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HOMework

DATE	PARTICULARS

NOTES



NOTES



NOTES



NOTES



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 <i>relative atomic</i> , <i>isotopic</i> , <i>molecular</i> and <i>formula masses</i> , based on the ^{12}C scale |
| 1.2 The mole and the Avogadro constant | a) define and use the term <i>mole</i> 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 <i>empirical</i> and <i>molecular formula</i>
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: <ol style="list-style-type: none"> reacting masses (from formulae and equations) volumes of gases (e.g. in the burning of hydrocarbons) 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 ${}^x_{\gamma}A$ for isotopes, where x is the nucleon number and γ 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**.

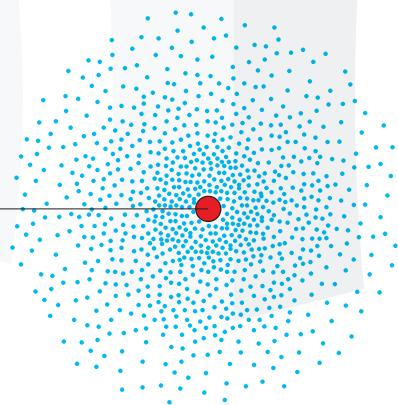
Atoms have 1 **uncharged** particle called a **neutron**.

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

1

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**

2

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

3

EXAMPLE

Calculate the mass of a carbon-12 atom.

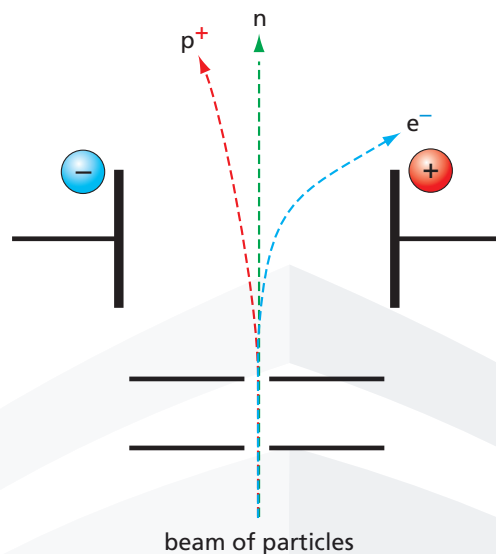
A **neutral** ^{12}C atom has *6 protons*, *6 neutrons*, and *6 electrons*.

Therefore, its mass is:

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

4

BEHAVIOUR OF SUB ATOMIC PARTICLES



5

ISOTOPES

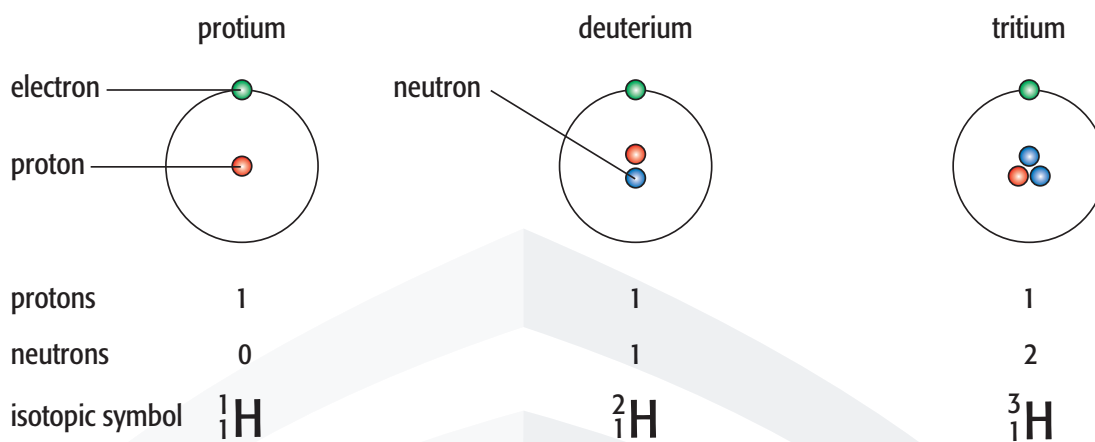
Isotopes are atoms with:

- 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.

6

ISOTOPES



7

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%

8

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.

9

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.

10

RELATIVE MASSES

Relative Formula Mass

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

11

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.

12

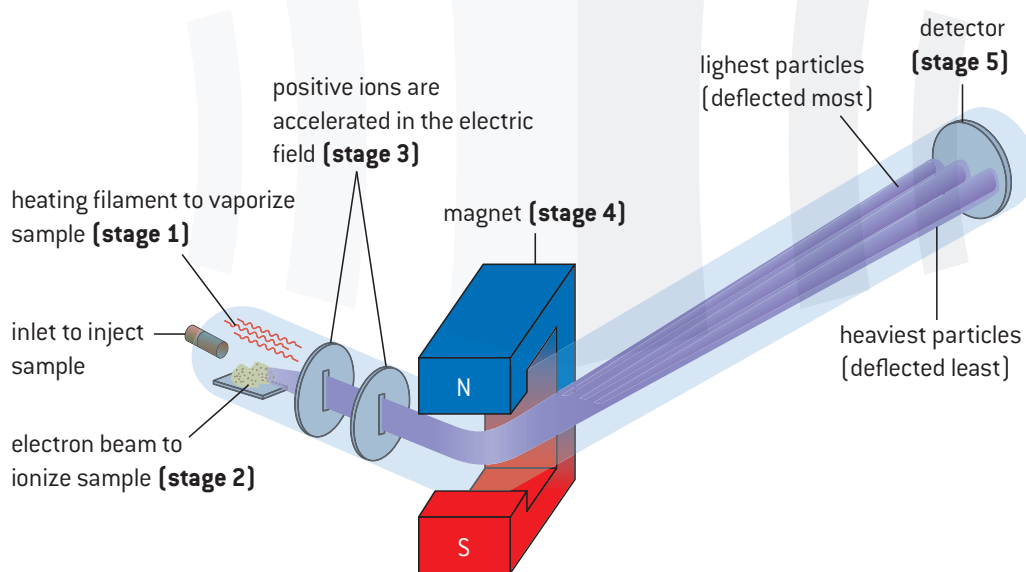
MASS SPECTROMETER

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.

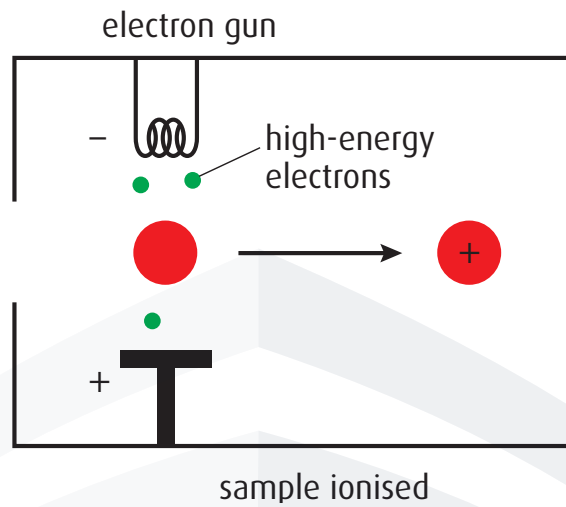
13

HOW DOES A MASS SPECTROMETER WORK?



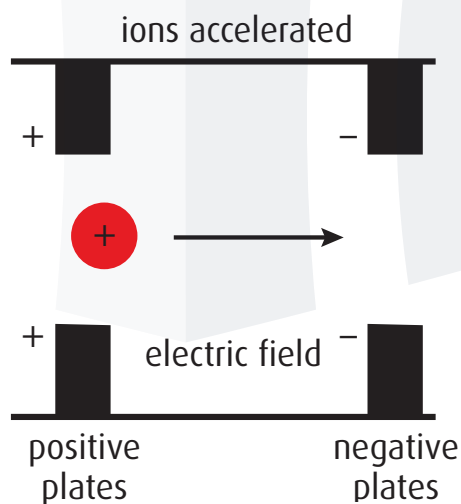
14

HOW DOES A MASS SPECTROMETER WORK?



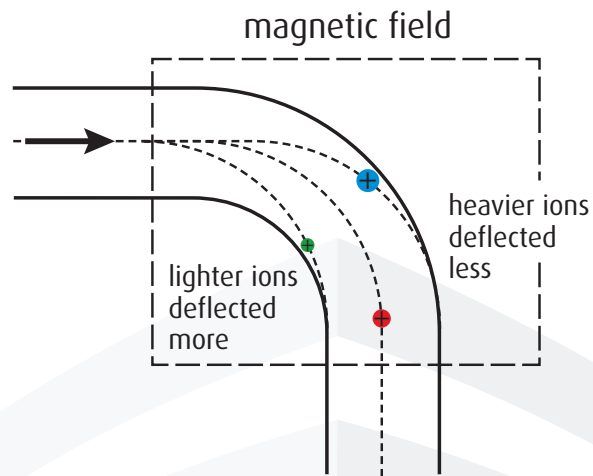
15

HOW DOES A MASS SPECTROMETER WORK?



16

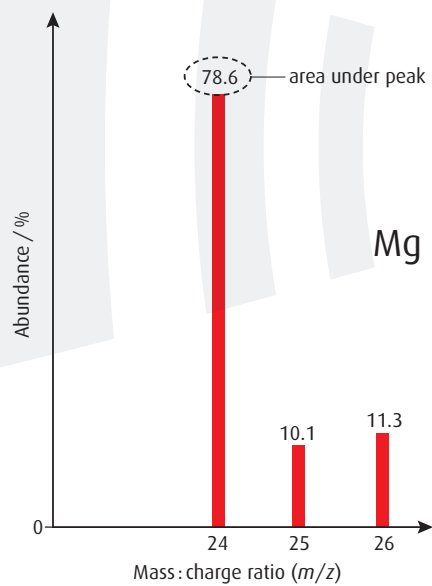
HOW DOES A MASS SPECTROMETER WORK?



17

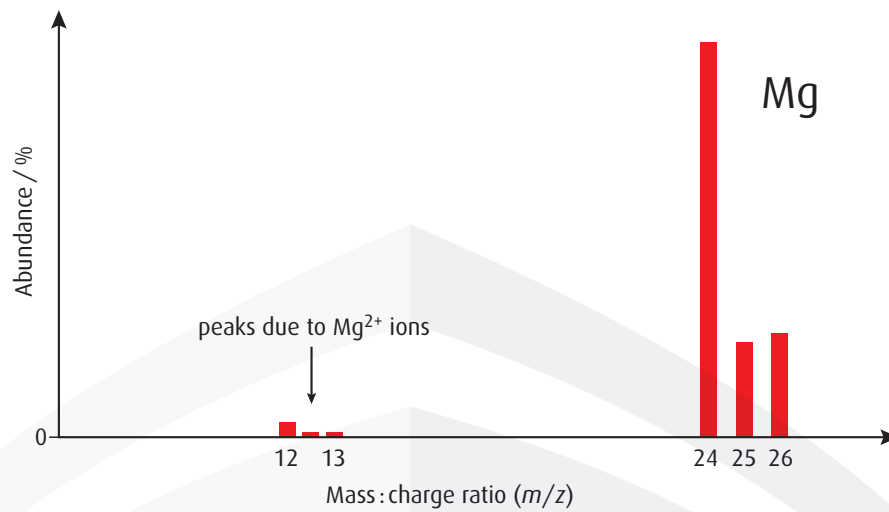
MASS SPECTRA

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.



18

MASS SPECTRA

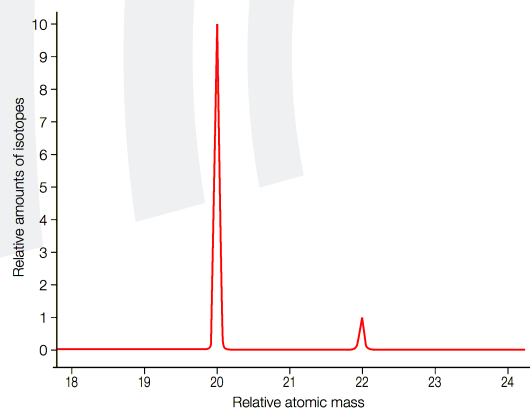


19

SKILL CHECK 2

The graph shows the mass spectrum of Neon.

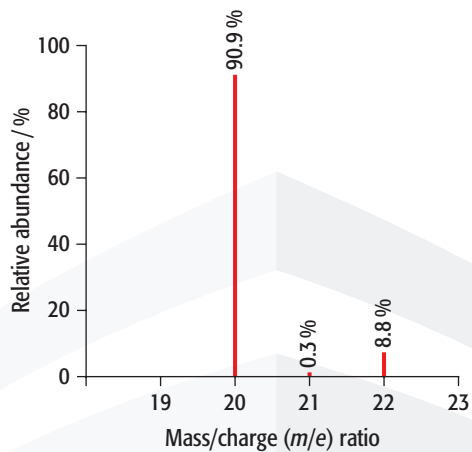
1. How many isotopes does Neon contain?
2. What are the relative isotopic masses of the isotopes of Neon?
3. What are the relative amounts of the isotopes of Neon?



20

SKILL CHECK 3

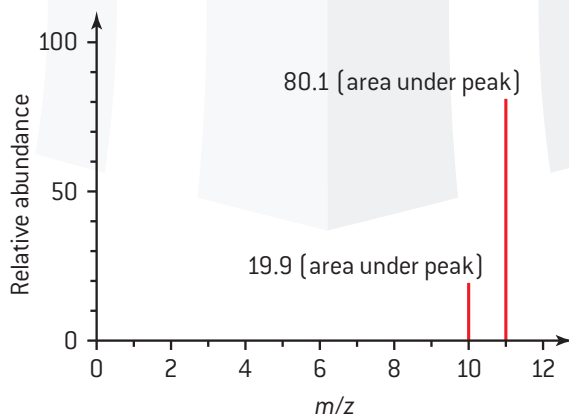
Calculate the average relative atomic mass of neon using the information below:



21

SKILL CHECK 4

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



22

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

23

SKILL CHECK 6

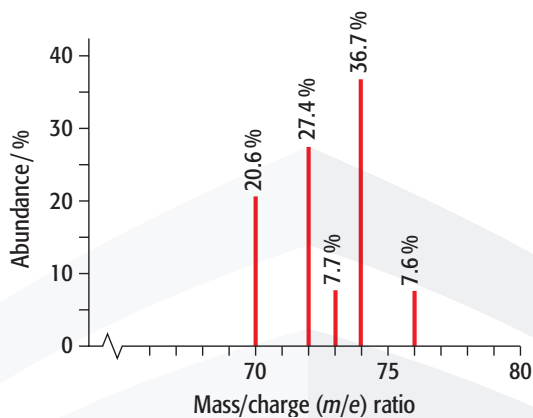
Calculate the average relative atomic mass of lead using the information below:

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

24

SKILL CHECK 7

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



25

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:

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

26

MASS SPECTRA: CALCULATING ABUNDANCE

therefore $39x + 4100 - 41x = 3910$

thus $-2x = -190$

$$x = 95$$

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

27

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.

28

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

29

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.

30

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?

31

SKILL CHECK 12

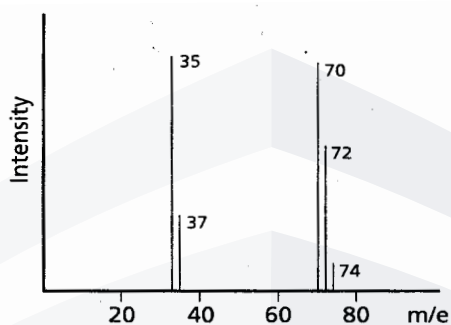
A sample of element X contains 69% of ^{63}X and 31% of ^{65}X . What is the relative atomic mass of X in this sample?

32

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):



33

MASS SPECTRA: MOLECULAR IONS

Cl_2^+ molecular ion produces three peaks:

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

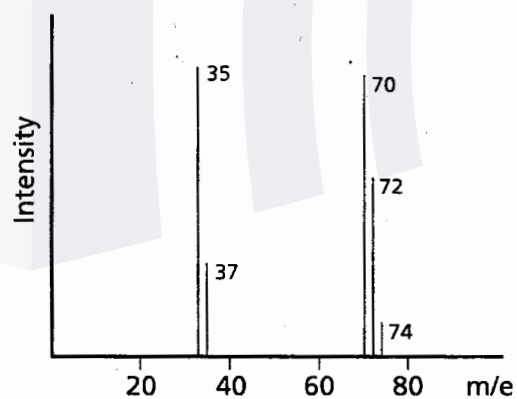
Species responsible: $^{70}\text{Cl}_2^+$

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

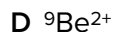
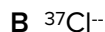


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ATOMIC STRUCTURE WS 1

SECTION A

1 Which one the following has more neutrons than electrons and more electrons than protons?



2 Chlorine exists as two isotopes ^{35}Cl with an abundance of 75.5% and ^{37}Cl with an abundance of 24.5%.

Phosphorus has only one isotope, ^{31}P . The mass spectrum of PCl_3 has four lines at $m/z = 136, 138, 140$ and 142 .

Which one of these lines will have the smallest height?

A 136

C 138

B 140

D 142

3 Antimony has two isotopes ^{121}Sb and ^{123}Sb . The relative atomic mass of a naturally occurring sample of antimony is measured as 121.75.

Which one of the following is the best approximate estimate of the percentage of ^{121}Sb present in the naturally occurring sample?

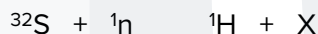
A 20%

C 40%

B 60%

D 80%

4 When sulfur, ^{32}S is bombarded with neutrons ^1_0n , two particles are formed. One of them is a hydrogen atom, ^1_1H and the other is an element, X.



Which one of the following correctly represents X?

A ^{32}S

C ^{33}S

B ^{32}P

D ^{33}P

5 What is the number of protons, electrons, and neutrons in boron-11?

A 5 protons, 5 electrons and 11 neutrons

C 5 protons, 5 electrons and 6 neutrons

B 5 protons, 5 electrons and 10.8 neutrons

D 11 protons, 11 electrons and 5 neutrons

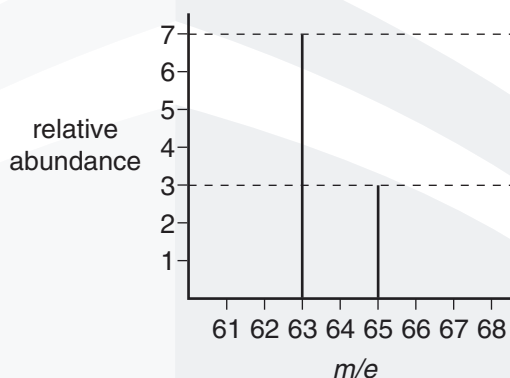
- 10 In the radioactive decay of an isotope of lead to an isotope of bismuth, a particle ${}_{-1}^0\text{X}$ is emitted.

Which particle is ${}_{-1}^0\text{X}$?

- A electron
- B ion
- C neutron
- D proton

[S'02 Q1]

- 11 The diagram shows the mass spectrum of a sample of naturally-occurring copper.



What is the relative atomic mass of this copper?

- A 63.3
- B 63.5
- C 63.6
- D 64.0

[S'02 Q3]

- 12 Which isotope of an element in the third period of the Periodic Table contains the same number of neutrons as ${}_{16}^{32}\text{S}$?

- A ${}_{11}^{23}\text{Na}$
- B ${}_{12}^{24}\text{Mg}$
- C ${}_{14}^{28}\text{Si}$
- D ${}_{15}^{31}\text{P}$

[S'03 Q3]

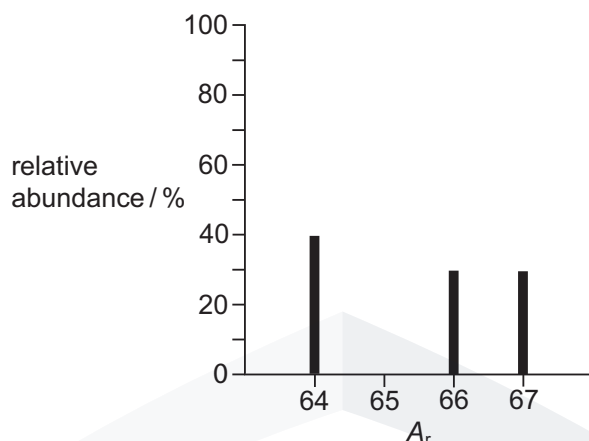
- 13 Unnilpentium is an artificial element. One of its isotopes is ${}_{105}^{262}\text{Unp}$.

Which of the following statements is correct?

- A ${}_{105}^{262}\text{Unp}$ has a nucleon number of 105.
- B The atom ${}_{105}^{260}\text{X}$ is an isotope of ${}_{105}^{262}\text{Unp}$.
- C There are 262 neutrons in ${}_{105}^{262}\text{Unp}$.
- D The proton number of ${}_{105}^{262}\text{Unp}$ is 262.

[W'03 Q4]

- 14 The diagram shows the mass spectrum of a sample of zinc. Use the data to calculate the relative atomic mass of the sample.



- A 65 B 65.25 C 65.5 D 65.66

[W'04 Q2]

- 15 It is now thought that where an element exists as several isotopes, the stable ones usually contain a 'magic number' of neutrons. One of these magic numbers is 126.

Which isotope is unstable?

- A ^{209}Bi B ^{208}Pb C ^{210}Po D ^{208}Tl

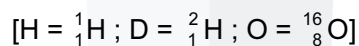
[W'04 Q4]

- 16 In which species are the numbers of electrons and neutrons equal?

- A ^9_4Be B $^{19}_9\text{F}$ C $^{23}_{11}\text{Na}^+$ D $^{18}_8\text{O}^{2-}$

[S'05 Q4]

- 17 Which ion has more electrons than protons and more protons than neutrons?



- A D^- B H_3O^+ C OD^- D OH^-

[W'05 Q2]

- 18 A sample of chlorine containing isotopes of mass numbers 35 and 37 was analysed in a mass-spectrometer.

How many peaks corresponding to Cl_2^+ were recorded?

- A 2 B 3 C 4 D 5

[S'06 Q2]

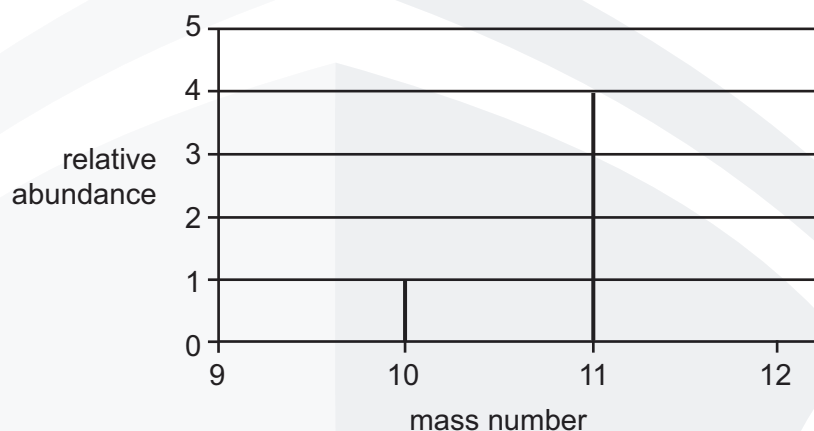
- 19 A radioactive isotope of thallium, ${}_{81}^{201}\text{Tl}$, is used to assess damage in heart muscles after a heart attack.

