | *8th* | *Group* |
|---|---|---|---|---|---|---|---|---|---|
| **1** | 736 | 1450 | 7740 | 10500 | 13600 | 18000 | 21700 | 25600 | 2 |
| **2** | 1680 | 3370 | 6040 | 8410 | 11000 | 15100 | 17900 | 91600 | 7 |
| **3** | 762 | 1540 | 3300 | 4390 | 8950 | 11900 | 14900 | 18200 | 4 |
| **4** | 418 | 3070 | 4600 | 6480 | 8120 | 10700 | 12300 | 14600 | 1 |
| **5** | 941 | 2080 | 3090 | 4140 | 7030 | 7870 | 16000 | 19500 | 6 |
| **6** | 577 | 1820 | 2740 | 11600 | 14800 | 18400 | 23400 | 27500 | 3 |
| **7** | 1310 | 3390 | 5320 | 7450 | 11000 | 13300 | 71000 | 84100 | 6 |
| **8** | 590 | 1150 | 4940 | 6480 | 8120 | 10700 | 12300 | 14600 | 2 |
| **9** | 1060 | 1900 | 2920 | 4960 | 6280 | 21200 | 25900 | 30500 | 5 |
| **10** | 2080 | 3950 | 6150 | 9290 | 12100 | 15200 | 19500 | 23000 | 0 |

# TASK 7 – Which has the higher ionisation energy?

## First ionisation energy

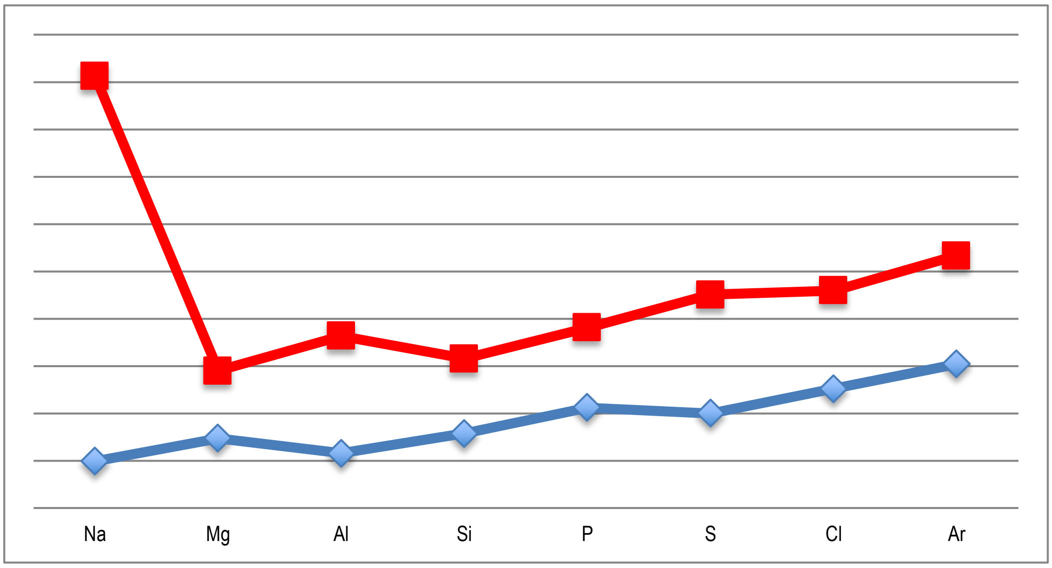
Circle the element with the higher first ionisation energy.

Give the electron structure of each atom. Use this to explain which has the higher first ionisation energy.

| | circle the higher one | electron structure | explanation |
|---|---|---|---|
| 1 | [✓ **argon**] v potassium | Ar **$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$**<br>K **$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$** | • **electron in Ar is from shell 3, in K it is from shell 4**<br>• **Ar has smaller atomic radius**<br>• **Ar has less shielding** |
| 2 | [✓ **phosphorus**] v sulfur | P **$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$**<br>S **$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$** | • **electron in P is from orbital with 1 electron, in S it is from an orbital with 2 electrons**<br>• **less electron-electron repulsion in P** |
| 3 | [✓ **magnesium**] v calcium | Mg **$1s^2\ 2s^2\ 2p^6\ 3s^2$**<br>Ca **$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$** | • **electron in Mg is from shell 3, in Ca it is from shell 4**<br>• **Mg has smaller atomic radius**<br>• **Mg has less shielding** |
| 4 | [✓ **magnesium**] v aluminium | Mg **$1s^2\ 2s^2\ 2p^6\ 3s^2$**<br>Al **$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$** | • **electron in Mg is from 3s, while in Al it is from 3p**<br>• **3p is higher energy than 3s** |
| 5 | oxygen v [✓ **fluorine**] | O **$1s^2\ 2s^2\ 2p^4$**<br>F **$1s^2\ 2s^2\ 2p^5$** | • **F has smaller atomic radius than O**<br>• **F has more protons than O** |

## Second ionisation energy

The diagram below shows the first ionisation energy for some elements. Sketch a line to show the second ionisation energy for these same elements.



Circle the element with the higher ***second*** ionisation energy and explain why it is higher.

Give the electron structure of each atom. Use this for your explanation.

| | circle the higher one | electron structure | explanation |
|---|---|---|---|
| 6 | [✓ sodium] v magnesium | Na$^+$ $1s^2\ 2s^2\ 2p^6$<br>Mg$^+$ $1s^2\ 2s^2\ 2p^6\ 3s^1$ | • electron in Na$^+$ is from shell 2, in Mg$^+$ it is from shell 3<br>• Na$^+$ has radius smaller<br>• Na$^+$ has less shielding |
| 7 | neon v [✓ sodium] | Ne$^+$ $1s^2\ 2s^2\ 2p^5$<br>Na$^+$ $1s^2\ 2s^2\ 2p^6$ | • Na$^+$ has smaller radius than Ne$^+$<br>• Na$^+$ has more protons than Ne |
| 8 | [✓ aluminium] v silicon | Al$^+$ $1s^2\ 2s^2\ 2p^6\ 3s^2$<br>Si$^+$ $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$ | • electron in Al$^+$ is from 3s orbital<br>• electron in Si$^+$ is from 3p orbital<br>• 3p is higher energy than 3s |