Which statement about ${}_{81}^{201}\text{Tl}$ is correct?

- A This isotope has a nucleon number of 120.
 B The number of electrons in one atom of this isotope is 81.
 C The number of neutrons in one atom of this isotope is 201.
 D ${}_{82}^{201}\text{X}$ is an isotope of ${}_{81}^{201}\text{Tl}$.

[S'06 Q4]

- 20 The isotopic composition of an element is indicated below.



What is the relative atomic mass of the element?

- A 10.2 B 10.5 C 10.8 D 11.0

[S'07 Q1]

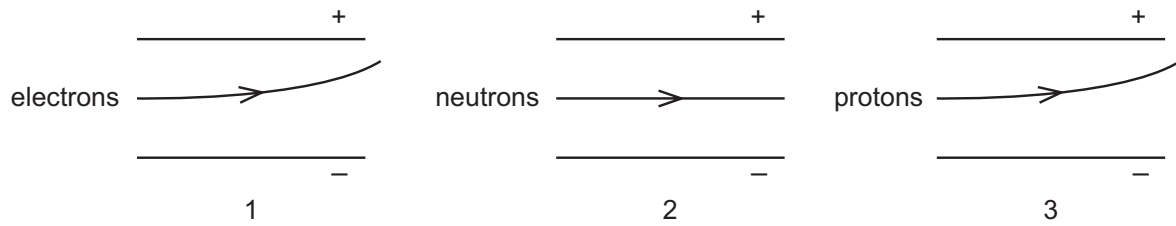
- 21 John Dalton's atomic theory, published in 1808, contained four predictions about atoms.

Which of his predictions is still considered to be correct?

- A Atoms are very small in size.
 B No atom can be split into simpler parts.
 C All the atoms of a particular element have the same mass.
 D All the atoms of one element are different in mass from all the atoms of other elements.

[S'07 Q3]

- 22 The diagrams show the possible paths of subatomic particles moving in an electric field in a vacuum.



Which diagrams are correct?

- A 1 and 2 only
 B 1 and 3 only
 C 2 and 3 only
 D 1, 2 and 3
- [S'07 Q4]
- 23 Skin cancer can be treated using a radioactive isotope of phosphorus, $^{32}_{15}\text{P}$. A compound containing the phosphide ion $^{32}_{15}\text{P}^{3-}$, wrapped in a plastic sheet, is strapped to the affected area.

What is the composition of the phosphide ion, $^{32}_{15}\text{P}^{3-}$?

	protons	neutrons	electrons
A	15	17	18
B	15	17	32
C	17	15	17
D	32	17	15

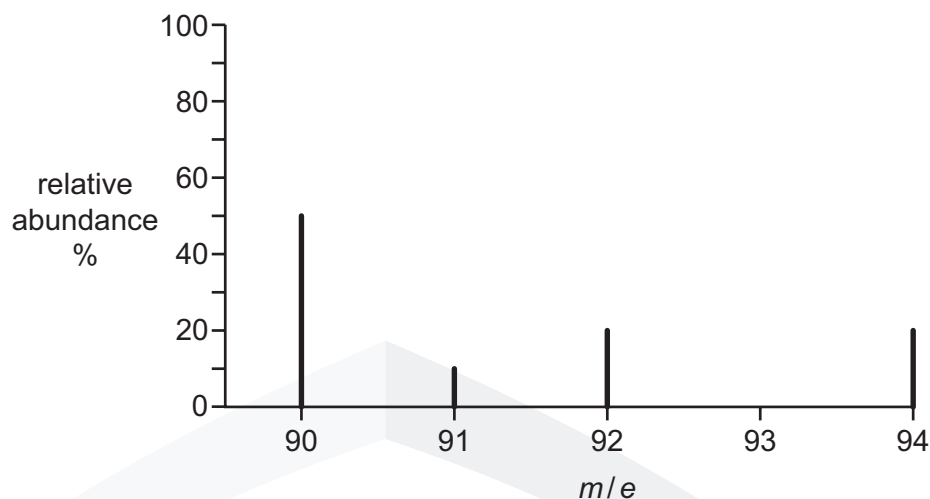
- [S'08 Q3]
- 24 Hard water contains calcium ions and hydrogencarbonate ions arising from dissolved calcium hydrogencarbonate, $\text{Ca}(\text{HCO}_3)_2$.

How many electrons are present in the hydrogencarbonate anion?

- A 30 B 31 C 32 D 33

[W'08 Q4]

- 25 An element **X** consists of four isotopes. The mass spectrum of **X** is shown in the diagram.



What is the relative atomic mass of **X**?

- A** 91.00 **B** 91.30 **C** 91.75 **D** 92.00 [W'09 1 Q4]
- 26 Helium, He, is the second element in the Periodic Table.
Tritium is the isotope of hydrogen ^3H .
What is the same in an atom of ^4He and an atom of ^3H ?
- A** the number of electrons
B the number of neutrons
C the number of protons
D the relative atomic mass [S'11 2 Q1]
- 27 In which species are the numbers of protons, neutrons and electrons all different?
- A** $^{11}_5\text{B}$ **B** $^{19}_9\text{F}^-$ **C** $^{23}_{11}\text{Na}^+$ **D** $^{24}_{12}\text{Mg}^{2+}$ [S'12 2 Q2]
- 28 The ^{68}Ge isotope is medically useful because it undergoes a natural radioactive process to give an isotope of a different element, ^{68}X , which can be used to detect tumours. This transformation of ^{68}Ge occurs when an electron enters the nucleus and changes a proton into a neutron.
Which statement about the composition of an atom of ^{68}X is correct?
- A** It has 4 electrons in its outer p orbitals.
B It has 13 electrons in its outer shell.
C It has 37 neutrons.
D Its proton number is 32. [S'12 1 Q2]

29 *Use of the Data Booklet is relevant to this question.*

In which species are the numbers of protons, neutrons and electrons **all** different?

- A ${}^{19}_9\text{F}^-$ B ${}^{23}_{11}\text{Na}^+$ C ${}^{31}_{15}\text{P}$ D ${}^{32}_{16}\text{S}^{2-}$

[S'10 1 Q1]

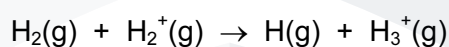
30 In which species are the numbers of protons, neutrons and electrons all different?

- A ${}^{27}_{13}\text{Al}$ B ${}^{35}_{17}\text{Cl}^-$ C ${}^{32}_{16}\text{S}^{2-}$ D ${}^{39}_{19}\text{K}^+$

[S'13 1 Q5]

31 *Use of the Data Booklet is relevant to this question.*

The most common ion-molecule reaction in gas clouds of the Universe is as shown.



What could be the composition of an H_3^+ ion?

	protons	neutrons	electrons
A	2	1	1
B	2	1	2
C	3	0	1
D	3	0	2

[S'14 3 Q4]

32 *Use of the Data Booklet is relevant to this question.*

In some types of spectroscopy, it is important to know if ions are isoelectronic. This means that they contain equal numbers of electrons.

Which ion is **not** isoelectronic with K^+ ?

- A Ca^{2+} B Cl^- C S^{2-} D Ti^{3+}

[W'14 3 Q2]

33 *Use of the Data Booklet is relevant to this question.*

In which option do all three particles have the same electronic configuration **and** the same number of neutrons?

- A ${}^{15}\text{N}^{3-}$ ${}^{16}\text{O}^{2-}$ ${}^{19}\text{F}^-$
 B ${}^{18}\text{O}^{2-}$ ${}^{19}\text{F}^-$ ${}^{20}\text{Ne}$
 C ${}^{19}\text{F}^-$ ${}^{20}\text{Ne}$ ${}^{23}\text{Na}^+$
 D ${}^{22}\text{Ne}$ ${}^{23}\text{Na}$ ${}^{24}\text{Mg}^{2+}$

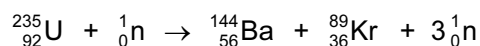
[S'15 2 Q1]

34 Which species contains the smallest number of electrons?

- A B^{3+} B Be^{2+} C H^{-} D He^{+}

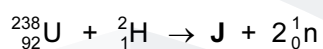
[M'16 2 Q4]

35 When nuclear reactions take place, the elements produced are different from the elements that reacted. Nuclear equations, such as the one below, are used to represent the changes that occur.



The nucleon (mass) number total is constant at 236 and the proton number total is constant at 92.

In another nuclear reaction, uranium-238 is reacted with deuterium atoms, ${}_1^2\text{H}$. An isotope of a new element, **J**, is formed as well as two neutrons.



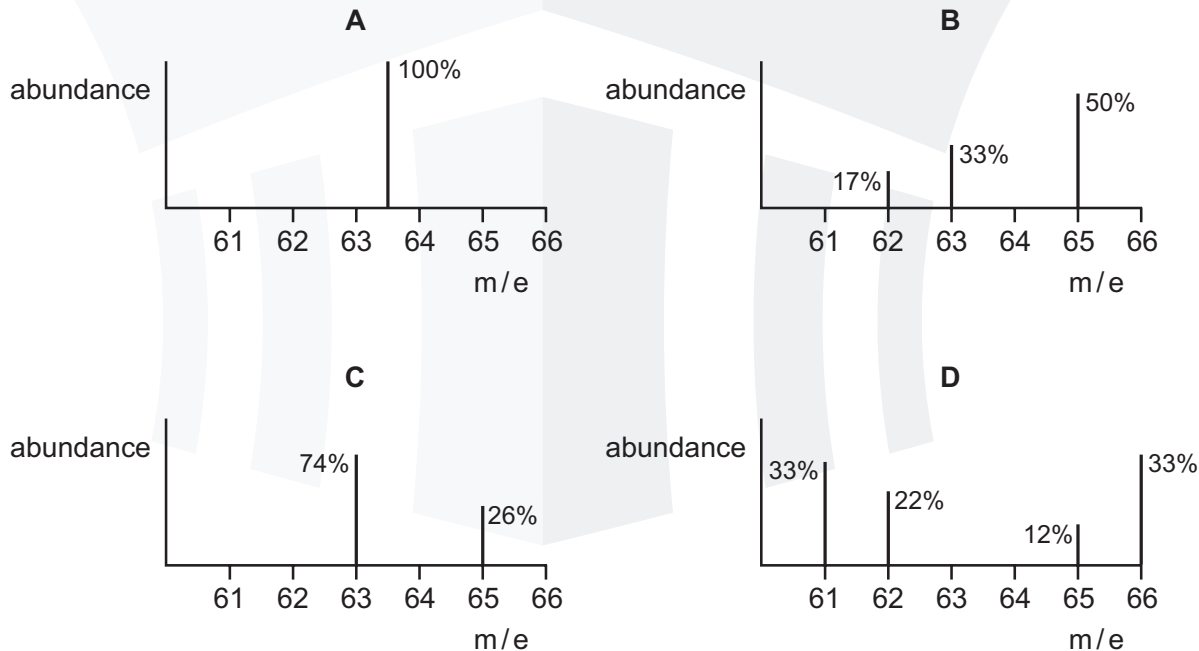
What is isotope **J**?

- A ${}^{238}\text{Np}$ B ${}^{238}\text{Pu}$ C ${}^{240}\text{Np}$ D ${}^{240}\text{Pu}$

[S'16 1 Q4]

36 The relative atomic mass of copper is 63.5.

Which chart is a correct mass spectrum that would lead to this value?



[S'16 3 Q4]

- 37 Neutrons are passed through an electric field. The mass of one neutron relative to $\frac{1}{12}$ the mass of a ^{12}C atom and any deflection in the electric field is recorded.

Which row is correct?

	mass of neutron	behaviour of beam of neutrons in an electric field
A	0	deflected
B	1	deflected
C	0	not deflected
D	1	not deflected

[S'18 3 Q2]

SECTION B

For each of the questions in this section, one or more of the three numbered statements 1 to 3 may be correct.

Decide whether each of the statements is or is not correct (you may find it helpful to put a tick against the statements that you consider to be correct).

The responses **A** to **D** should be selected on the basis of

A	B	C	D
1, 2 and 3 are correct	1 and 2 only are correct	2 and 3 only are correct	1 only is correct

No other combination of statements is used as a correct response.

- 1 The isotope cobalt-60 (${}^{60}_{27}\text{Co}$) is used to destroy cancer cells in the human body.

Which statements about an atom of cobalt-60 are correct?

- 1 It contains 33 neutrons.
- 2 Its nucleus has a relative charge of 27+.
- 3 It has a different number of neutrons from the atoms of other isotopes of cobalt.

[S'04 Q31]

- 2 The relative molecular mass of a molecule of chlorine is 72.

Which properties of the atoms in this molecule are the same?

- 1 radius
- 2 nucleon number
- 3 relative isotopic mass

[S'05 Q31]

- 3 *Use of the Data Booklet is relevant to this question.*

The technetium-99 isotope (${}^{99}\text{Tc}$) is radioactive and has been found in lobsters and seaweed adjacent to nuclear fuel reprocessing plants.

Which statements are correct about an atom of ${}^{99}\text{Tc}$?

- 1 It has 13 more neutrons than protons.
- 2 It has 43 protons.
- 3 It has 99 nucleons.

[S'07 Q31]

- 4 On a scale in which the mass of a ^{12}C atom is 12 the relative molecular mass of a particular sample of chlorine is 72.

Which properties of the atoms in this sample are always the same?

- 1 radius
- 2 nucleon number
- 3 isotopic mass

[S'09 1 Q31]

- 5 The phosphide ion $^{31}_{15}\text{P}^{3-}$ and sulfide ion $^{32}_{16}\text{S}^{2-}$ have the same number of which sub-atomic particles?

- 1 neutrons
- 2 electrons
- 3 protons

[S'12 2 Q32]

- 6 The $^1\text{H}_3^+$ ion was first characterised by J. J. Thomson over a century ago. ^6Li is a rare isotope of lithium which forms the $^6\text{Li}^+$ ion.

Which statements are correct?

- 1 Both ions contain the same number of protons.
- 2 Both ions contain the same number of electrons.
- 3 Both ions contain the same number of neutrons.

[S'04 3 Q31]

- 7 In 2011 an international group of scientists agreed to add two new elements to the Periodic Table. Both elements had been made artificially and were called ununquadium (Uuq) and ununhexium (Uuh).

	Uuq	Uuh
proton number	114	116
nucleon number	289	292

Which statements about these elements are correct?

- 1 One atom of Uuh has one more neutron than one atom of Uuq.
- 2 One Uuq^{2-} ion has the same number of electrons as one atom of Uuh.
- 3 One Uuh^+ ion has the same number of electrons as one Uuq^- ion.

[S'14 3 Q31]

- 8 Which statements are correct when referring to the isotopes of a single element?

- 1 The isotopes have different masses.
- 2 The isotopes have different numbers of nucleons.
- 3 The isotopes have different chemical reactions.

[S'14 3 Q32]

9 Use of the Data Booklet is relevant to this question.

Which statements about the phosphide ion, $^{31}\text{P}^{3-}$, and the chloride ion, $^{35}\text{Cl}^-$, are correct?

- 1 They have the same number of electrons.
- 2 They have the same number of neutrons.
- 3 They have the same number of protons.

[S'15 2 Q31]

10 X is a particle with 18 electrons and 20 neutrons.

What could be the symbol of X?

- 1 $^{38}_{18}\text{Ar}$
- 2 $^{40}_{20}\text{Ca}^{2+}$
- 3 $^{39}_{19}\text{K}^+$

[S'16 1 Q31]

11 A sample of boron contains aluminium as the only impurity. A mass spectrum of the mixture shows three lines corresponding to three ions, X^+ , Y^+ and Z^+ .

ion	X^+	Y^+	Z^+
m/e	10	11	27
percentage abundance	15.52	74.48	10.00

Which statements are correct?

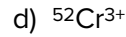
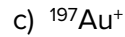
- 1 There are more electrons in Z^+ than in X^+ .
 - 2 The A_r of boron in the sample is 10.83 to four significant figures.
 - 3 There are more protons in Y^+ than in X^+ .
- 12 In which pairs do both species have the same number of electrons?

- 1 ^{35}Cl and ^{37}Cl
- 2 $^{35}\text{Cl}^-$ and ^{40}Ar
- 3 ^{40}Ar and $^{40}\text{K}^+$

[S'18 2 Q32]

ATOMIC STRUCTURE WS 2

1 Give the numbers of protons, neutrons and electrons present in each of the following atoms:



2 This question concerns the following five species:



a) Which two species have the same number of neutrons?

b) Which two species have the same ratio of neutrons to protons?

c) Which two species do not have 10 electrons?

3 The element Rhenium (Re) has two main isotopes, ^{185}Re with an abundance of 37.1% and ^{187}Re with an abundance of 62.9%.

Calculate the weighted mean atomic mass of rhenium.

4 Antimony has two main isotopes, ^{121}Sb and ^{123}Sb . A forensic scientist was asked to help a crime investigation by analysing the antimony in a bullet. This was found to contain 57.3% of ^{121}Sb and 42.7% of ^{123}Sb .

a) Calculate the relative atomic mass of the sample of antimony from the bullet. (*Write your answer to three significant figures*)

b) State one similarity and one difference between isotopes in terms of subatomic particles.

.....

.....

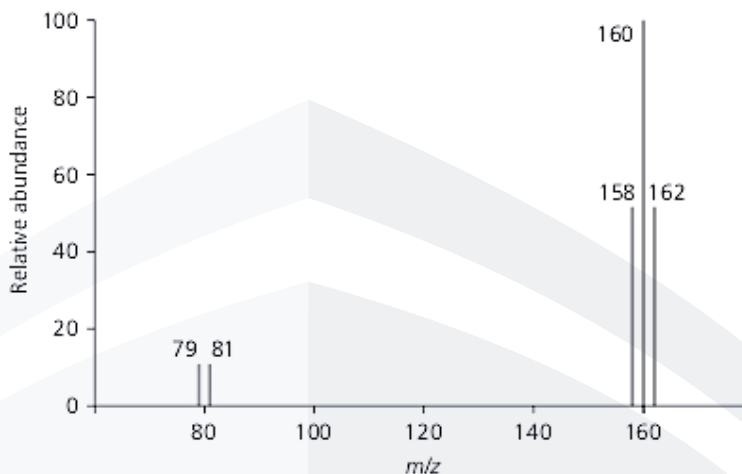
.....

- 5 Bromine exists as a molecule with two bromine atoms combined together. Bromine has two isotopes: bromine-79 and bromine-81

a) A molecule of bromine containing two atoms of bromine can be written as $^{79}\text{Br}_2$. Write the formulae for the two other possible molecules of bromine.

.....

b) The mass spectrum of molecules of bromine is shown below:



i. Explain why these peaks are observed.

.....

.....

.....

ii. The peaks at 79 and 81 are the same height. What does this tell you about the relative abundances of the two isotopes?

.....

.....

iii. Explain why the peak at 160 is twice the height of the peaks at 158 and 162.

.....

.....

.....

- 6 a) Explain why the relative atomic mass of copper is not an exact whole number?

.....

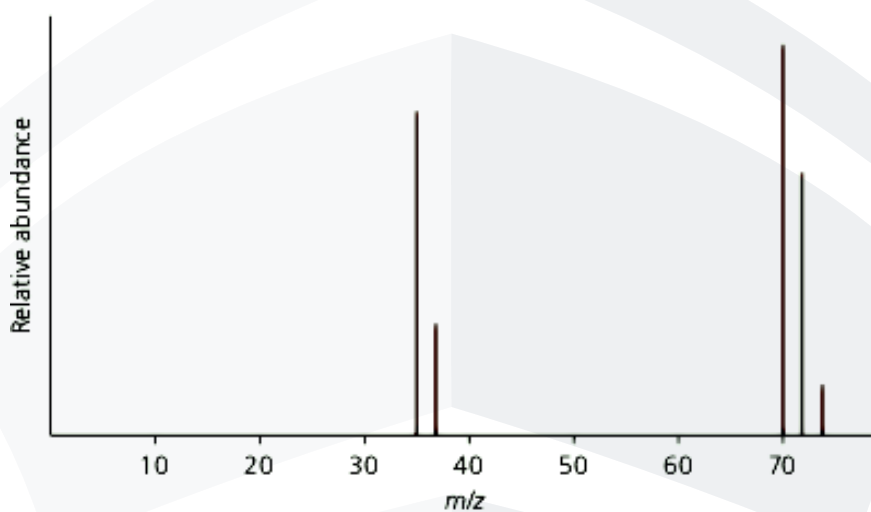
.....

.....

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

- 7 Chlorine exists as a molecule with two chlorine atoms combined together. Chlorine has two isotopes: chlorine-35 and chlorine-37.

The mass spectrum of chlorine is shown below:



- a) The peak at 35 is three times as high as the peak at 37. Calculate the relative atomic mass of chlorine.

.....

.....

- b) Explain why the peaks are observed at 70, 72 and 74.

.....

.....

- c) The heights of the peaks at 70, 72 and 74 are in the ratio 9 : 6 : 1. Explain why the heights are in this ratio.

.....

.....

.....

- 8 The data about silicon in the table below were obtained from a mass spectrometer.

m/z	% abundance
28	92.2
29	4.7
30	3.1

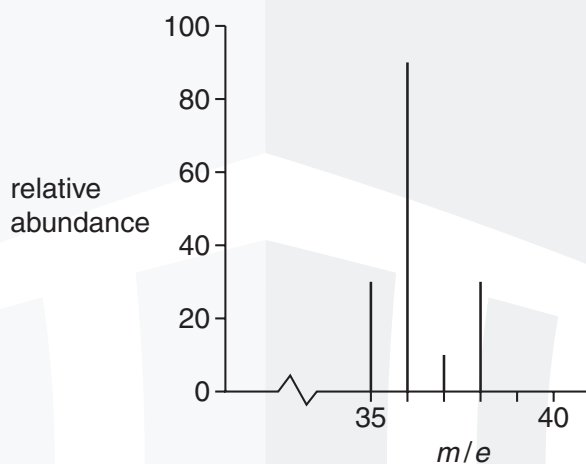
Calculate the relative atomic mass of silicon to one decimal place.

- 9 (a) Define *an isotope* in terms of its sub-atomic particles.

.....

[1]

- (b) In a mass spectrometer some hydrogen chloride molecules will split into atoms. The mass spectrum of HCl is given. Chlorine has two isotopes. The hydrogen involved here is the isotope ^1_1H only.



- (i) What particle is responsible for the peak at mass 35?
- (ii) What particle is responsible for the peak at mass 38?

[2]

- (c) Use the relative heights of the peaks to determine the proportions of the two isotopes of chlorine. Explain simply how you obtained your answer.

[2]

(d) Use your answer to (c) to explain why chlorine has a relative atomic mass of 35.5.

[1]

[S'03 Q1]

10 Iron and cobalt are adjacent elements in the Periodic Table. Iron has three main naturally occurring isotopes, cobalt has one.

(a) Explain the meaning of the term *isotope*.

.....

.....

..... [2]

(b) The most common isotope of iron is ^{56}Fe ; the only naturally occurring isotope of cobalt is ^{59}Co .

Use the *Data Booklet* to complete the table below to show the atomic structure of ^{56}Fe and of ^{59}Co .

isotope	number of		
	protons	neutrons	electrons
^{56}Fe			
^{59}Co			

[3]

(c) A sample of iron has the following isotopic composition by mass.

isotope mass	54	56	57
% by mass	5.84	91.68	2.17

(i) Define the term *relative atomic mass*.

.....

.....

.....

.....

- (ii) By using the data above, calculate the relative atomic mass of iron to **three** significant figures.

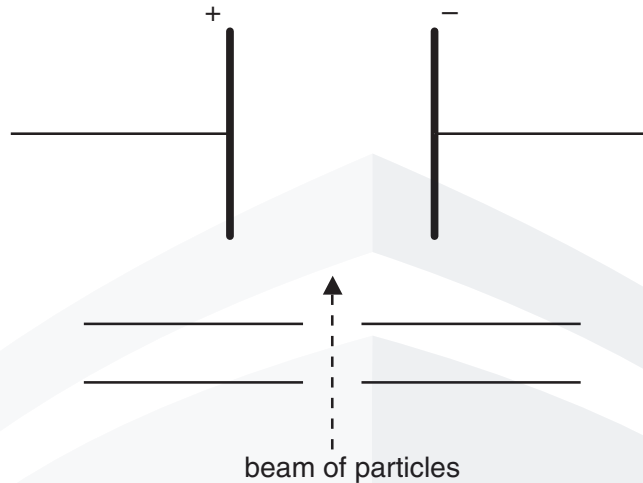
[5]

[S'05 Q1]



- 11 In the 19th and 20th centuries, scientists established the atomic theory and showed that three sub-atomic particles, electron, neutron and proton, exist. The masses and charges of these three particles were subsequently determined.

When separate beams of electrons, neutrons or protons are passed through an electric field in the apparatus below, they behave differently.



- (a) (i) Which of these three particles will be deflected the most by the electric field?

.....

- (ii) In which direction will this particle be deflected?

.....

- (iii) Explain your answer.

.....

[4]

- (b) (i) Define the term *proton number*.

.....

- (ii) Why is the proton number of an atom of an element usually different from the nucleon number of an atom of the element?

.....

[2]

- (c) Protons and neutrons have been used in nuclear reactions which result in the formation of artificial elements. In such processes, protons or neutrons are accelerated to high speeds and then fired like 'bullets' at the nucleus of an atom of an element.

Suggest why neutrons are more effective than protons as 'nuclear bullets'.

.....
..... [2]

- (d) In some cases, when neutrons are fired at atoms of an element, the neutrons become part of the nucleus of those atoms.

What effect does the presence of an extra neutron have on the chemical properties of the new atoms formed? Explain your answer.

.....
.....
..... [2]

[Total: 10]

[W'06 Q1]

12 Magnesium, Mg, and radium, Ra, are elements in Group II of the Periodic Table.

Magnesium has three isotopes.

(a) Explain the meaning of the term *isotope*.

.....

 [2]

A sample of magnesium has the following isotopic composition by mass.

isotope mass	24	25	26
% by mass	78.60	10.11	11.29

(b) Calculate the relative atomic mass, A_r , of magnesium to **four** significant figures.

$A_r = \dots\dots\dots$ [2]

Radium, proton number 88, and uranium, proton number 92, are radioactive elements.

The isotope ^{226}Ra is produced by the radioactive decay of the uranium isotope ^{238}U .

(c) Complete the table below to show the atomic structures of the isotopes ^{226}Ra and ^{238}U .

isotopes	number of		
	protons	neutrons	electrons
^{226}Ra			
^{238}U			

[3]

(d) Radium, like other Group II elements, forms a number of ionic compounds.

(i) What is the formula of the radium cation?

.....

(ii) Use the *Data Booklet* to suggest a value for the energy required to form one mole of the gaseous radium cation you have given in (i) from one mole of gaseous radium atoms. Explain your answer.

.....

.....

..... [3]

[W'09 1 Q1]

13 The element magnesium, Mg, proton number 12, is a metal which is used in many alloys which are strong and light.

Magnesium has several naturally occurring isotopes.

(a) What is meant by the term *isotope*?

.....

.....

..... [2]

(b) Complete the table below for two of the isotopes of magnesium.

isotope	number of protons	number of neutrons	number of electrons
^{24}Mg			
^{26}Mg			

[2]

A sample of magnesium had the following isotopic composition:

^{24}Mg , 78.60%; ^{25}Mg , 10.11%; ^{26}Mg , 11.29%.

(c) Calculate the relative atomic mass, A_r , of magnesium in the sample.
Express your answer to an appropriate number of significant figures.

[2]

[W'10 3 Q1]

14 Sulfur, S, and polonium, Po, are both elements in Group VI of the Periodic Table.

Sulfur has three isotopes.

(a) Explain the meaning of the term *isotope*.

.....

.....

..... [2]

(b) A sample of sulfur has the following isotopic composition by mass.

isotope mass	32	33	34
% by mass	95.00	0.77	4.23

Calculate the relative atomic mass, A_r , of sulfur to **two** decimal places.

$$A_r = \dots\dots\dots$$

[2]

(c) Isotopes of polonium, proton number 84, are produced by the radioactive decay of several elements including thorium, Th, proton number 90.

The isotope ^{213}Po is produced from the thorium isotope ^{232}Th .

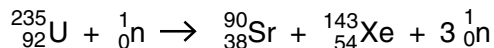
Complete the table below to show the atomic structures of the isotopes ^{213}Po and ^{232}Th .

isotope	number of		
	protons	neutrons	electrons
^{213}Po			
^{232}Th			

[3]

Radiochemical reactions, such as nuclear fission and radioactive decay of isotopes, can be represented by equations in which the nucleon (mass) numbers must balance and the proton numbers must also balance.

For example, the nuclear fission of uranium-235, ${}_{92}^{235}\text{U}$, by collision with a neutron, ${}_0^1\text{n}$, produces strontium-90, xenon-143 and three neutrons.



In this equation, the nucleon (mass) numbers balance because: $235 + 1 = 90 + 143 + (3 \times 1)$.

The proton numbers also balance because: $92 + 0 = 38 + 54 + (3 \times 0)$.

(d) In the first stage of the radioactive decay of ${}_{90}^{232}\text{Th}$, the products are an isotope of element *E* and an alpha-particle, ${}_2^4\text{He}$.

(i) By considering nucleon and proton numbers only, construct a balanced equation for the formation of the isotope of *E* in this reaction.



Show clearly the nucleon number and proton number of the isotope of *E*.

nucleon number of the isotope of *E*

proton number of the isotope of *E*

(ii) Hence state the symbol of the element *E*.

.....

[3]

[W'11 3 Q1]

15 (a) Explain what is meant by the term *nucleon number*.

.....

..... [1]

(b) Bromine exists naturally as a mixture of two stable isotopes, ${}^{79}\text{Br}$ and ${}^{81}\text{Br}$, with relative isotopic masses of 78.92 and 80.92 respectively.

(i) Define the term *relative isotopic mass*.

.....

.....

..... [2]

- (ii) Using the relative atomic mass of bromine, 79.90, calculate the relative isotopic abundances of ^{79}Br and ^{81}Br .

[3]

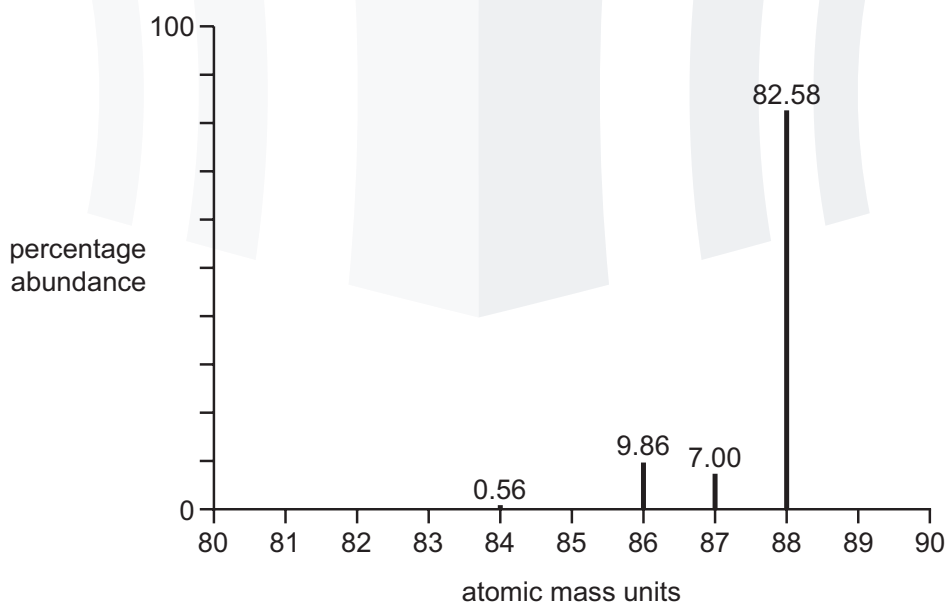
- (c) Bromine reacts with the element **A** to form a compound with empirical formula ABr_3 . The percentage composition by mass of ABr_3 is **A**, 4.31; Br, 95.69.

Calculate the relative atomic mass, A_r , of **A**.
Give your answer to **three** significant figures.

A_r of **A** = [3]

[S'14 2 Q1]

- 16** A sample of strontium, atomic number 38, gave the mass spectrum shown. The percentage abundances are given above each peak.



(ii) Explain why there are four different peaks in the mass spectrum of strontium.

.....
..... [1]

(iii) Calculate the atomic mass, A_r , of this sample of strontium.
Give your answer to **three** significant figures.

$A_r =$ [2]

[W'14 2 Q1]



- 17 (a) Chemists recognise that atoms are made of three types of particle.

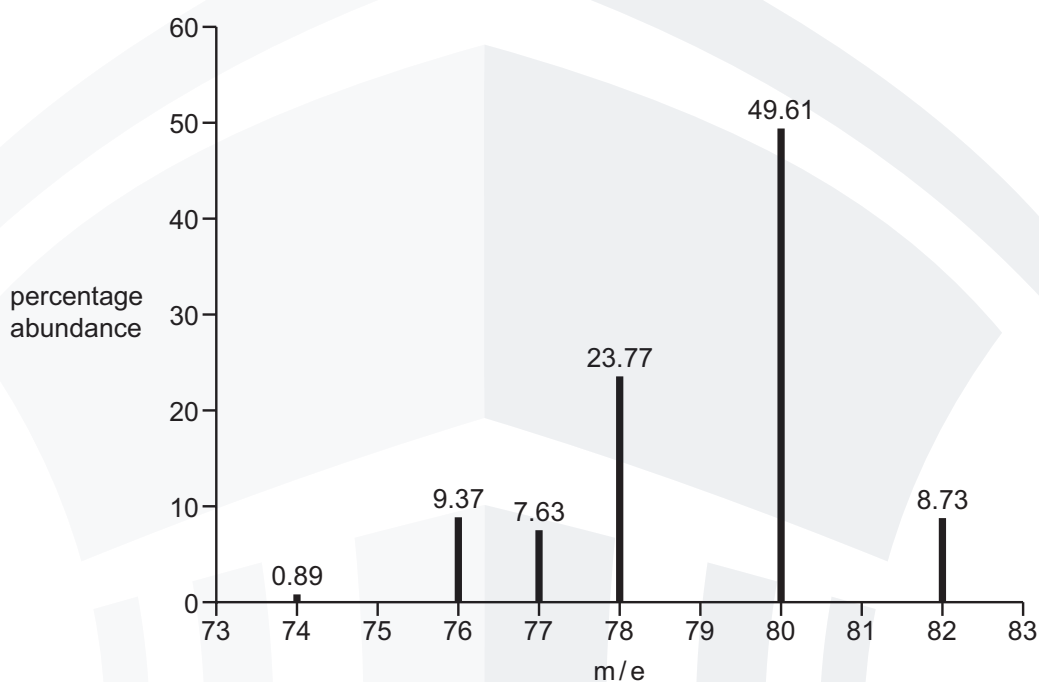
Complete the following table with their names and properties.

name of particle	relative mass	relative charge
		0
	1/1836	

[3]

- (b) The relative atomic mass of an element can be determined using data from its mass spectrum.

The mass spectrum of element X is shown, with the percentage abundance of each isotope labelled.



- (i) Define the terms *relative atomic mass* and *isotope*.

relative atomic mass

.....

.....

isotope

.....

[3]

- (ii) Use the data in the mass spectrum to calculate the relative atomic mass, A_r , of **X**.
Give your answer to **two** decimal places and suggest the identity of **X**.

A_r of **X**

identity of **X**

[2]

- (c) The element tellurium, Te, reacts with chlorine to form a single solid product, with a relative formula mass of 270. The product contains 52.6% chlorine by mass.

- (i) Calculate the molecular formula of this chloride.

molecular formula [3]

[M'15 1 Q1]

- 18 (a) Chemists recognise that atoms are made of three types of particle.

Complete the following table with their names and properties.

name of particle	relative mass	relative charge
		+1
	1/1836	

[3]

- (b) Most elements exist naturally as a mixture of isotopes, each with their own relative isotopic mass. The mass spectrum of an element reveals the abundances of these isotopes, which can be used to calculate the relative atomic mass of the element.

Magnesium has three stable isotopes. Information about two of these isotopes is given.

isotope	relative isotopic mass	percentage abundance
^{24}Mg	24.0	79.0
^{26}Mg	26.0	11.0

- (i) Define the term *relative isotopic mass*.

.....

 [2]

- (ii) The relative atomic mass of magnesium is 24.3.

Calculate the percentage abundance and hence the relative isotopic mass of the third isotope of magnesium. Give your answer to **three** significant figures

percentage abundance =

isotopic mass =

[3]

(c) Neon has three stable isotopes.

isotope	mass number	percentage abundance
1		9.25
2	20	90.48
3	21	0.27

(i) Define the term *relative atomic mass*.

.....
..... [2]

(ii) Use the relative atomic mass of neon, 20.2, to calculate the mass number of isotope 1.

mass number = [2]

[S'15 3 Q1]

20

(a) Complete the table to show the composition and identity of some atoms and ions.

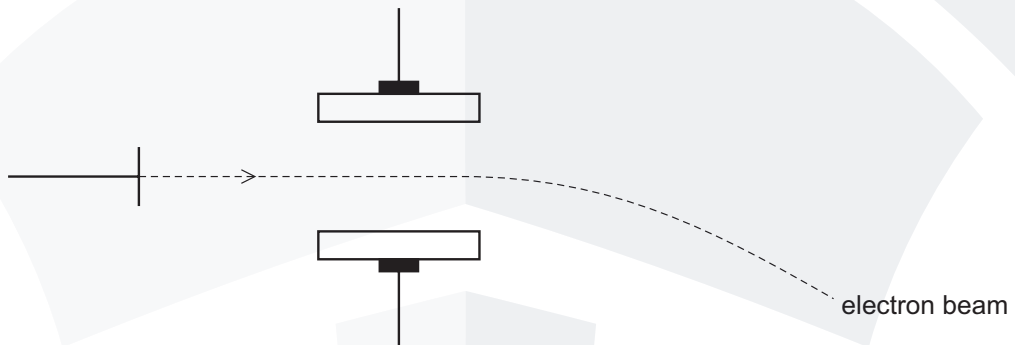
name of element	nucleon number	atomic number	number of protons	number of neutrons	number of electrons	overall charge
lithium	6	3	+1
oxygen	9	10
.....	54	26	26	24
.....	17	18	0

[4]

(b) Beams of protons, neutrons and electrons behave differently in an electric field due to their differing properties.

The diagram shows the path of a beam of electrons in an electric field.

Add and label lines to represent the paths of beams of protons and neutrons in the same field.



[3]

- (d) A sample of strontium exists as a mixture of four isotopes. Information about three of these isotopes is given in the table.

mass number	86	87	88
abundance	9.86%	7.00%	82.58%

- (i) Calculate the abundance of the fourth isotope.

abundance = % [1]

- (ii) The relative atomic mass of this sample of strontium is 87.71.

Calculate the mass number of the fourth isotope.

mass number = [2]

[S'16 1 Q1]

21

A sample of oxygen exists as a mixture of three isotopes. Information about two of these isotopes is given in the table.

mass number	16	17
abundance	99.76%	0.04%

(i) Calculate the abundance of the third isotope.

abundance = % [1]

(ii) The relative atomic mass of this sample of oxygen is 16.0044.

Calculate the mass number of the third isotope. You **must** show your working.

mass number = [2]

[S'16 2 Q1]

- 22 A naturally occurring sample of cerium contains only **four** isotopes. Data for **three** of the isotopes are shown in the table.

isotope	^{136}Ce	^{138}Ce	^{140}Ce	^{142}Ce
relative isotopic mass	135.907	137.906	139.905	to be calculated
percentage abundance	0.185	0.251	88.450	to be calculated

The A_r of the sample is 140.116.

Use these data to calculate the **relative isotopic mass** of the fourth isotope in this sample of cerium.

Give your answer to **three** decimal places.

relative isotopic mass = [3]

[M'17 Q1]

2 Atomic structure

2.3 Electrons: energy levels, atomic orbitals, ionisation energy



ELECTRONIC CONFIGURATION

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:

2.3 Electrons: energy levels, atomic orbitals, ionisation energy, electron affinity

- a) describe the number and relative energies of the s, p and d orbitals for the principal quantum numbers 1, 2 and 3 and also the 4s and 4p orbitals
- b) describe and sketch the shapes of s and p orbitals
- c) state the electronic configuration of atoms and ions given the proton number and charge, using the convention $1s^22s^22p^6$, etc.
- d)
 - (i) explain and use the term *ionisation energy*
 - (ii) explain the factors influencing the ionisation energies of elements
 - (iii) explain the trends in ionisation energies across a Period and down a Group of the Periodic Table (see also Section 9.1)
- e) deduce the electronic configurations of elements from successive ionisation energy data
- f) interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table
- g) explain and use the term *electron affinity*

DISCLAIMER

A complete discussion of the experimental evidence for the modern theory of atomic structure is beyond the scope of the CIE A Level Syllabus.

In this chapter only the results of the theoretical treatment will be described. These results will have to be memorized as “rules of the game,” but they will be used so extensively throughout the general chemistry course that the notation used will soon become familiar.

1

ELECTRON ARRANGEMENT

The electronic configuration describes the arrangement of electrons in atoms.

An atom's electrons are arranged outside the nucleus in energy levels (or shells).

Each shell or energy level holds a certain maximum number of electrons.

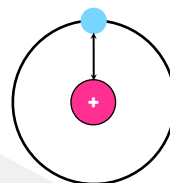
The energy of levels becomes greater as they go further from the nucleus and electrons fill energy levels in order.

2

IONISATION ENERGY

Ionisation energy is a measure of the energy needed to remove an electron from a gaseous atom or ion. It measures how strongly an atom or ion holds on to its electrons.

Attraction between the nucleus and an electron



The greater the pull of the nucleus, the harder it will be to pull an electron away from an atom.

3

FIRST IONISATION ENERGY

Ionisation energies give evidence for the arrangement of electrons in atoms in shells and sub-shells.

The first ionisation energy for an element is the energy needed to remove **one mole** of electrons from **one mole** of **gaseous atoms**.



4

SUCCESSIVE IONISATION ENERGIES

Successive ionisation energies for the same element measure the energy to remove a second, third, fourth electron and so on.

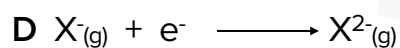
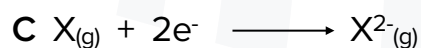
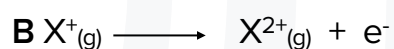


It is possible to measure energy changes involving ions which do not normally appear in chemical reactions.

5

SKILL CHECK 1

Which equation represents the second ionisation energy of an element X?



6

SKILL CHECK 2

Write equations to represent the first ionisation of:

- (a) potassium
- (b) argon
- (c) bromine
- (d) fluorine

7

SKILL CHECK 3

The successive ionisation energies kJmol^{-1} of element X are listed below. **Identify the group in the periodic table in which X occurs.**

Ionisation energies of X:

1st	2nd	3rd	4th	5th	6th	7th
950	1800	2700	4800	6000	12300	15000

8

SUCCESSIVE IONISATION ENERGIES

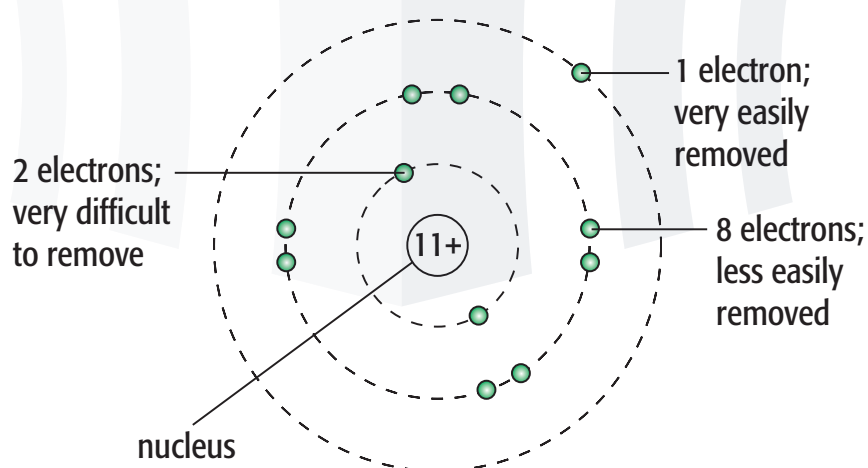
After an electron has been removed the rest of them will be more strongly attracted by the nucleus.

Hence more energy is required to pull the 2nd electron and thus the 2nd I.E. is greater than the 1st I.E.

Successive ionisation energies are always greater than the previous one.

9

SUCCESSIVE IONISATION ENERGIES



10

EVIDENCE OF ENERGY LEVELS

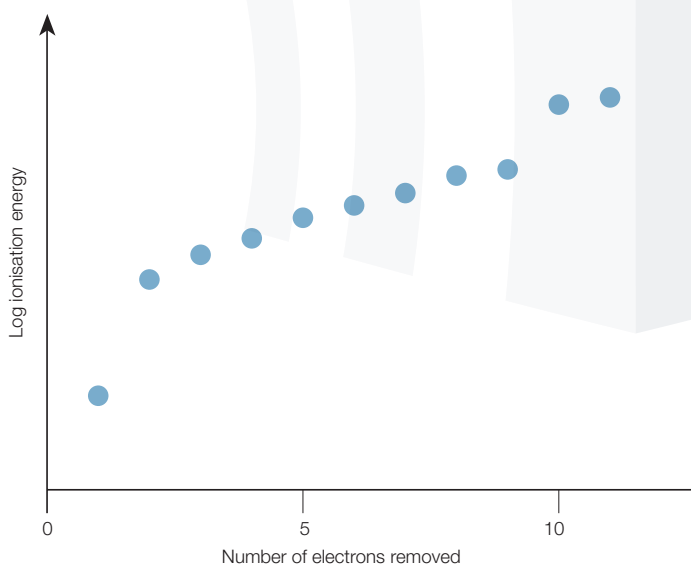
The arrangement of electrons in an atom of any element can be deduced from the values of successive ionisation energies.

The successive I.E of sodium illustrate the change clearly.

electron removed	1	2	3	4	5	6	7	8	9	10	11
ionisation energy	500	4600	6900	9500	13400	16600	20100	25500	28900	141000	158000

11

IONISATION ENERGIES OF SODIUM



The graph shows successive ionisation energies against the number of electrons removed for sodium.

12

IONISATION ENERGIES OF SODIUM

There is a big difference between **some** successive ionisation energies. For sodium the first big difference occurs between the 1st and 2nd ionisation energies.

These **large changes** indicate that for the **second** of these two ionisation energies, the electron being removed is from a shell **closer** to the nucleus.

13

IONISATION ENERGIES OF SODIUM

electron removed	1	2	3	4	5	6	7	8	9	10	11
ionisation energy	500	4600	6900	9500	13400	16600	20100	25500	28900	141000	158000

There is a **big jump** in the value of the **second** ionisation energy. This suggests that the second electron is in a shell closer to the nucleus than the first electron.

Taken together, the 1st and 2nd ionisation energies suggest that sodium has **one electron** in its **outer shell**.

14

IONISATION ENERGIES OF SODIUM

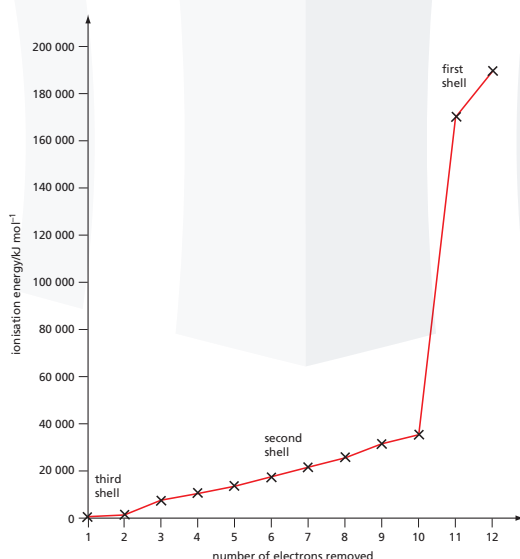
electron removed	1	2	3	4	5	6	7	8	9	10	11
ionisation energy	500	4600	6900	9500	13400	16600	20100	25500	28900	141000	158000

From the second to the ninth electrons removed there is only a **gradual** change in successive ionisation energies. This suggests that all these eight electrons are in the **same** shell.

There is a **big jump** in the value of the 10th ionisation energy. This suggests that the 10th electron is in a shell **closer** to the nucleus than the 9th electron.

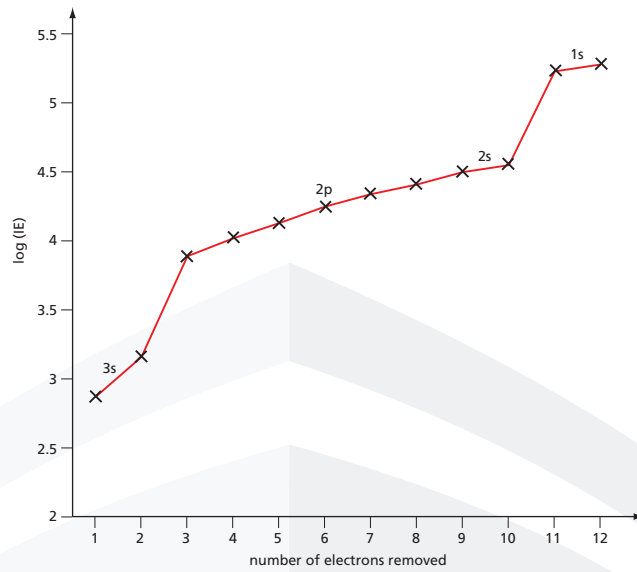
15

IONISATION ENERGIES OF MAGNESIUM



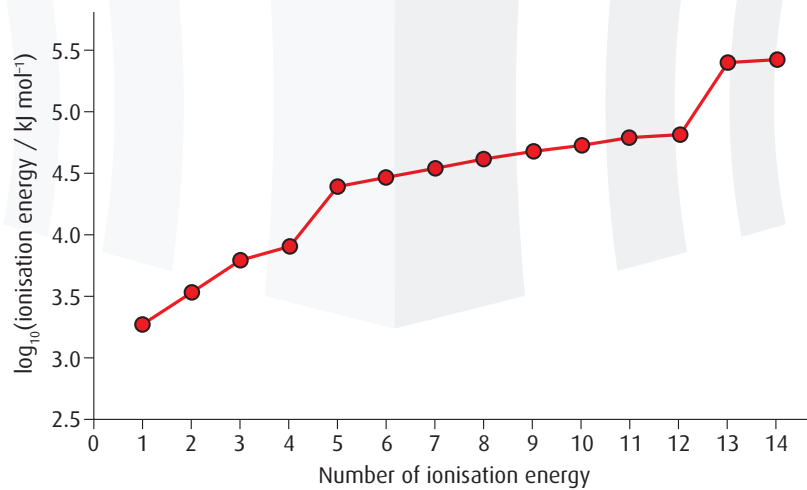
16

IONISATION ENERGIES OF MAGNESIUM



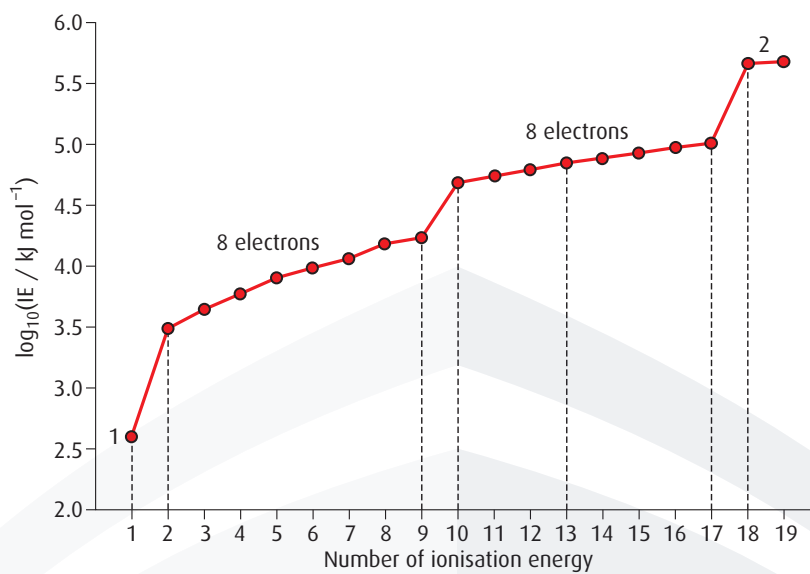
17

IONISATION ENERGIES OF SILICON



18

IONISATION ENERGIES OF POTASSIUM



19

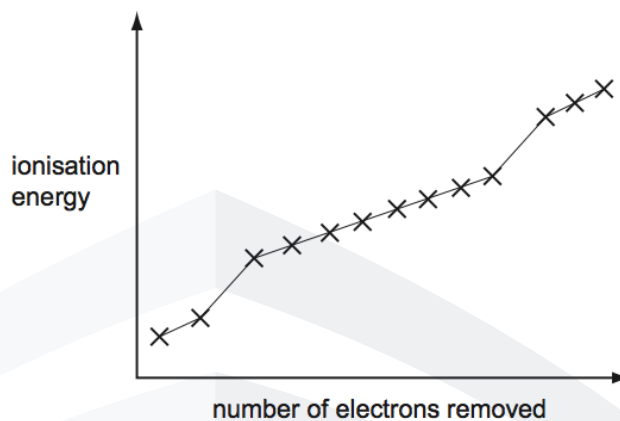
SKILL CHECK 4

Write an equation to represent the 5th ionisation energy of Fluorine.

20

SKILL CHECK 5

The graph shows the first thirteen ionisation energies for element X.



What group is X in?

21

SKILL CHECK 6

The first ionisation energies of four consecutive elements in the Periodic table are:

Sodium = 494 kJ mol⁻¹

Magnesium = 736 kJ mol⁻¹

Aluminium = 577 kJ mol⁻¹

Silicon = 786 kJ mol⁻¹

- Explain the general increase in ionisation energies from Sodium to Silicon.
- Explain why Aluminium has a lower first ionisation energy than Magnesium.

22

SKILL CHECK 7

The first six ionisation energies of an element are, or 1090, 2250, 4610, 6220, 37,800, and 47,300 kJ mol⁻¹. Which group in the Periodic Table does this element belong to? Explain your decision.

23

SKILL CHECK 8

The successive ionisation energies ΔH_i , of an element X are shown in the table below. Which group in the Periodic Table does X belong to?

	Number of electrons removed									
	1	2	3	4	5	6	7	8	9	10
$\Delta H_i / \text{kJ mol}^{-1}$	1000	2260	3390	4540	7010	8500	27100	31670	36580	43140

24

SUCCESSIVE IONISATION ENERGIES

We can use successive ionisation energies in this way to confirm:

- The simple electronic configuration of elements.
- The number of electrons in the outer shell of an element and hence the group to which the element belongs.

The successive ionisation energies for an element rise and there are big jumps in value each time electrons start to be removed from the next shell in towards the nucleus.

25

IONISATION ENERGIES OF OXYGEN

electron removed	1	2	3	4	5	6	7	8
ionisation energy	1310	3390	5320	7450	11000	13300	71300	84100

Large increases can be used to predict the group of any element. The electron configuration of oxygen is 2,6.

Since the large change is after the removal of 6 electrons, it signifies that there are 6 electrons in the shell farthest from the nucleus.

Therefore, Oxygen is in Group VI.

26

SUCCESSIVE IONISATION ENERGIES

Element	ELECTRONS REMOVED											
	1	2	3	4	5	6	7	8	9	10	11	
1	H	1310										
2	He	2370	5250									
3	Li	519	7300	11800								
4	Be	900	1760	14850	21000							
5	B	799	2420	3660	25000	32800						
6	C	1090	2350	4620	6220	37800	47300					
7	N	1400	2860	4580	7480	9450	53300	64400				
8	O	1310	3390	5320	7450	11000	13300	71300	84100			
9	F	1680	3370	6040	8410	11000	15200	17900	92000	106000		
10	Ne	2080	3950	6150	9290	12200	15200	20000	23000	117000	131400	
11	Na	494	4560	6940	9540	13400	16600	20100	25500	28900	141000	158700

27

SKILL CHECK 9

The successive ionisation energies, in kJ mol^{-1} , of different elements are given below. Which groups are the following elements in?

	1	2	3	4	5	6	7	8
A	799	2420	3660	25000				
B	736	1450	7740	10500				
C	418	3070	4600	5860				
D	870	1800	3000	3600	5800	7000	13200	
E	950	1800	2700	4800	6000	12300		

28

SKILL CHECK 10

The successive ionisation energies of beryllium are 900, 1757, 14,849 and 21,007 kJ mol⁻¹.

- What is the atomic number of beryllium?
- Why do successive ionisation energies of beryllium always get more endothermic?
- To which group of the Periodic Table does this element belong?

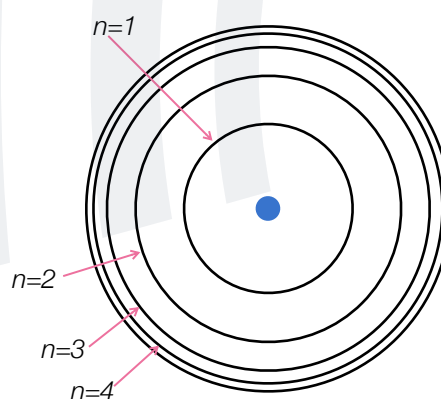
29

SHELLS (ENERGY LEVELS)

The principal energy levels are designated $n = 1, 2, 3$, and so forth.

The energy levels are **not** equally spaced.

The energy gap between successive levels gets increasingly smaller as the levels move further from the nucleus.



30

SUB-LEVELS (SUB-SHELLS)

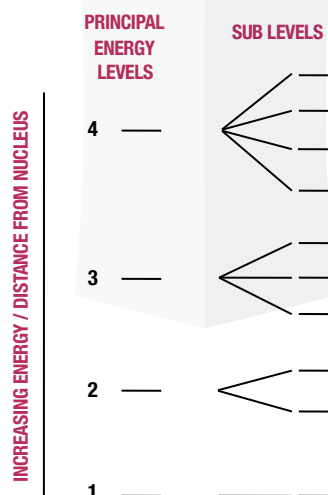
Electron shells are numbered 1,2,3 etc. These numbers are known as the **principle quantum numbers**.

Each energy level (shell) consists of a number of sub-levels (sub-shells), labeled **s, p, d, or f**.

Energy Level	Number of sub-levels	Name of sub-levels
1	1	s
2	2	s, p
3	3	s, p, d
4	4	s, p, d, f

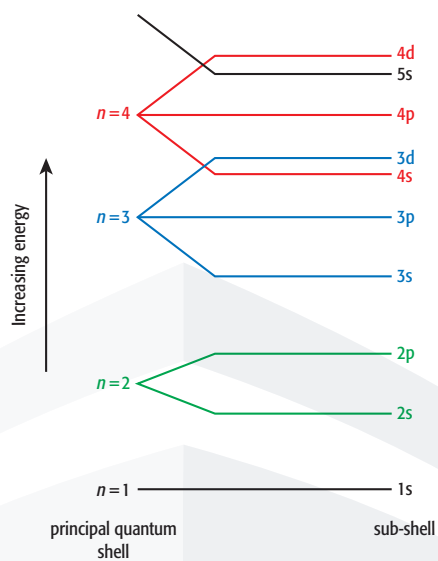
31

SUB-LEVELS (SUB-SHELLS)



32

SUB-LEVELS (SUB-SHELLS)



SUB-LEVELS

Each sub-level can hold a certain maximum number of electrons.

Type of sub-level	Maximum # of electrons
s	2
p	6
d	10
f	14

ORBITALS

An **atomic orbital** is a region of space around the nucleus of an atom which can be occupied by one or two electrons **only**.

Each sub-level contains a **fixed number** of orbitals that contain electrons.

Type of sub-level	Maximum # of electrons	Number of orbitals
s	2	1
p	6	3
d	10	5
f	14	7

35

ORBITALS

Electrons are viewed as charged clouds and the region, which encloses almost all the charge cloud, is the orbital.

The region in space where the probability of finding an electron in maximum is called the orbital.

The boundary surface encloses the region where the probability of finding an electron is high.

The orbitals are of different **three-dimensional** shapes and are named **s, p, d, f** etc.

36

ORBITALS

The cluster of dots show the probability of finding an electron at different distances from the nucleus.



37

SHELLS, SUB SHELLS AND ORBITALS

Energy Level	Type of sub-level	Number of orbitals	Maximum # of electrons
1	s	1	2
2	s	1	2
	p	3	6
3	s	1	2
	p	3	6
	d	5	10
4	s	1	2
	p	3	6
	d	5	10

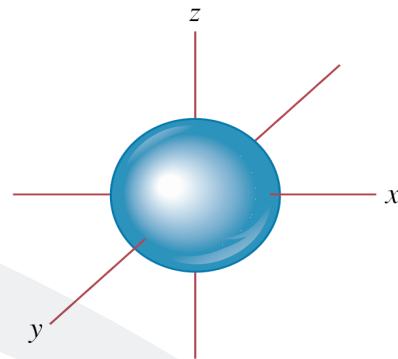
38

“S” ORBITAL

The s orbital is spherically shaped. There is **only one** s orbital for each shell.

The 2s orbital in the second principal quantum shell has the same shape as the 1s orbital in the first quantum shell.

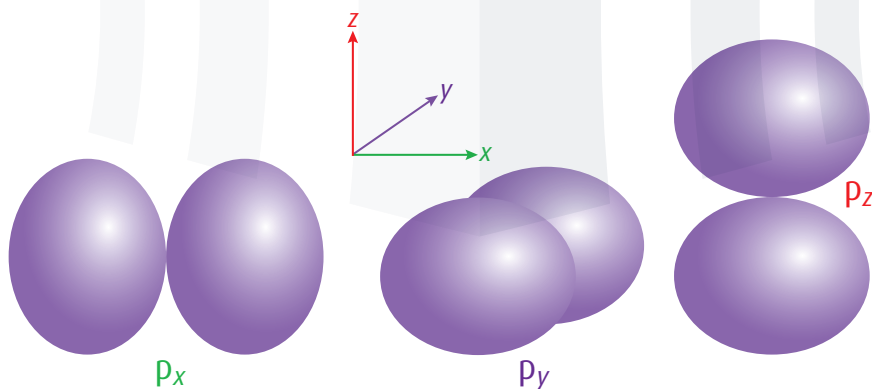
They are both spherical, but electrons in the 2s orbital have more energy than electrons in the 1s orbital.



39

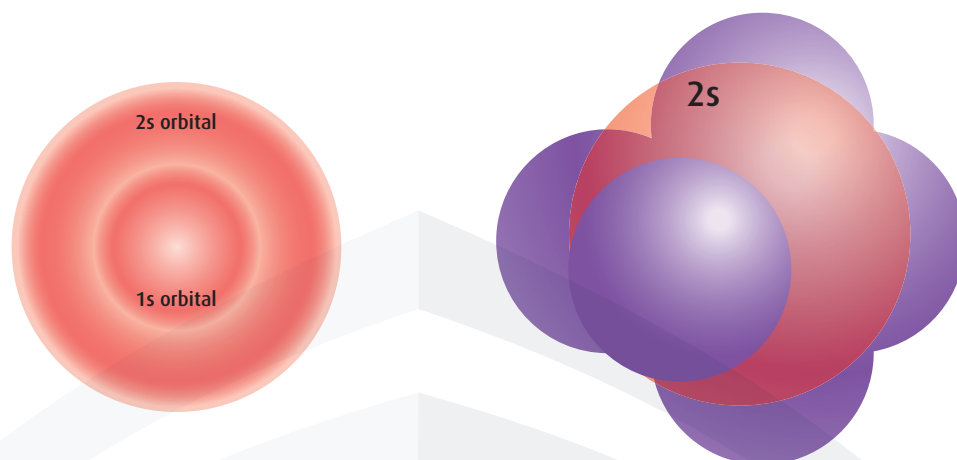
“P” ORBITAL

For each shell (**except the first**), there are three p orbitals.



40

THE FIRST TWO SHELLS



41

ELECTRONIC CONFIGURATION

Electrons are distributed in different energy levels in the atom of the element.

The order in which they fill up the sub-levels is governed by **stability**.

When electrons fill up the orbitals having the **least energy** they attain **maximum stability**.

There are three principles that describe how electrons fill up in orbitals.

Aufbau Principle: Electrons enter the orbital that is available with the **lowest** energy. The orbitals are arranged in the order of increasing energy and the electrons are added until the proper number of electrons for the element have been accommodated

42

ELECTRONIC CONFIGURATION

Pauli's Exclusion Principle: No orbital can accommodate more than two electrons. If there are two electrons in an orbital, they must have opposite spin.

Hund's Rule of Maximum Multiplicity: When there are a number of orbitals of equal energy, electrons first fill them up individually and then get paired. By filling up individually, **mutual repulsion** between electrons is avoided and thereby maximum stability is achieved.

43

ELECTRON SPIN

Electrons are all identical. The only way of distinguishing them is by describing how their **energies** and **spatial distributions** differ.

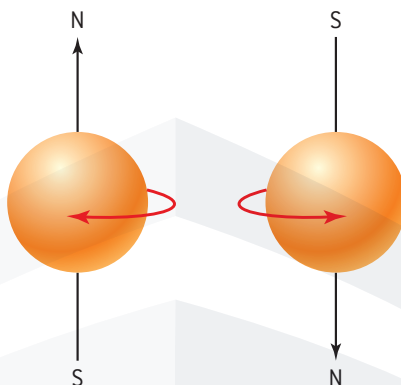
Thus an electron in a 1s orbital is different from an electron in a 2s orbital because it occupies a different region of space **closer to the nucleus**, causing it to have **less** potential energy.

An electron in a $2p_x$ orbital differs from an electron in a $2p_y$ orbital because although they have exactly the same potential energy, they occupy different regions of space.

44

ELECTRON SPIN

There can only be two electrons in each orbital, and they must have opposite directions of spin.



45

ELECTRON SPIN

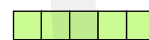
For convenience, an “**electrons-in-boxes**” notation is used to represent the electrons in these atomic orbitals:



s sub-level



p sub-level



d sub-level

Each box represents one orbital:

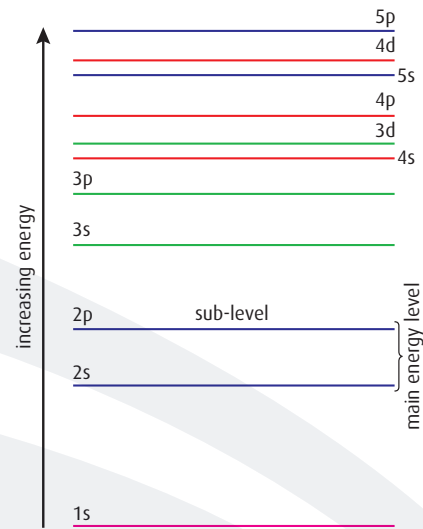


an orbital with electrons in opposite spins

46

ORDER OF FILLING ORBITALS

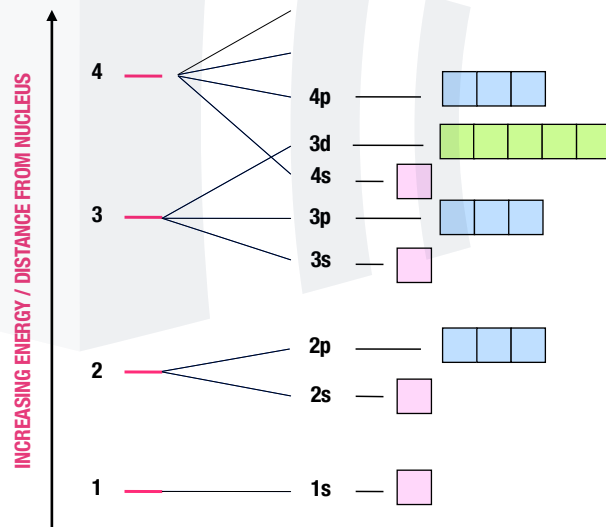
The **principal energy levels** (shells) get closer together as you get further from the nucleus. This results in an overlap of sub-levels.



47

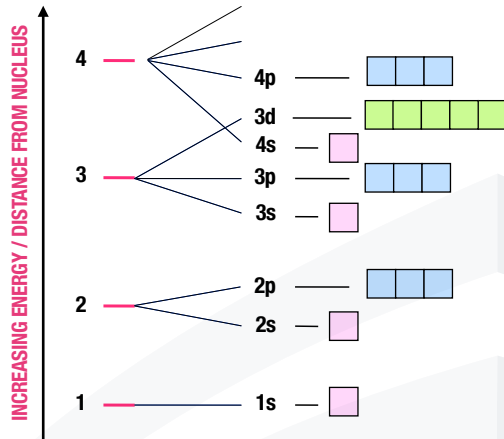
ORDER OF FILLING ORBITALS

The first example of this overlap occurs when the 4s orbital is filled before the 3d orbital



48

THE 'AUFBAU' PRINCIPAL



The following sequence will show the 'building up' of the electronic structures of the first 36 elements in the periodic table.

Electrons are shown as **half-headed** arrows and can spin in one of two directions.

Orbitals are color-coded as below:

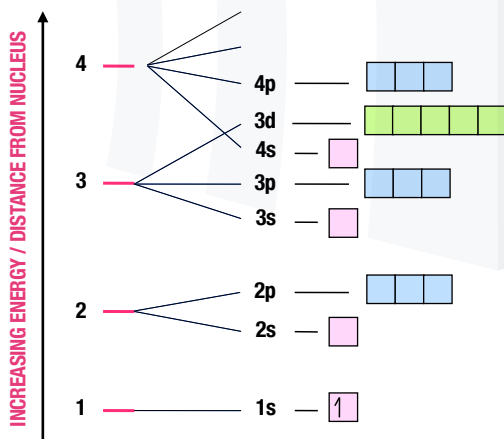
s orbitals □

p orbitals □

d orbitals □

49

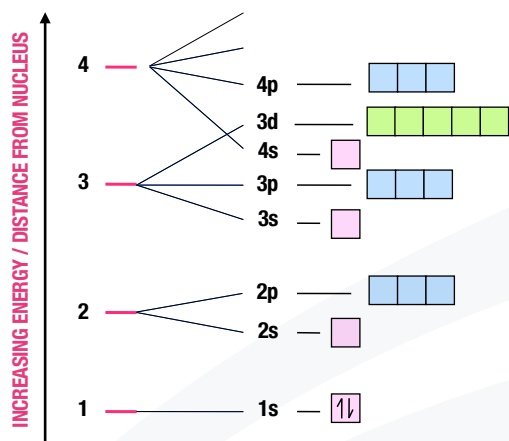
HYDROGEN


 $1s^1$

Hydrogen atoms have one electron. This goes into a vacant orbital in the lowest available energy level.

50

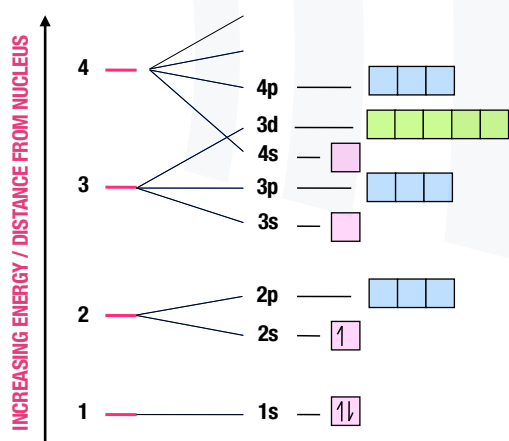
HELIUM



Every orbital can contain 2 electrons, provided the electrons are spinning in opposite directions. The two electrons in a helium atom both go in the 1s orbital.

51

LITHIUM

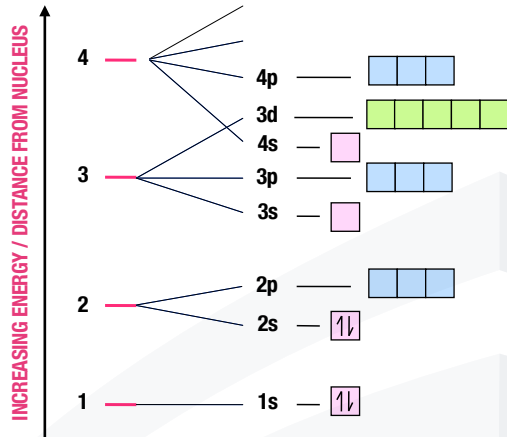


1s orbitals can hold a maximum of two electrons so the third electron in a lithium atom must go into the next available orbital of higher energy. This will be further from the nucleus in the second principal energy level.

The second principal level has two types of orbital (s and p). An s orbital is lower in energy than a p.

52

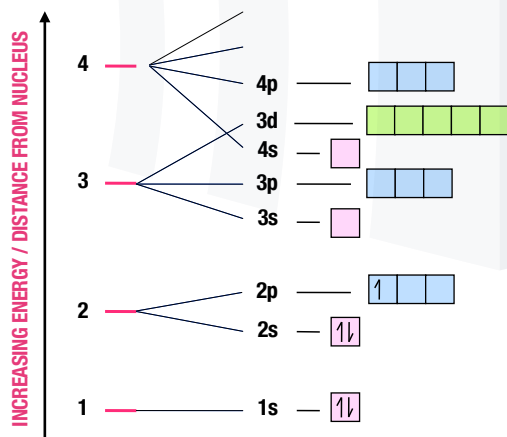
BERYLLIUM



Beryllium atoms have four electrons so the fourth electron pairs up in the 2s orbital. The 2s sub level is now full.

53

BORON

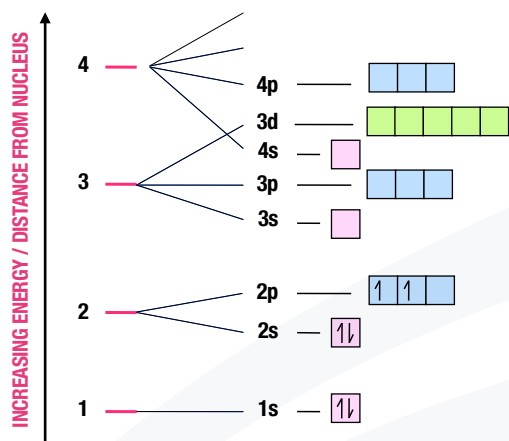


As the 2s sub level is now full, the fifth electron goes into one of the three p orbitals in the 2p sub level.

The 2p orbitals are slightly higher in energy than the 2s orbital.

54

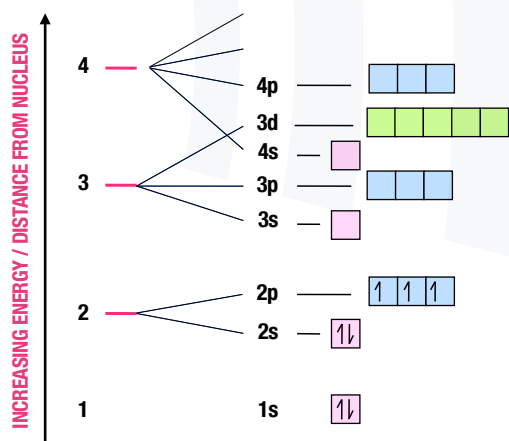
CARBON



The next electron in doesn't pair up with the one already there. This would give rise to **repulsion between the similarly charged species**. Instead, it goes into another p orbital which means **less repulsion, lower energy and more stability**.

55

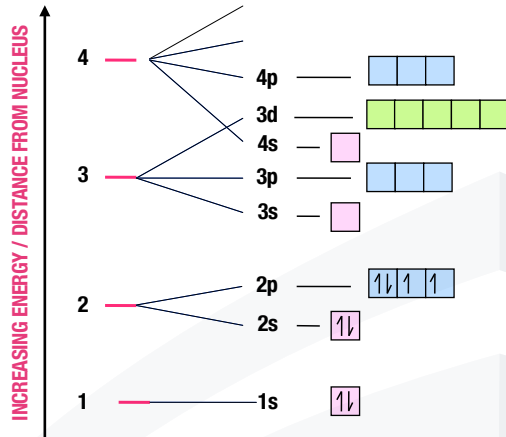
NITROGEN



The next electron will not pair up but goes into a vacant p orbital. All three electrons are now unpaired. This gives **less repulsion, lower energy and therefore more stability**.

56

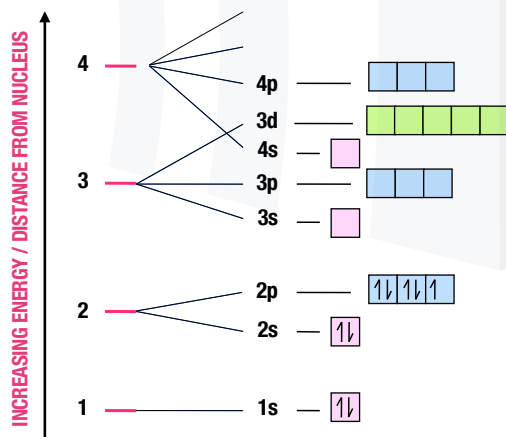
OXYGEN



With all three orbitals half-filled, the eighth electron in an oxygen atom must now pair up with one of the electrons already there.

57

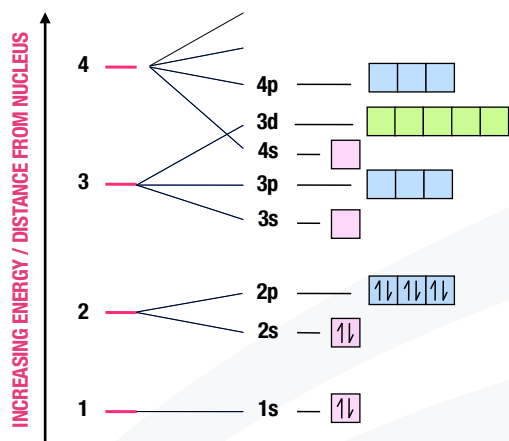
FLUORINE



The electrons continue to pair up with those in the half-filled orbitals.

58

NEON



The electrons continue to pair up with those in the half-filled orbitals.

The 2p orbitals are now completely filled and so is the second principal energy level.

In the older system of describing electronic configurations, this would have been written as 2,8.

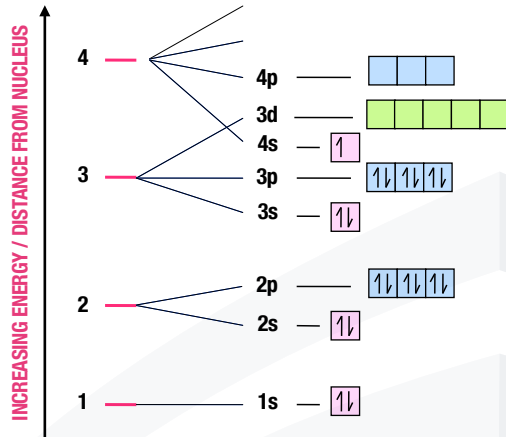
59

SODIUM TO ARGON



60

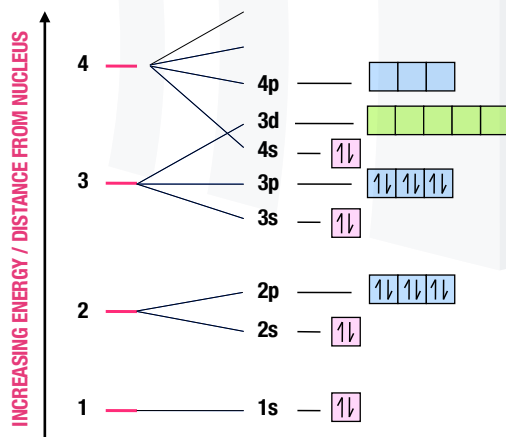
POTASSIUM



Because the principal energy levels get closer together as you go further from the nucleus coupled with the splitting into sub energy levels, the 4s orbital is of a **LOWER ENERGY** than the 3d orbitals so it gets filled first.

61

CALCIUM



As expected, the next electron pairs up to complete a filled 4s orbital.

62

ELEMENTS WITH PROTON NUMBERS 1 TO 10

Period 1									H								He
Atomic no.									1								2
Electron shell structure									1								2
Electron sub-shell structure									$1s^1$								$1s^2$

Period 2	Li	Be	B	C	N	O	F	Ne
Atomic no.	3	4	5	6	7	8	9	10
Electron shell structure	2, 1	2, 2	2, 3	2, 4	2, 5	2, 6	2, 7	2, 8
Electron sub-shell structure	$1s^2$ $2s^1$	$1s^2$ $2s^2$	$1s^2$ $2s^2 2p^1$	$1s^2$ $2s^2 2p^2$	$1s^2$ $2s^2 2p^3$	$1s^2$ $2s^2 2p^4$	$1s^2$ $2s^2 2p^5$	$1s^2$ $2s^2 2p^6$

63

ELEMENTS WITH PROTON NUMBERS 11 TO 20

Period 3	Na	Mg	Al	Si	P	S	Cl	Ar
Atomic no.	11	12	13	14	15	16	17	18
Electron shell structure	2, 8, 1	2, 8, 2	2, 8, 3	2, 8, 4	2, 8, 5	2, 8, 6	2, 8, 7	2, 8, 8
Electron sub-shell structure	$1s^2$ $2s^2 2p^6$ $3s^1$	$1s^2$ $2s^2 2p^6$ $3s^2$	$1s^2$ $2s^2 2p^6$ $3s^2 3p^1$	$1s^2$ $2s^2 2p^6$ $3s^2 3p^2$	$1s^2$ $2s^2 2p^6$ $3s^2 3p^3$	$1s^2$ $2s^2 2p^6$ $3s^2 3p^4$	$1s^2$ $2s^2 2p^6$ $3s^2 3p^5$	$1s^2$ $2s^2 2p^6$ $3s^2 3p^6$

Period 4	K	Ca
Atomic no.	19	20
Electron shell structure	2, 8, 8, 1	2, 8, 8, 2
Electron sub-shell structure	$1s^2$ $2s^2 2p^6$ $3s^2 3p^6$ $4s^1$	$1s^2$ $2s^2 2p^6$ $3s^2 3p^6$ $4s^2$

SKILL CHECK 11

Copy and complete the following information for the quantum shell with **principal quantum number 3**.

- (a) total number of sub-shells
- (b) total number of orbitals
- (c) number of different types of orbital
- (d) maximum number of electrons in the shell

65

SKILL CHECK 12

An atom has eight electrons. Which diagram shows the electronic configuration of this atom in its lowest energy state?

- A**

↑↓	↑↓	↑↓	↑↓		
----	----	----	----	--	--
- B**

↑↓	↑↓	↑↓	↑	↑	
----	----	----	---	---	--
- C**

↑↓	↑↓	↑↓	↑		↑
----	----	----	---	--	---
- D**

↑↓	↑↓	↑	↑	↑	↑
----	----	---	---	---	---

66

SKILL CHECK 13

Fill in the outer electrons of a phosphorus atom in the boxes below.



67

SKILL CHECK 14

Give the electron orbital configuration for the ground state of the following atoms or ions:

- (a) N
- (b) O^{2-}
- (c) Ca^{2+}
- (d) Al^{3+}
- (e) P^{3-}

68

SKILL CHECK 15

Write the full electronic configuration of:

- (a) ^{75}As
- (b) $^{75}\text{As}^{3-}$
- (c) ^{32}S
- (d) $^{32}\text{S}^{2-}$

69

SKILL CHECK 16

Name all element in the third period (row) of the periodic table with the following:

- a** three valence electrons
- b** four $3p$ electrons
- c** six $3p$ electrons
- d** two $3s$ electrons and no $3p$ electrons

70

EXCEPTIONS IN TRANSITION ELEMENTS

Though the s orbital is at lower energy level than the d of the penultimate shell, after the filling of the d sub-level, the order changes.

The d electrons, because of the shape of the d orbital, penetrate into the region of space between the nucleus and the s orbital and repel the s electrons and push them to higher energy level.

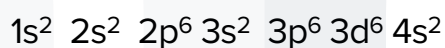
Before filling: $1s\ 2s\ 2p\ 3s\ 3p\ 4s\ 3d$

After filling: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^x\ 4s^2$

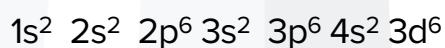
71

EXCEPTIONS IN TRANSITION ELEMENTS

Thus the electronic configuration of iron is



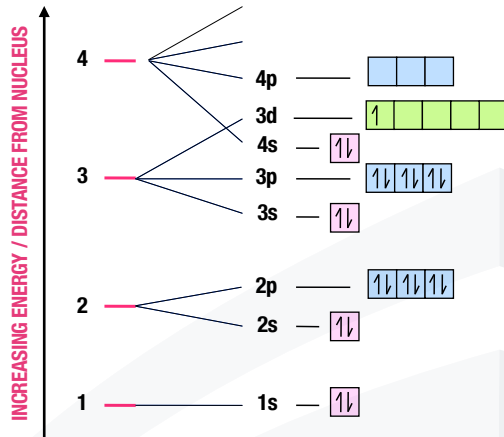
and not



Remember: 3d is higher than 4s in terms of energy levels!

72

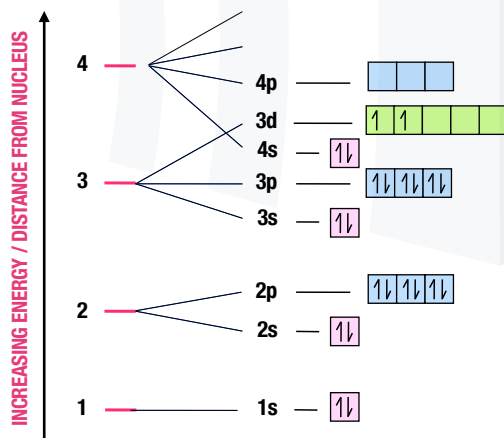
SCANDIUM



With the lower energy 4s orbital filled, the next electrons can now fill the 3d orbitals. There are five d orbitals. They are filled according to Hund's Rule.

73

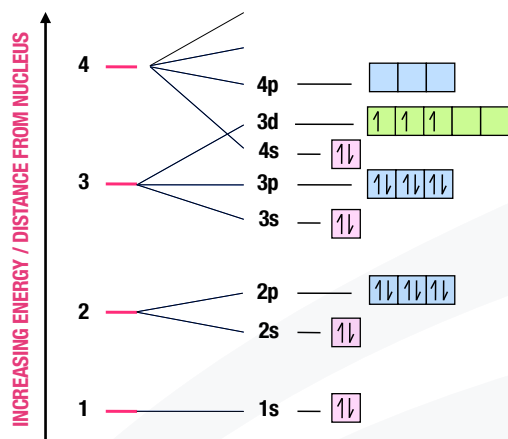
TITANIUM



The 3d orbitals are filled according to Hund's rule so the next electron doesn't pair up but goes into an empty orbital in the same sub level.

74

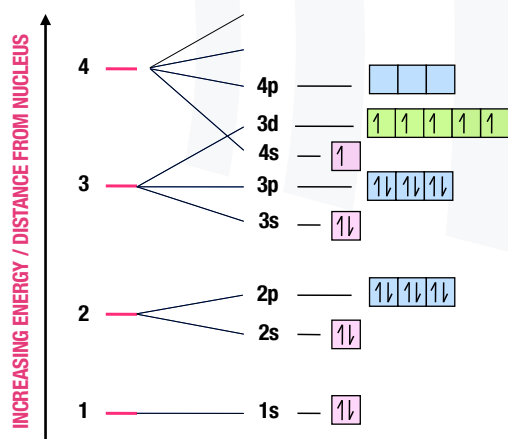
VANADIUM



The 3d orbitals are filled according to Hund's rule so the next electron doesn't pair up but goes into an empty orbital in the same sub level.

75

CHROMIUM

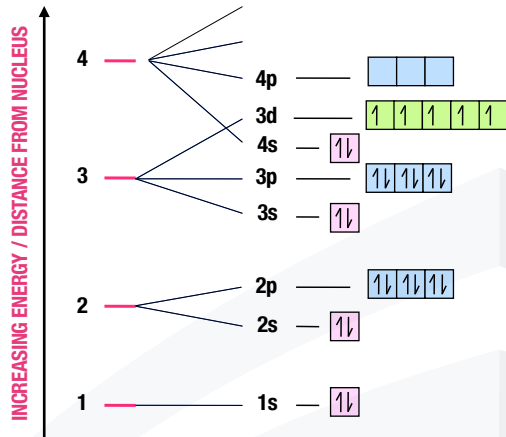


One would expect the configuration of chromium atoms to end in $3d^4 4s^2$.

To achieve a more stable arrangement of lower energy, one of the 4s electrons is promoted into the 3d to give six unpaired electrons with lower repulsion.

76

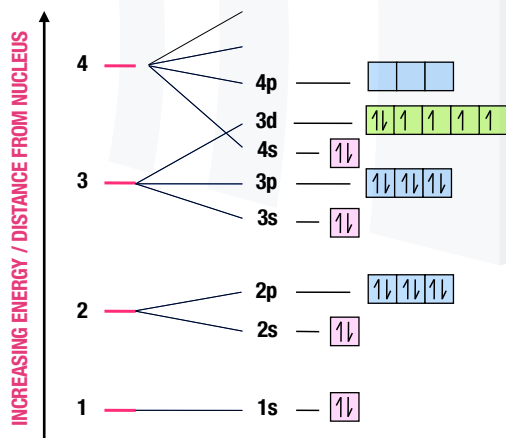
MANGANESE



The new electron goes into the 4s to restore its filled state.

77

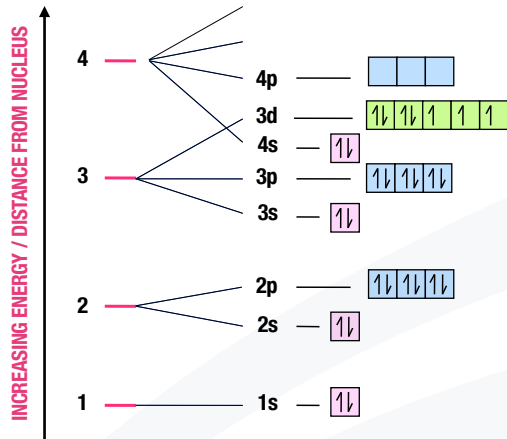
IRON



Orbitals are filled according to Hund's Rule. They continue to pair up.

78

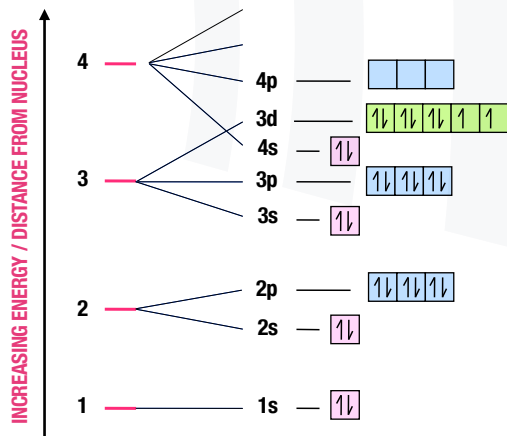
COBALT



Orbitals are filled according to Hund's Rule. They continue to pair up.

79

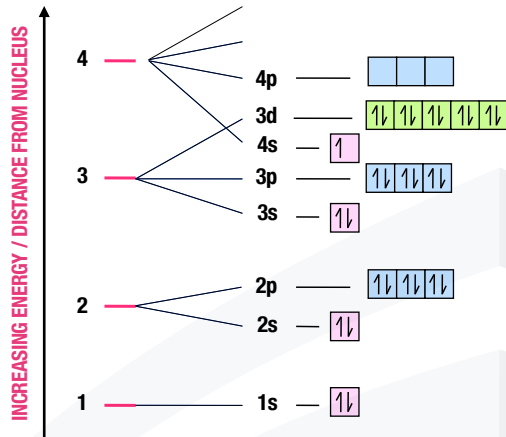
NICKEL



Orbitals are filled according to Hund's Rule. They continue to pair up.

80

COPPER

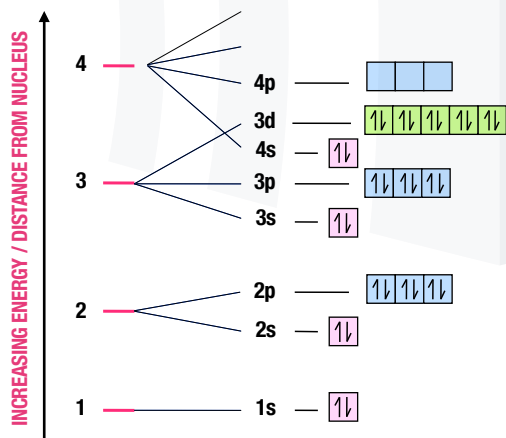


One would expect the configuration of chromium atoms to end in $3d^9 4s^2$.

To achieve a more stable arrangement of lower energy, one of the 4s electrons is promoted into the 3d.

81

ZINC

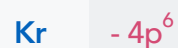


The electron goes into the 4s to restore its filled state and complete the 3d and 4s orbital filling.

82

GALLIUM TO KRYPTON

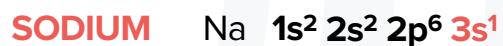
The 4p orbitals are filled in exactly the same way as those in the 2p and 3p sub levels:



83

ELECTRONIC CONFIGURATION OF IONS

Metallic elements, belonging to Group I, II and III form positively charged ions by losing electrons in their outermost shell, so that the ions may be iso-electronic with the preceding noble gas.

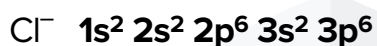


(1 electron removed from the 3s orbital)

84

ELECTRONIC CONFIGURATION OF IONS

Non-metallic elements belonging to Group V, VI and VII form negative ions by accepting electrons so that they achieve the noble gas configuration:



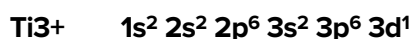
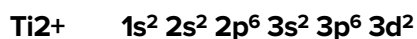
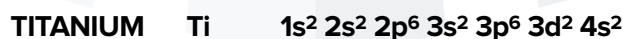
(1 electron added to the 3p orbital)

85

TRANSITION METAL IONS

When transition metals form ions, electrons are lost first from the outermost s orbital and then from the penultimate d sub-level.

Electrons in the 4s orbital are removed before any electrons in the 3d orbitals.



86

SKILL CHECK 17

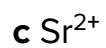
Write electronic configurations for the following ions:



87

SKILL CHECK 18

Write the electron configuration for each ion.



88

SKILL CHECK 19

Q. What is the order of increasing energy of the listed orbitals in the atom of titanium?

- A 3s 3p 3d 4s
- B 3s 3p 4s 3d
- C 3s 4s 3p 3d
- D 4s 3s 3p 3d

89

SKILL CHECK 20

A simple ion X^+ contains eight protons.

What is the electronic configuration of X^+ ?

- A $1s^2 2s^1 2p^6$
- B $1s^2 2s^2 2p^3$
- C $1s^2 2s^2 2p^5$
- D $1s^2 2s^2 2p^7$

90

SKILL CHECK 21

Write down the electronic configurations of the following ions:

A bromide

B magnesium

C iron(II)

D copper (II)

E iron(III)

91

SKILL CHECK 22

Q. Determine the number of unpaired electrons in each of these atoms:

A phosphorus

B chromium

C oxygen

92

SKILL CHECK 23

Use the periodic table to determine the element corresponding to each electron configuration.

- A $[\text{Ar}] 4s^2 3d^{10} 4p^6$
- B $[\text{Ar}] 4s^2 3d^2$
- C $[\text{Kr}] 5s^2 4d^{10} 5p^2$
- D $[\text{Kr}] 5s^2$

93

PERIODIC TABLE

The modern Periodic Table is arranged such that elements with similar electronic configuration lie in vertical groups.

Thus elements with electronic configuration ending up as ns^1 are put in one group while those that end up as ns^2 are put in another group.

The elements that fill up the s orbital of the highest energy level are said to belong to the s block, comprising of Groups 1 and 2.

94

PERIODIC TABLE

The elements that similarly fill up the p orbitals of the highest energy are said to belong to the p block, which comprises of Groups 13 to 0.

So there are two columns in the s block and six columns in the p block.

The elements that fill up the d sub-level of the penultimate shell are called the d block elements or the Transition Metal series.

95

SKILL CHECK 24

Write down the last term of the electronic configuration for the elements in the table, the sequence for Hydrogen has been entered for you. Label the s, p and d blocks on the table.

1s ¹																		

96

ELECTRONIC CONFIGURATION WS 1

1 Complete the electronic configurations of atoms of the following elements:

a) Phosphorus: [Ne].....

b) Cobalt: [Ar].....

2 Fill in the outer electrons of a phosphorus atom in the boxes below:

$3s$	<input style="width: 40px; height: 20px; border: 1px solid black;" type="text"/>	$3p$	<input style="width: 40px; height: 20px; border: 1px solid black;" type="text"/>	<input style="width: 40px; height: 20px; border: 1px solid black;" type="text"/>	<input style="width: 40px; height: 20px; border: 1px solid black;" type="text"/>
------	--	------	--	--	--

3 The successive ionisation energies of an element, X, are given in the table. To which group of the periodic table does element X belong?

Ionisation	Ionisation energy/ kJ mol^{-1}
1st	1 000
2nd	2 260
3rd	3 390
4th	4 540
5th	6 990
6th	8 490
7th	27 100
8th	31 700
9th	36 600
10th	43 100

.....

5 Write down the complete electronic configurations for the following elements:

a) Mn:

b) Mn^{2+} :

c) Cu^{2+} :

- 6 a) Explain what you understand by the word 'orbital' as applied to electrons.

.....
.....

- b) Draw an s- and a p- orbital.

- c) How does a 1s orbital differ from a 2s orbital?

.....

- d) How many electrons are there in:

i. a 3d orbital?

ii. orbitals with a principal quantum number of 3?

ELECTRONIC CONFIGURATION WS 2

- 1 Successive ionisation energies of an element X in kJ/mol are as follows:

578	1817	2745	11578	14831	18378
-----	------	------	-------	-------	-------

Which one of the following is X?

- A boron
 B carbon
 C aluminium
 D silicon
- 2 Which one of the rows giving information about the fourth period of the periodic table is correct?

	Total number of orbitals	The number of different types of orbital	Maximum number of electrons in the shell
A	4	2	8
B	9	2	18
C	9	3	8
D	9	3	18

- 3 What is the order of increasing energy of the orbitals within a single energy level?
- A $d > s < f < p$
 B $s < p < d < f$
 C $p < s < f < d$
 D $f < d < p < s$
- 4 What is the condensed electronic configuration for Co^{3+} ?
- A $[\text{Ar}]4s^23d^5$
 B $[\text{Ar}]4s^23d^4$
 C $[\text{Ar}]3d^6$
 D $[\text{Ar}]4s^13d^5$
- 5 Which are the values of the successive ionisation energies for an element in Group 14 of the periodic table?
- A 496, 738, 578, 789, 1012, 1000
 B 578, 1817, 2745, 11578, 14831, 18378
 C 1086, 2353, 4621, 6223, 37832, 47278
 D 1314, 1000, 941, 869, 812

- 6 Which are the values for the first ionisation energies of consecutive elements in the same period?
- A 496, 738, 578, 789, 1012, 1000 C 1086, 2353, 4621, 6223, 37832, 47278
- B 578, 1817, 2745, 11578, 14831, 18378 D 1314, 1000, 941, 869, 812

- 7 *Use of the Data Booklet is relevant to this question.*

In the gas phase, aluminium and a transition element require the same amount of energy to form one mole of an ion with a 2+ charge.

What is the transition element?

- A Co
B Cr
C Cu
D Ni

[W'02 3]

- 8 The successive ionisation energies, in kJ mol^{-1} , of an element X are given below.

870 1800 3000 3600 5800 7000 13 200

What is X?

- A ${}_{33}\text{As}$ B ${}_{40}\text{Zr}$ C ${}_{52}\text{Te}$ D ${}_{53}\text{I}$

[S'03 4]

- 9 Which of the following particles would, on losing an electron, have a half-filled set of p orbitals?

- A C^- B N C N^- D O^+

[S'04 5]

- 10 The table gives the successive ionisation energies for an element X.

	1st	2nd	3rd	4th	5th	6th
ionisation energy / kJ mol^{-1}	950	1800	2700	4800	6000	12300

What could be the formula of the chloride of X?

- A XCl B XCl_2 C XCl_3 D XCl_4

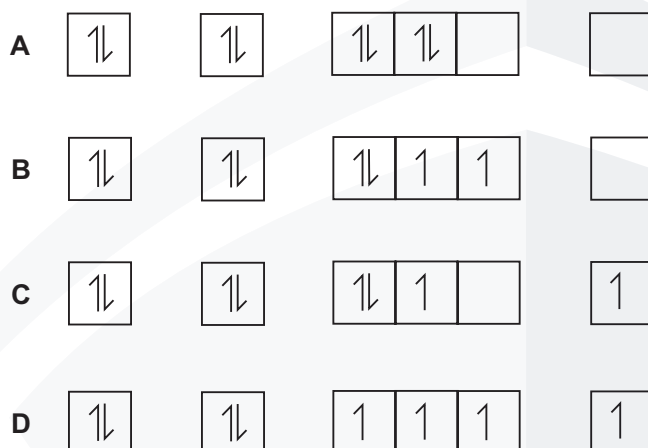
[W'03 5]

- 11 What is the order of increasing energy of the listed orbitals in the atom of titanium?
- A 3s 3p 3d 4s
 B 3s 3p 4s 3d
 C 3s 4s 3p 3d
 D 4s 3s 3p 3d

[S'04 4]

- 12 An atom has eight electrons.

Which diagram shows the electronic configuration of this atom in its lowest energy state?



[W'04 5]

- 13 The first six ionisation energies of four elements, **A** to **D**, are given.

Which element is most likely to be in Group IV of the Periodic Table?

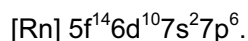
ionisation energy / kJ mol ⁻¹	1st	2nd	3rd	4th	5th	6th
A	494	4560	6940	9540	13400	16600
B	736	1450	7740	10500	13600	18000
C	1090	2350	4610	6220	37800	47000
D	1400	2860	4590	7480	9400	53200

[S'05 3]

- 14 What is the electronic configuration of an element with a **second** ionisation energy higher than that of each of its neighbours in the Periodic Table?
- A $1s^2 2s^2 2p^6 3s^2$
 B $1s^2 2s^2 2p^6 3s^2 3p^1$
 C $1s^2 2s^2 2p^6 3s^2 3p^2$
 D $1s^2 2s^2 2p^6 3s^2 3p^3$

[S'05 3]

- 15 In 1999, researchers working in the USA believed that they had made a new element and that it had the following electronic structure.



In which group of the Periodic Table would you expect to find this element?

- A II B IV C VI D 0

[S'11 2 13]

- 16 Gallium nitride, GaN, could revolutionise the design of electric light bulbs because only a small length used as a filament gives excellent light at low cost.

Gallium nitride is an ionic compound containing the Ga^{3+} ion.

What is the electron arrangement of the nitrogen ion in gallium nitride?

- A $1s^2 2s^2$
 B $1s^2 2s^2 2p^3$
 C $1s^2 2s^2 2p^4$
 D $1s^2 2s^2 2p^6$

[S'06 3]

- 17 *Use of the Data Booklet is relevant to this question.*

The electronic structures of calcium, krypton, phosphorus and an element X are shown.

Which electronic structure is that of element X?

- A $1s^2 2s^2 2p^6 3s^2 3p^3$
 B $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
 C $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
 D $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

[W'06 3]

- 18 *Use of the Data Booklet is relevant to this question.*

In forming ionic compounds, elements generally form an ion with the electronic structure of a noble gas.

Which ion does **not** have a noble gas electronic structure?

- A I^- B Rb^+ C Sn^{2+} D Sr^{2+}

[W'07 2]

- 19 In which pair do both atoms have one electron only in an s orbital in their ground states?

- A Ca, Sc B Cu, Be C H, He D Li, Cr

[W'08 3]

- 20 The first seven ionisation energies of an element between lithium and neon in the Periodic Table are as follows.

1310 3390 5320 7450 11 000 13 300 71 000 kJ mol^{-1}

What is the outer electronic configuration of the element?

- A $2s^2$ B $2s^2 2p^1$ C $2s^2 2p^4$ D $2s^2 2p^6$

[S'09 13]

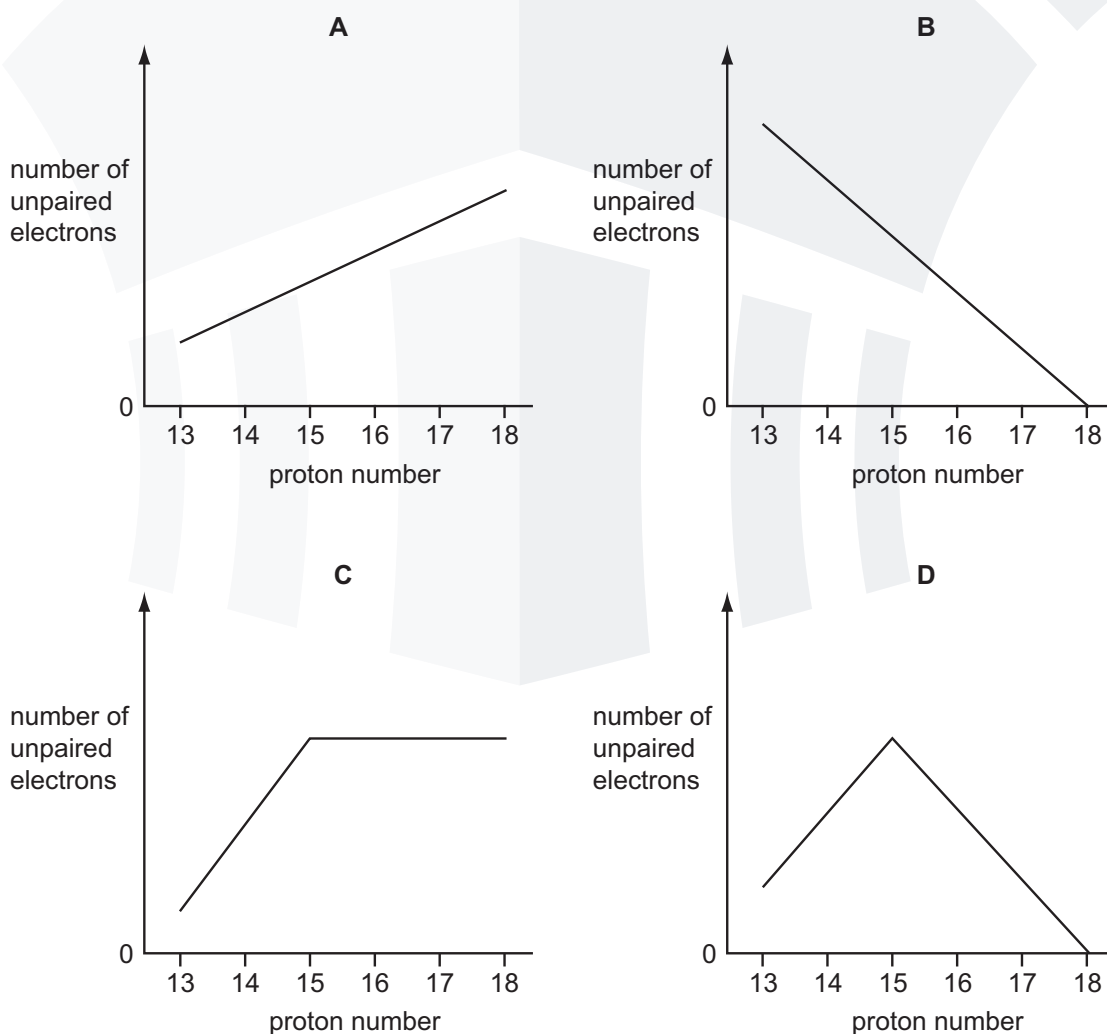
- 21 Which element has an equal number of electron pairs and of unpaired electrons within orbitals of principal quantum number 2?

- A beryllium
B carbon
C nitrogen
D oxygen

[W'11 13]

- 22 Use of the Data Booklet is relevant to this question.

Which graph represents the number of unpaired p orbital electrons for atoms with proton numbers 13 to 18?



[S'09 14]

23 In which set do all species contain the same number of electrons?

- A Co^{2+} , Co^{3+} , Co^{4+}
- B F^- , Br^- , Cl^-
- C Na^+ , Mg^{2+} , Al^{3+}
- D K_2SO_4 , K_2SeO_4 , K_2TeO_4

[W'13 2 4]

24 Element X forms X^- ions that can be oxidised to element X by acidified potassium manganate(VII).

What could be the values of the first four ionisation energies of X?

	1st	2nd	3rd	4th
A	418	3070	4600	5860
B	577	1820	2740	11 600
C	590	1150	4940	6480
D	1010	1840	2040	4030

[W'13 3 4]

25 Atoms of element X have six unpaired electrons.

What could be element X?

- A carbon
- B chromium
- C iron
- D selenium

[S'14 11]

26 For the element sulfur, which pair of ionisation energies has the largest difference between them?

- A third and fourth ionisation energies
- B fourth and fifth ionisation energies
- C fifth and sixth ionisation energies
- D sixth and seventh ionisation energies

[M'16 2 2]

- 27 Elements X and Y are in the same group of the Periodic Table.

The table shows the first six ionisation energies of X and Y in kJ mol^{-1} .

	1st	2nd	3rd	4th	5th	6th
X	800	1600	2400	4300	5400	10 400
Y	1000	1800	2700	4800	6000	12 300

What could be the identities of X and Y?

	X	Y
A	antimony, Sb	arsenic, As
B	arsenic, As	antimony, Sb
C	selenium, Se	tellurium, Te
D	tellurium, Te	selenium, Se

[S'16 2 3]

- 28 Which isolated gaseous atom has a total of five electrons occupying spherically shaped orbitals?

- A** boron
- B** fluorine
- C** sodium
- D** potassium

[S'16 2 5]

- 30 Sodium azide, NaN_3 is an explosive used to inflate airbags in cars when they crash. It consists of positive sodium ions and negative azide ions.

What are the numbers of electrons in the sodium ion and the azide ion?

	sodium ion	azide ion
A	10	20
B	10	22
C	12	20
D	12	22

- 31 What is the electronic configuration of an isolated Ni^{2+} ion?

- A** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
- B** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$
- C** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$
- D** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8$

- 32 Which ion has the same electronic configuration as Cl^- ?

- A** F^-
- B** P^+
- C** Sc^{3+}
- D** Si^{4+}

33 This question refers to isolated gaseous atoms.

In which atom are all electrons paired?

- A** Ba **B** Br **C** S **D** Si

[S'18 1 Q1]

34 Element X has a higher first ionisation energy than element Y.

Two students state what they believe is one factor that helps to explain this.

student 1 "X has a higher first ionisation energy than Y because an atom of X has more protons in its nucleus than an atom of Y."

student 2 "X has a higher first ionisation energy than Y because X has a smaller atomic radius than Y."

Only **one** of the two students is correct.

What could X and Y be?

	X	Y
A	carbon	boron
B	magnesium	aluminium
C	oxygen	nitrogen
D	oxygen	sulfur

[S'18 1 Q10]

35 The electronic configuration of an atom of sulfur is $1s^2 2s^2 2p^6 3s^2 3p^4$.



How many valence shell and unpaired electrons are present in one sulfur atom?

	valence shell electrons	unpaired electrons
A	2	1
B	4	2
C	6	0
D	6	2

[S'18 2 Q2]

36 The table refers to the electron distribution in the second shell of an atom with eight protons.

Which row is correct for this atom?

	orbital shape 		orbital shape 	
	orbital type	number of electrons	orbital type	number of electrons
A	p	2	s	4
B	p	4	s	2
C	s	2	p	4
D	s	4	p	2

[S'18 3 Q3]

SECTION B

For each of the questions in this section, one or more of the three numbered statements **1** to **3** may be correct.

Decide whether each of the statements is or is not correct (you may find it helpful to put a tick against the statements that you consider to be correct).

The responses **A** to **D** should be selected on the basis of

A	B	C	D
1, 2 and 3 are correct	1 and 2 only are correct	2 and 3 only are correct	1 only is correct

No other combination of statements is used as a correct response.

1 In which pairs do both species have the same number of unpaired p electrons?

- 1 O and Cl^+
- 2 F^+ and Ga^-
- 3 P and Ne^+

[S'12 3 32]

2 Use of the Data Booklet is relevant to this question.

The isotope ^{99}Tc is radioactive and has been found in lobsters and seaweed adjacent to nuclear fuel reprocessing plants.

Which statements are correct about an atom of ^{99}Tc ?

- 1 It has 13 more neutrons than protons.
- 2 It has 43 protons.
- 3 It has 99 nucleons.

[S'07 31]

3 Which statements are correct when referring to the atoms ^{23}Na and ^{24}Mg ?

- 1 They have the same number of full electron orbitals.
- 2 They have the same number of neutrons.
- 3 They are both reducing agents.

[S'13 3 32]

4 Carbon and nitrogen are adjacent in the Periodic Table.

Which properties do they both have?

- 1 There is an empty 2p orbital in one atom of the element.
- 2 The principal quantum number of the highest occupied orbital is 2.
- 3 They form compounds in which their atoms form bonds with four other atoms.

[S'13 132]



ELECTRONIC CONFIGURATION WS 3

1 Electrons are arranged in energy levels.

(a) An orbital is a region in which an electron may be found.

Draw diagrams to show the shape of an s orbital and of a p orbital.



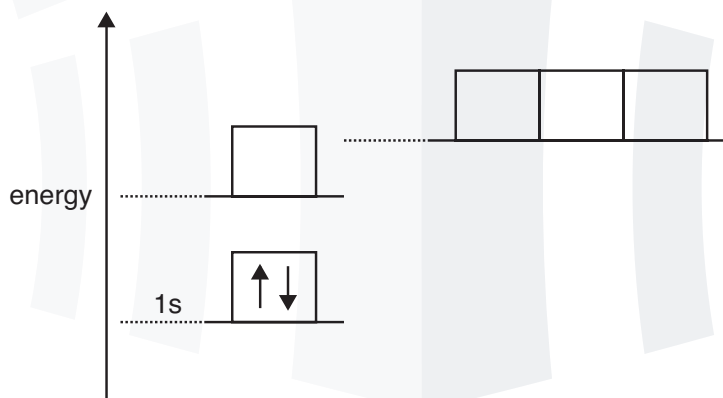
[2]

(b) Complete the table below to show how many electrons **completely** fill each of the following.

	number of electrons
a d orbital	
a p sub-shell	
the third shell ($n = 3$)	

[3]

(c) The energy diagram below is for the eight electrons in an oxygen atom. The diagram is incomplete as it only shows the two electrons in the 1s level.



Complete the diagram for the oxygen atom by:

(i) adding labels for the other sub-shell levels, [1]

(ii) adding arrows to show how the other electrons are arranged. [1]

- (d) Successive ionisation energies provide evidence for the arrangement of electrons in atoms. **Table 1.1** shows the eight successive ionisation energies of oxygen.

Table 1.1

ionisation number	1st	2nd	3rd	4th	5th	6th	7th	8th
ionisation energy/kJ mol ⁻¹	1314	3388	5301	7469	10989	13327	71337	84080

- (i) Define the term **first ionisation energy**.

.....
.....
.....
..... [3]

- (ii) Write an equation, with state symbols, to represent the **third** ionisation energy of oxygen.

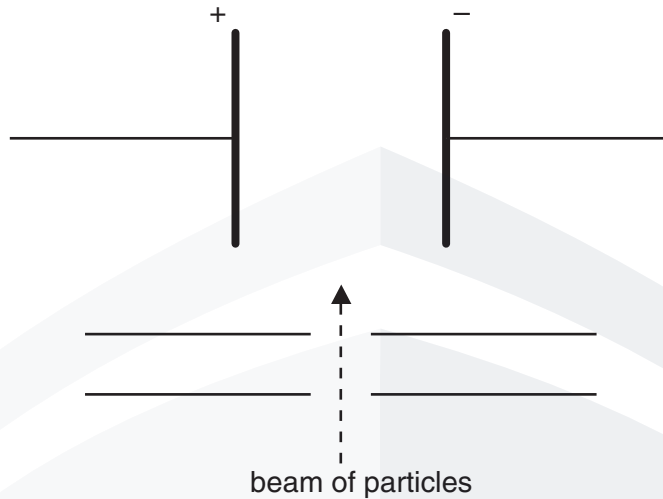
..... [2]

- (iii) Explain how the information in **Table 1.1** provides evidence for two electron shells in oxygen.

.....
.....
.....
..... [2]

- 3 In the 19th and 20th centuries, scientists established the atomic theory and showed that three sub-atomic particles, electron, neutron and proton, exist. The masses and charges of these three particles were subsequently determined.

When separate beams of electrons, neutrons or protons are passed through an electric field in the apparatus below, they behave differently.



- (a) (i) Which of these three particles will be deflected the most by the electric field?

.....

- (ii) In which direction will this particle be deflected?

.....

- (iii) Explain your answer.

.....

.....

[4]

- (b) (i) Define the term *proton number*.

.....

.....

- (ii) Why is the proton number of an atom of an element usually different from the nucleon number of an atom of the element?

.....

.....

[2]

- (c) Protons and neutrons have been used in nuclear reactions which result in the formation of artificial elements. In such processes, protons or neutrons are accelerated to high speeds and then fired like ‘bullets’ at the nucleus of an atom of an element.

Suggest why neutrons are more effective than protons as ‘nuclear bullets’.

.....
..... [2]

- (d) In some cases, when neutrons are fired at atoms of an element, the neutrons become part of the nucleus of those atoms.

What effect does the presence of an extra neutron have on the chemical properties of the new atoms formed? Explain your answer.

.....
.....
..... [2]

[Total: 10]

- 4 The first six successive ionisation energies of an element **D** are shown in Table 4.1 below.

Table 4.1

element	ionisation energy / kJ mol^{-1}					
	1st	2nd	3rd	4th	5th	6th
D	1086	2353	4621	6223	37832	47278

- (a) Define the term **first ionisation energy**.

.....

.....

.....

..... [3]

- (b) Write an equation, with state symbols, to represent the **third** ionisation energy of element **D**.

..... [2]

- (c) Use Table 4.1 to deduce which group of the Periodic Table contains element **D**. Explain your answer.

group

explanation

.....

..... [3]

- 5 (a) Explain what is meant by the term *ionisation energy*.

.....

 [3]

- (b) The first seven ionisation energies of an element, **A**, in kJ mol^{-1} , are

1012 1903 2912 4957 6274 21269 25398.

- (i) State the group of the Periodic Table to which **A** is most likely to belong. Explain your answer.

.....

 [2]

- (ii) Complete the electronic configuration of the element in Period 2 that is in the same group as **A**.

$1s^2$ [1]

- (c) Another element, **Z**, in the same period of the Periodic Table as **A**, reacts with chlorine to form a compound with empirical formula ZCl_2 . The percentage composition by mass of ZCl_2 is **Z**, 31.13; **Cl**, 68.87.

- (i) Define the term *relative atomic mass*.

.....
 [2]

- (ii) Calculate the relative atomic mass, A_r , of **Z**.
 Give your answer to **three** significant figures.

A_r of **Z** = [2]

NOTES



9 The Periodic Table: chemical periodicity

This topic illustrates the regular patterns in some physical properties of the elements in the Periodic Table.

9.1 Periodicity of physical properties of the elements in the third period



PERIODIC TRENDS

9 The Periodic Table: chemical periodicity

This topic illustrates the regular patterns in chemical and physical properties of the elements in the Periodic Table.

Learning outcomes

Candidates should be able to:

9.1 Periodicity of physical properties of the elements in the third period

- describe qualitatively (and indicate the periodicity in) the variations in atomic radius, ionic radius, melting point and electrical conductivity of the elements (see the *Data Booklet*)
- explain qualitatively the variation in atomic radius and ionic radius
- interpret the variation in melting point and electrical conductivity in terms of the presence of simple molecular, giant molecular or metallic bonding in the elements
- explain the variation in first ionisation energy (see the *Data Booklet*)
- explain the strength, high melting point and electrical insulating properties of ceramics in terms of their giant structure; to include magnesium oxide, aluminium oxide and silicon dioxide

PERIODICITY

The outer electronic configuration is a periodic function, it repeats ever so often. Many physical and chemical properties are influenced by the outer shell configuration of an atom and hence also exhibit periodicity, such as:

atomic radius, ionic radius, ionisation energy, electron affinity, electronegativity, electrical conductivity, melting point and boiling point

The first two periods in the periodic table are not typical...

Period 1 (H, He) contains only two elements

Period 2 elements at the top of each group have small sizes and high I.E. values

Period 3 (Na-Ar) is the most suitable period for studying trends

1

ATOMIC RADIUS

The atomic radius is basically used to describe the size of an atom. Larger the atomic radius, larger the atom.

Atomic radius increases down a group.

This is because, as we go down a group in the periodic table the atoms have increasingly more electron shells.

In each new period the outer-shell electrons enter a new energy level and so are located further away from the nucleus.

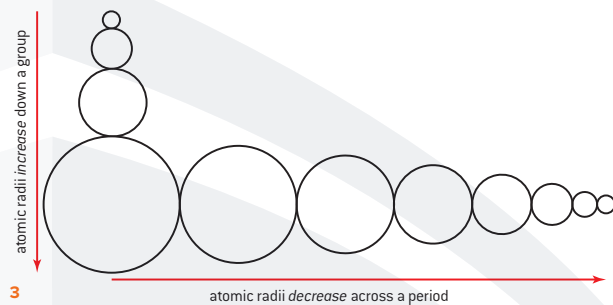
2

ATOMIC RADIUS

Atomic radius decreases across a period

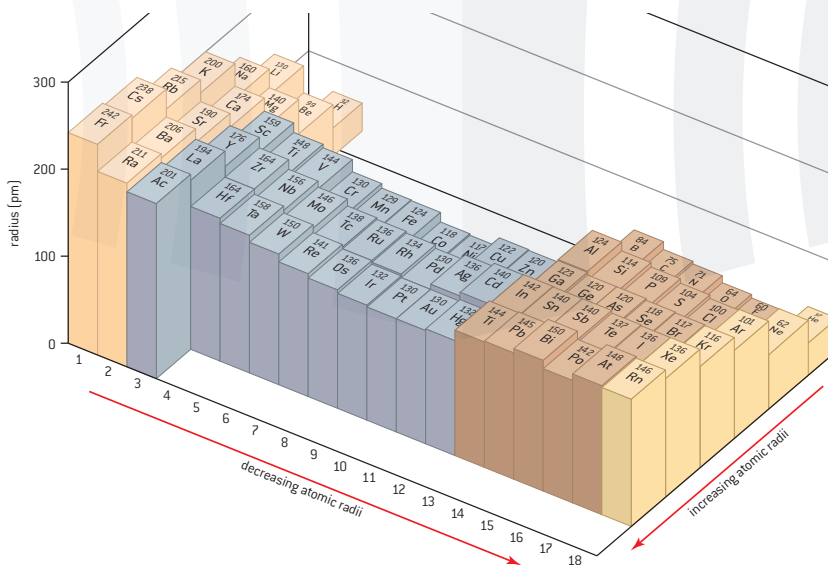
The magnitude of the positive charge of the nucleus increases, its “pull” on all of the electrons increases, hence the number of shells remain the same and the electrons are drawn closer to the nucleus.

This results in a contraction of the atomic radius and therefore a decrease in atomic size.



3

ATOMIC RADIUS



4

ATOMIC RADIUS MEASUREMENTS

The radius of an atom is determined by the distance between the center of the nucleus and the boundary of the region where the valence electrons have a probability of being located.

Since the probability of finding an electron in an atom extends up to infinity it is impossible to determine the exact size of the atom.

Hence atomic radius is taken as half the distance between the centre of two adjacent atoms in a molecule or in a closed packed system.

The bond between two adjacent atoms may be covalent, metallic or simply van der Waal's forces.

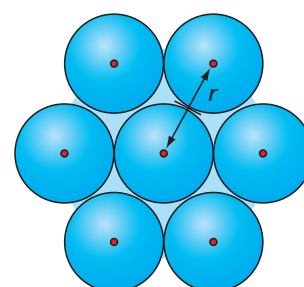
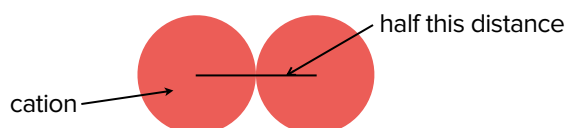
5

ATOMIC RADIUS

Chemists use X-ray diffraction and other techniques to measure the distance between the nuclei of atoms.

The atomic radius of an atom cannot be defined precisely because it depends on the type of bonding and on the number of bonds.

Metallic radius in metals is half the distance between the inter-nuclear distance of what are effectively ions.



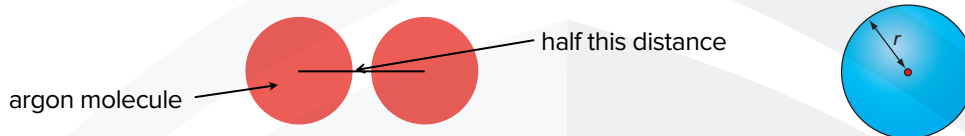
6

ATOMIC RADIUS MEASUREMENTS

- **Covalent radius** is half the distance between the nuclei of atoms joined by a covalent bond. The values are measured by X-ray or electron diffraction.

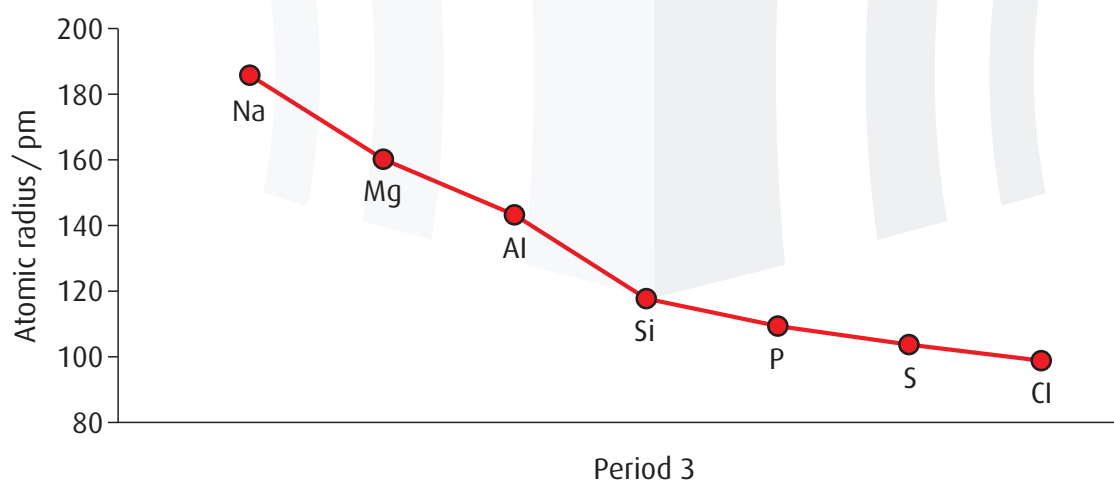


- **Van der Waal's radius** is half the distance between two monoatomic molecules (two atoms held by van der Waal's forces)



7

ATOMIC RADIUS



8

SKILL CHECK 1

Put the following elements in order of increasing atomic radius. Justify your answers:

A Mg, S, Si

B Mg, K, Al

C Si, Cl, K

9

SKILL CHECK 2

Explain why the ionic radius of a Group 2 ion is smaller than the atomic radius of the corresponding Group 2 atom.

10

IONIC RADIUS

Positive ions (cations) are smaller than the parent atom.

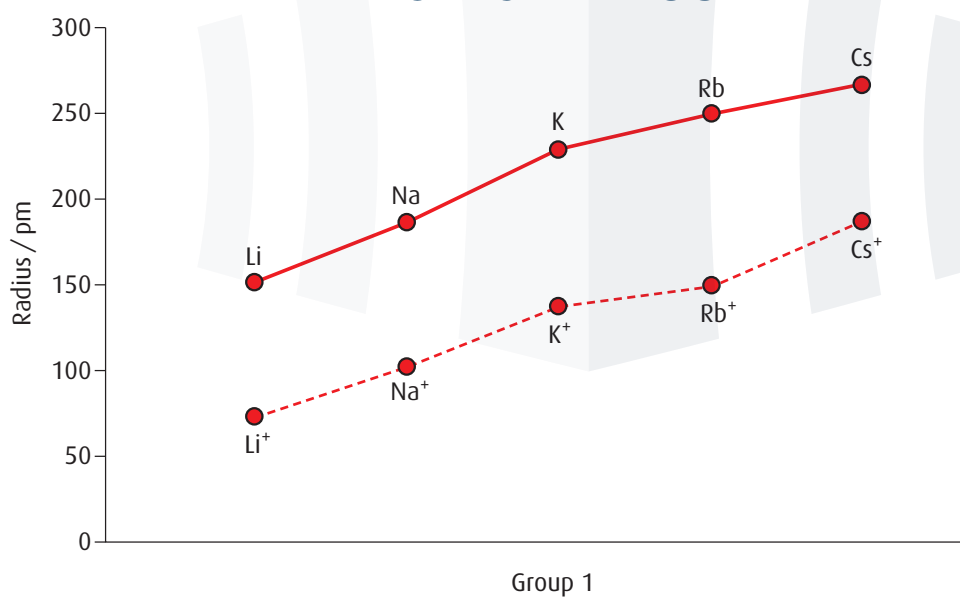
The cation has more protons than electrons (an increased nuclear charge).

The excess nuclear charge pulls the remaining electrons closer to the nucleus.

Also, cation formation often results in the loss of all outer-shell electrons, resulting in a significant decrease in radius.

11

IONIC RADIUS



12

IONIC RADIUS

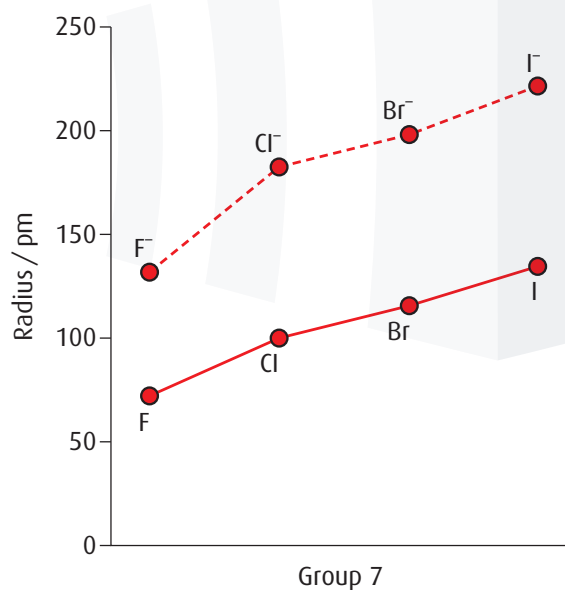
Negative ions (anions) are larger than the parent atom.

The anion has more electrons than protons.

Owing to the excess negative charge, the nuclear “pull” on each individual electron is reduced. The electrons are held less tightly, resulting in a larger anion radius in contrast to the neutral atom.

13

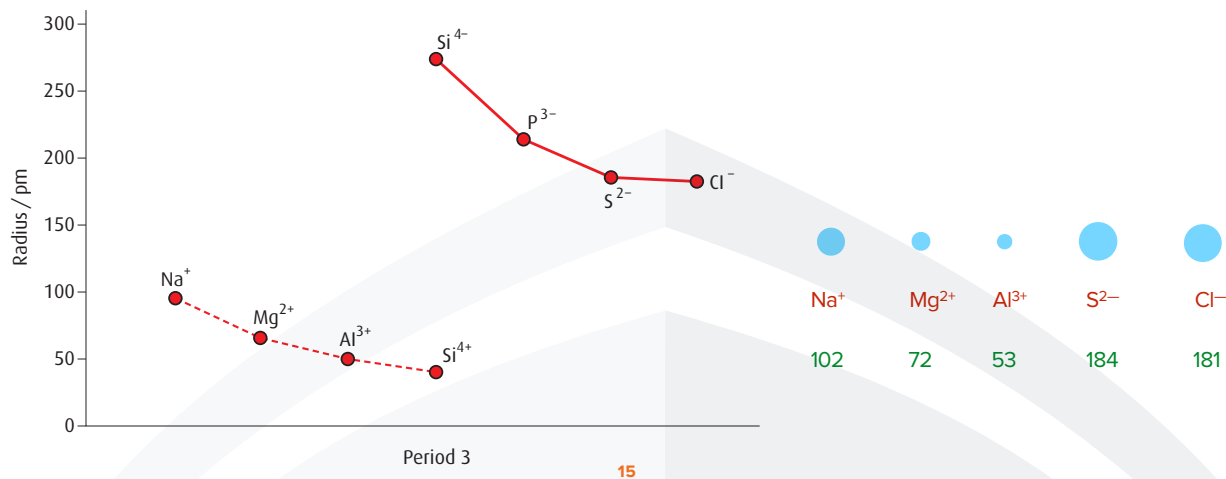
IONIC RADIUS



14

IONIC RADIUS ACROSS A PERIOD

Across a period the radii of ions with the same electron configuration decreases as nuclear charge increases.



IONIC RADIUS IN ISOELECTRONIC PARTICLES

particle	N ³⁻	O ²⁻	F ⁻	Ne	Na ⁺	Mg ²⁺	Al ³⁺
nuclear charge	7	8	9	10	11	12	13
electrons	10	10	10	10	10	10	10

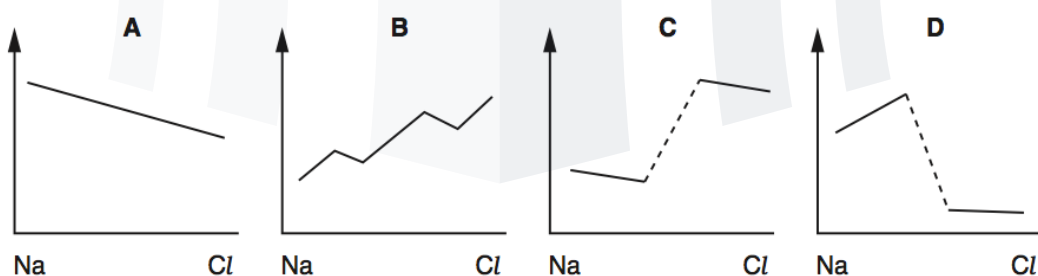
SKILL CHECK 3

Explain why the ionic radii of halides are larger than atomic radii of the corresponding halogens

17

SKILL CHECK 4

Which diagram represents the change in ionic radius of the elements across the third period (Na to Cl)?



18

SKILL CHECK 5

The species Ar, K^+ and Ca^{2+} are isoelectronic (have the same number of electrons).

In what order do their radii increase?

	smallest \longrightarrow largest		
A	Ar	Ca^{2+}	K^+
B	Ar	K^+	Ca^{2+}
C	Ca^{2+}	K^+	Ar
D	K^+	Ar	Ca^{2+}

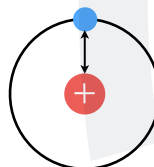
19

WHAT IS IONISATION ENERGY?

Ionisation Energy is the amount of energy needed to remove electrons from atoms.

The ionisation energy of an atom measures how strongly an atom holds its electrons.

Attraction between the nucleus and an electron

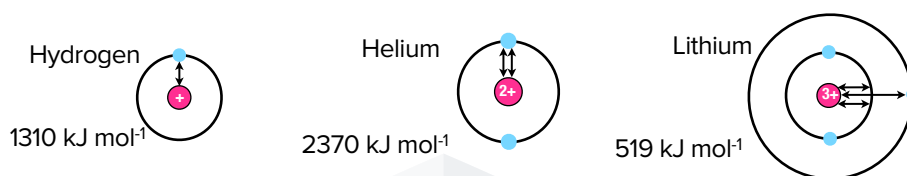


As electrons are negatively charged and protons in the nucleus are positively charged, there will be an attraction between them. The greater the pull of the nucleus, the harder it will be to pull an electron away from an atom.

20

WHAT AFFECTS IONISATION ENERGY?

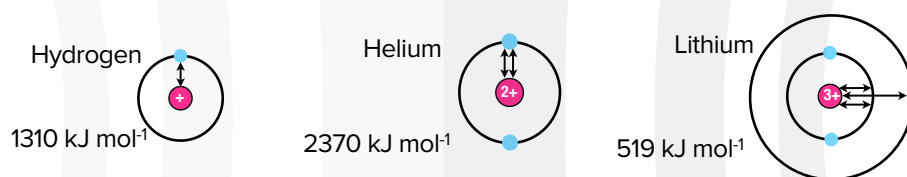
The value of the 1st Ionisation Energy depends on the electronic structure



Helium has two protons in the nucleus. The nuclear charge is greater so the pull on the outer electrons is larger. More energy will be needed to pull an electron out of the atom.

21

WHAT AFFECTS IONISATION ENERGY?



Lithium atoms have 3 protons so you would expect the pull on electrons to be greater. However, the 1st I.E. of Li is lower than that of He because

1. Filled inner shells exert a shielding effect - lowers the effective nuclear pull and,
2. Electrons are further away from the nucleus- lowers effective nuclear attraction.

22

FACTORS INFLUENCING IONISATION ENERGY

Nuclear Charge

As nuclear charge increases the attractive force would increase and hence more energy would be needed to overcome the increasing nuclear attraction.

Atomic Radius

As the atomic radius increases, the outermost electron would be further away from the nucleus experiencing a weaker attractive force. Hence the value decreases with increasing size.

Attraction decreases very rapidly with distance. An electron close to the nucleus will be much more strongly attracted than one further away.

23

FACTORS INFLUENCING IONISATION ENERGY

Shielding effect/Screening

Electrons in full inner shells repel electrons in outer shells. Full inner shells of electrons prevent the full nuclear charge being felt by the outer electrons.

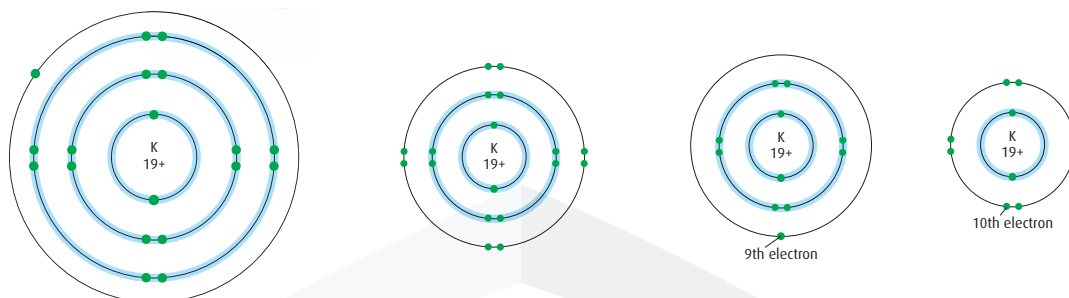
The inner electron orbitals effectively screen or shield the outermost electrons from the nucleus, due to which the ionisation energy decreases.

The lessening of the pull of the nucleus by the inner electrons is known as shielding.

It is due to the shielding effect that the electrons in the outer shell are attracted by the effective nuclear charge which is less than the full charge on the nucleus.

24

FACTORS INFLUENCING IONISATION ENERGY



25

FACTORS INFLUENCING IONISATION ENERGY

Nature of sub level

Electrons in the s orbital are closer to the nucleus as compared to the electrons in the p orbital of the same shell.

Hence the s electrons are the more firmly held and require a greater amount of energy to be removed as compared to the p electrons which are slightly further.

Also, the p orbital of the same energy level will experience the shielding effect of the s electrons from the same shell in addition to previous s orbitals.

Note: Only S Filled Orbitals Provide Shielding

26

FACTORS INFLUENCING IONISATION ENERGY

Stability of Certain Configurations

Two electrons in the same orbital experience a bit of repulsion from each other. This offsets the attraction of the nucleus so that the paired electrons are removed rather more easily.

Completely filled sub levels are more stable than others requiring large amounts of energy for their disruption. This additional stability is associated with half filled sub levels also.

Stability of completely filled sub levels > Stability of half-filled sub levels > Stability of other configurations

27

IONISATION ENERGY DOWN A GROUP

Ionisation energy decreases down a group.

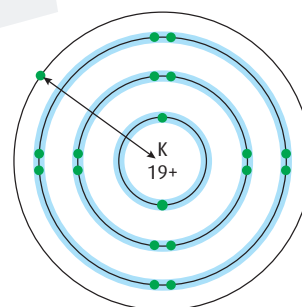
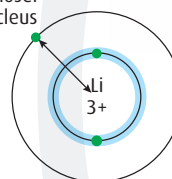
Despite an increased nuclear charge the outer electron is easier to remove. This is due to greater distance from the nucleus and increased shielding.

Down the group, as the number of shells increase, the outer electrons are farther away from the nucleus.

Potassium has a lower first ionisation energy than lithium.

28

electron closer to the nucleus



IONISATION ENERGY DOWN A GROUP

Also, down the group each successive element contains more electrons in the shells between the nucleus and the outermost electrons which increases the shielding effect.

This increased shielding causes the outermost electrons to be held less tightly to the nucleus.

The increased shielding effect and increased atomic radius/size outweigh the increase in nuclear charge. Therefore ionisation energy decreases.

29

IONISATION ENERGY ACROSS A PERIOD

General Trend: Ionisation energy increases across a Period

Across a period, the number of protons and the number of electrons increase by one each.

The additional proton increases the nuclear charge.

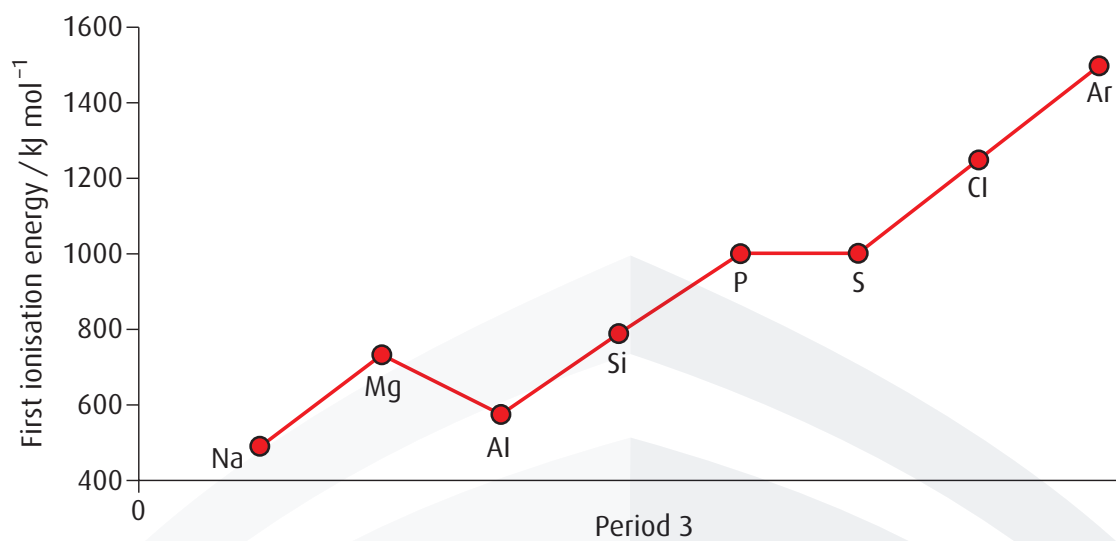
The additional electron is added to the same outer shell in each of the elements.

A higher nuclear charge more strongly attracts the outer electrons in the same shell, but the electron-shielding effect from inner-level electrons remains the same.

Thus, more energy is required to remove an electron because the attractive force on them is higher.

30

IONISATION ENERGY ACROSS A PERIOD



31

SKILL CHECK 6

For each of the following pairs, state which element has the higher first ionisation energy and explain your answer:

A Mg and Al

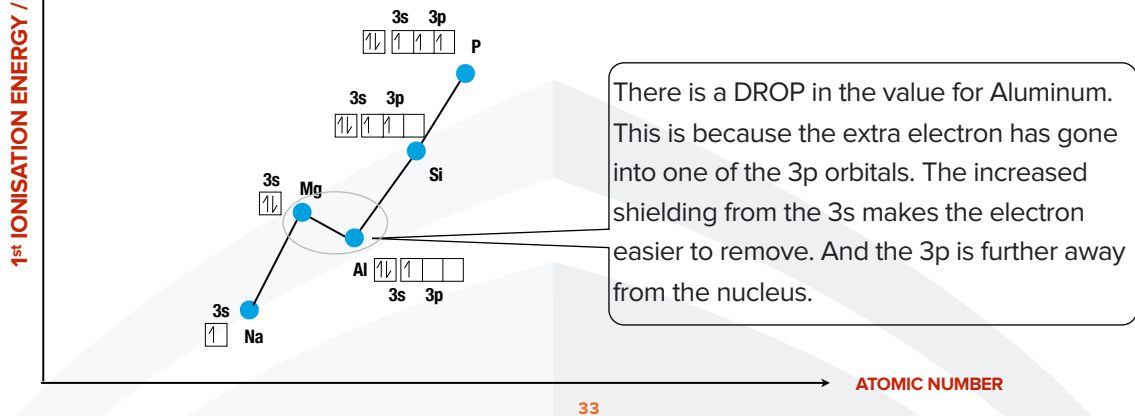
B Mg and Ca

C Ne and Na

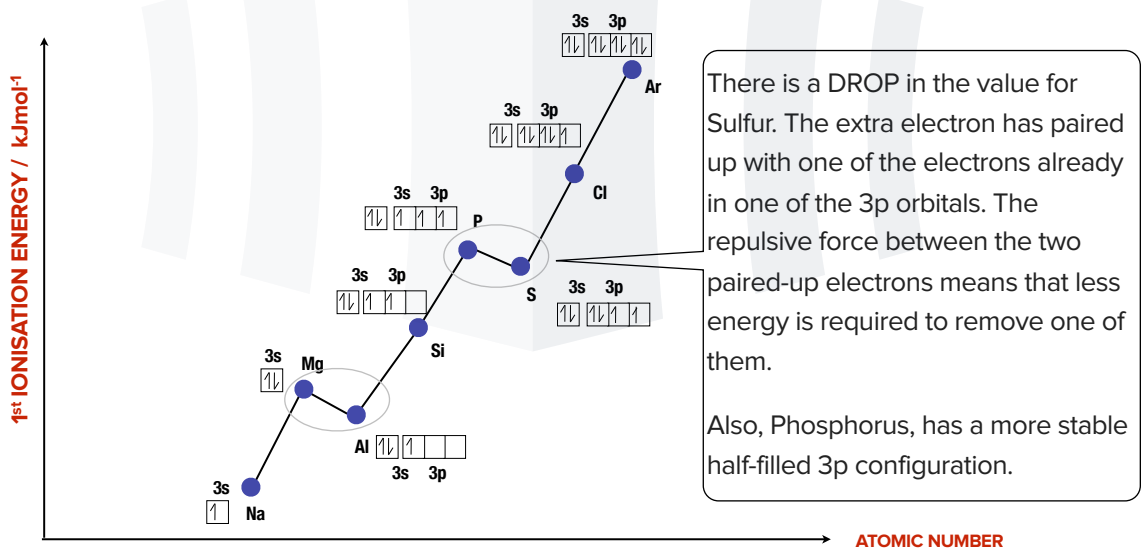
32

1ST IONISATION ENERGIES OF PERIOD 3

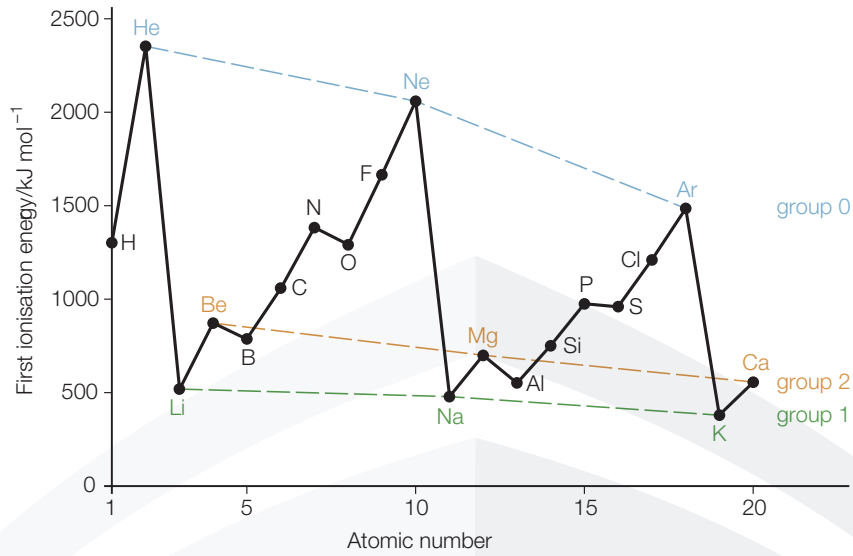
Along a Period as electrons are being added on to the same shell the magnitude of the ionisation energy increases due to the increase in the nuclear charge, a decrease in atomic size and no extra shielding.



1ST IONISATION ENERGIES OF PERIOD 3

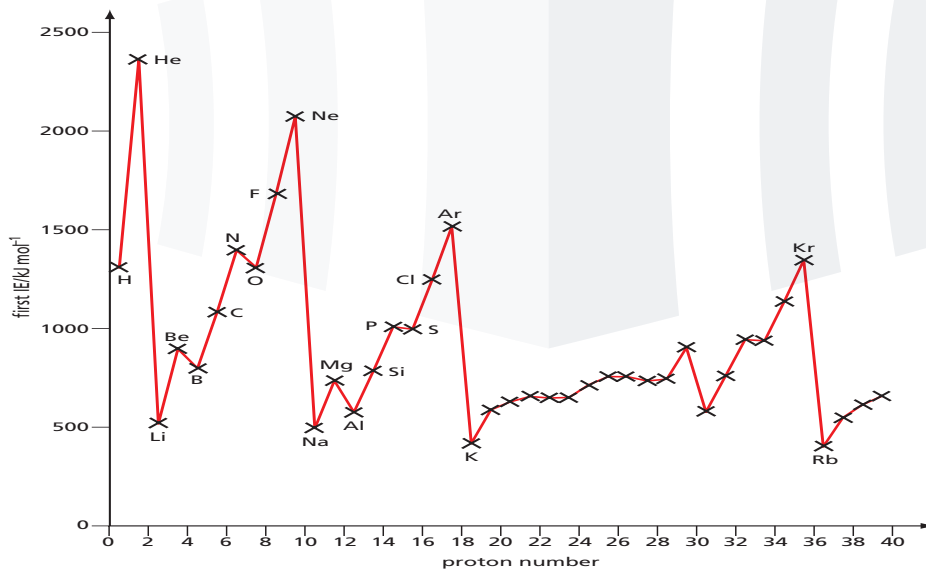


IONISATION ENERGIES OF ELEMENTS



35

IONISATION ENERGIES OF ELEMENTS



36

SKILL CHECK 7

Use of the Data Booklet is relevant to this question.

The elements radon (Rn), francium (Fr) and radium (Ra) have consecutive proton numbers in the Periodic Table.

What is the order of their first ionisation energies?

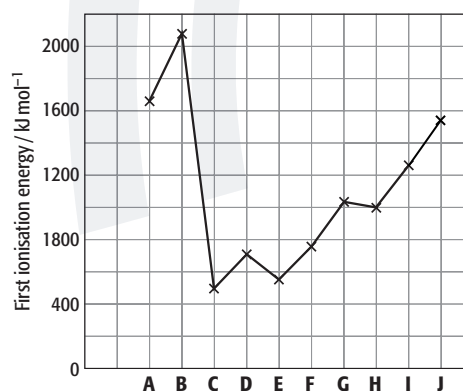
	least endothermic	→	most endothermic
A	Fr	Ra	Rn
B	Fr	Rn	Ra
C	Ra	Fr	Rn
D	Rn	Ra	Fr

37

SKILL CHECK 8

The 1st ionisation energies of several elements with consecutive atomic numbers are shown in the graph below. The letters are not the symbols of the elements.

- Which of the elements A to I belong to Group I in the Periodic Table? Explain your answer.
- Which of the elements A to I could have the electronic configuration $1s^2 2s^2 2p^6 3s^2$?
- Explain the rise in 1st ionisation energy between element E and element G.
- Estimate the 1st ionisation energy of element J.



38

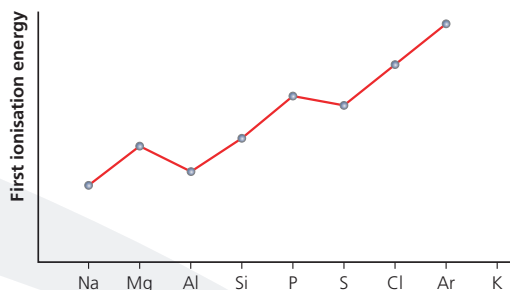
SKILL CHECK 9

The first ionisation of elements sodium to argon is shown below.

A Explain why the general trend from sodium to argon is upwards but why the value for sulfur is less than that for phosphorus.

B Mark on the graph where the value for potassium would be.

C Explain why the value for the second ionisation of sodium is very much larger than that of its first ionisation.



39

SKILL CHECK 10

Which experience a greater effective nuclear charge: the valence electrons in beryllium or the valence electrons in nitrogen? Why?

40

PERIODIC TRENDS WS 1

SECTION A

1 Which species represented by the following formulae has the largest radius?

- A P^{3-} B Cl^{-} C Ar D K^{+}

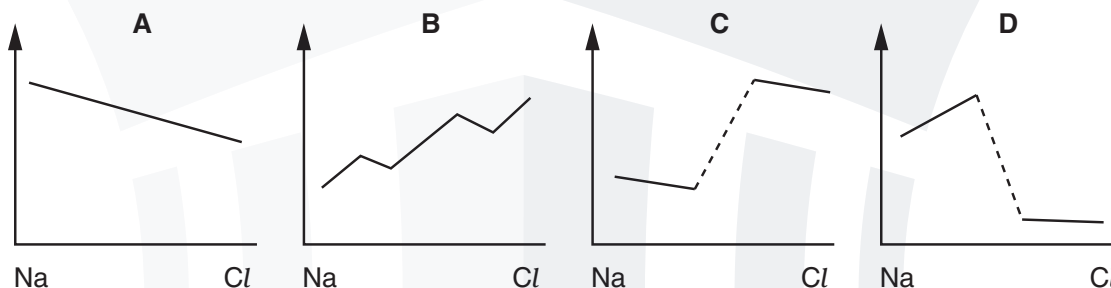
2 Use of the Data Booklet is relevant to this question.

In the gas phase, aluminium and a transition element require the same amount of energy to form one mole of an ion with a 2+ charge.

What is the transition element?

- A Co
B Cr
C Cu
D Ni

3 Which diagram represents the change in ionic radius of the elements across the third period (Na to Cl)?



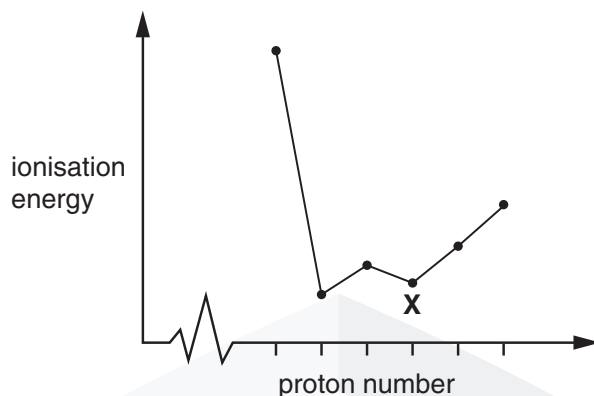
4 What is the electronic configuration of an element with a **second** ionisation energy higher than that of each of its neighbours in the Periodic Table?

- A $1s^2 2s^2 2p^6 3s^2$
B $1s^2 2s^2 2p^6 3s^2 3p^1$
C $1s^2 2s^2 2p^6 3s^2 3p^2$
D $1s^2 2s^2 2p^6 3s^2 3p^3$

5 In which pair is the radius of the second atom greater than that of the first atom?

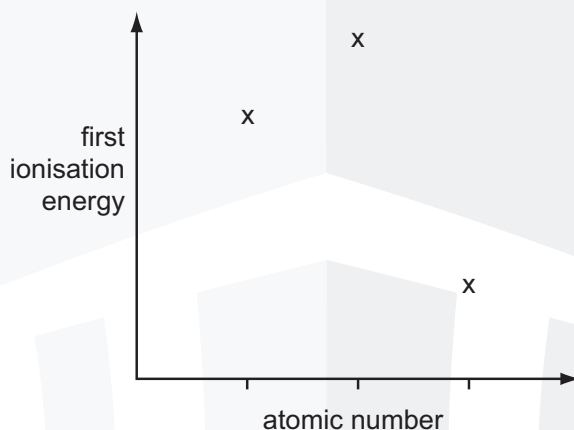
- A Na, Mg B Sr, Ca C P, N D Cl, Br

- 6 The sketch below shows the variation of first ionisation energy with proton number for six elements of consecutive proton numbers between 1 and 18 (H to Ar).



What is the identity of the element X?

- A Mg B Al C Si D P
- 7 Three successive elements in the Periodic Table have first ionisation energies which have the pattern shown in the diagram.



What could be the first element of this sequence?

- A C B N C F D Na
- 8 Which group of particles is in order of increasing size?

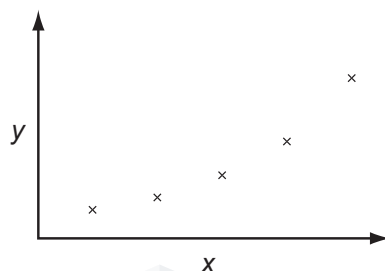
- A N O F
 B N^{3-} O^{2-} F^-
 C Na^+ Mg^{2+} Al^{3+}
 D Na^+ Ne F^-

[W'06 Q2]

[S'09 1 Q12]

- 9 Use of the Data Booklet is relevant to this question.

The sketch graph shows the variation of one physical or chemical property with another for the Group II elements.



What are the correct labels for the axes?

	x-axis	y-axis
A	atomic number	mass number
B	atomic number	melting point
C	first ionisation energy	atomic number
D	first ionisation energy	atomic radius

[W'07 1 Q14]

- 10 Why is the first ionisation energy of phosphorus greater than the first ionisation energy of silicon?

- A** A phosphorus atom has one more proton in its nucleus.
B The atomic radius of a phosphorus atom is greater.
C The outer electron in a phosphorus atom is more shielded.
D The outer electron in a phosphorus atom is paired.

[W'10 1 Q13]

- 11 The value of the second ionisation energy of calcium is 1150 kJ mol^{-1} .

Which equation correctly represents this statement?

- A** $\text{Ca(g)} \rightarrow \text{Ca}^{2+}(\text{g}) + 2\text{e}^-$; $\Delta H^\ominus = +1150 \text{ kJ mol}^{-1}$
B $\text{Ca}^+(\text{g}) \rightarrow \text{Ca}^{2+}(\text{g}) + \text{e}^-$; $\Delta H^\ominus = +1150 \text{ kJ mol}^{-1}$
C $\text{Ca}^+(\text{g}) \rightarrow \text{Ca}^{2+}(\text{g}) + \text{e}^-$; $\Delta H^\ominus = -1150 \text{ kJ mol}^{-1}$
D $\text{Ca(g)} \rightarrow \text{Ca}^{2+}(\text{g}) + 2\text{e}^-$; $\Delta H^\ominus = -1150 \text{ kJ mol}^{-1}$

[S'12 2 Q18]

- 12 Sodium and sulfur react together to form sodium sulfide, Na_2S .

How do the atomic radius and ionic radius of sodium compare with those of sulfur?

	atomic radius	ionic radius
A	sodium > sulfur	sodium > sulfur
B	sodium > sulfur	sodium < sulfur
C	sodium < sulfur	sodium > sulfur
D	sodium < sulfur	sodium < sulfur

[M'1 Q12]

- 13 From which particle is the removal of an electron the most difficult?

A $\text{Cl}^-(\text{g})$ **B** $\text{F}^-(\text{g})$ **C** $\text{K}^+(\text{g})$ **D** $\text{Na}^+(\text{g})$

[W'11 2 Q3]

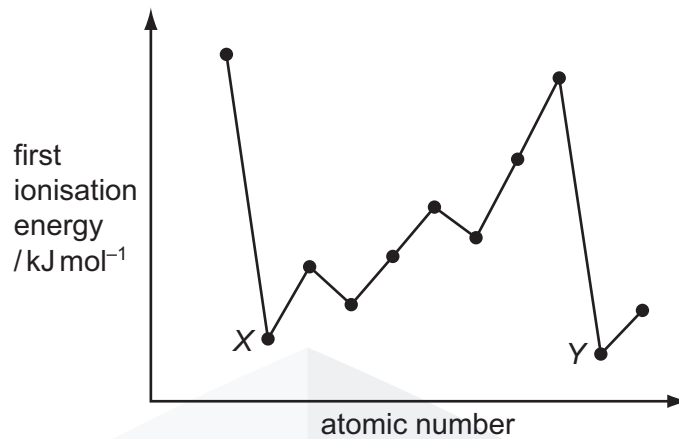
- 14 The species Ne , Na^+ and Mg^{2+} are isoelectronic. This means that they have the same number of electrons.

In which order do their radii increase?

	smallest	→	largest
A	Ne	Na^+	Mg^{2+}
B	Ne	Mg^{2+}	Na^+
C	Mg^{2+}	Ne	Na^+
D	Mg^{2+}	Na^+	Ne

[S'14 3 Q16]

15 The diagram shows the first ionisation energies of 11 consecutive elements.



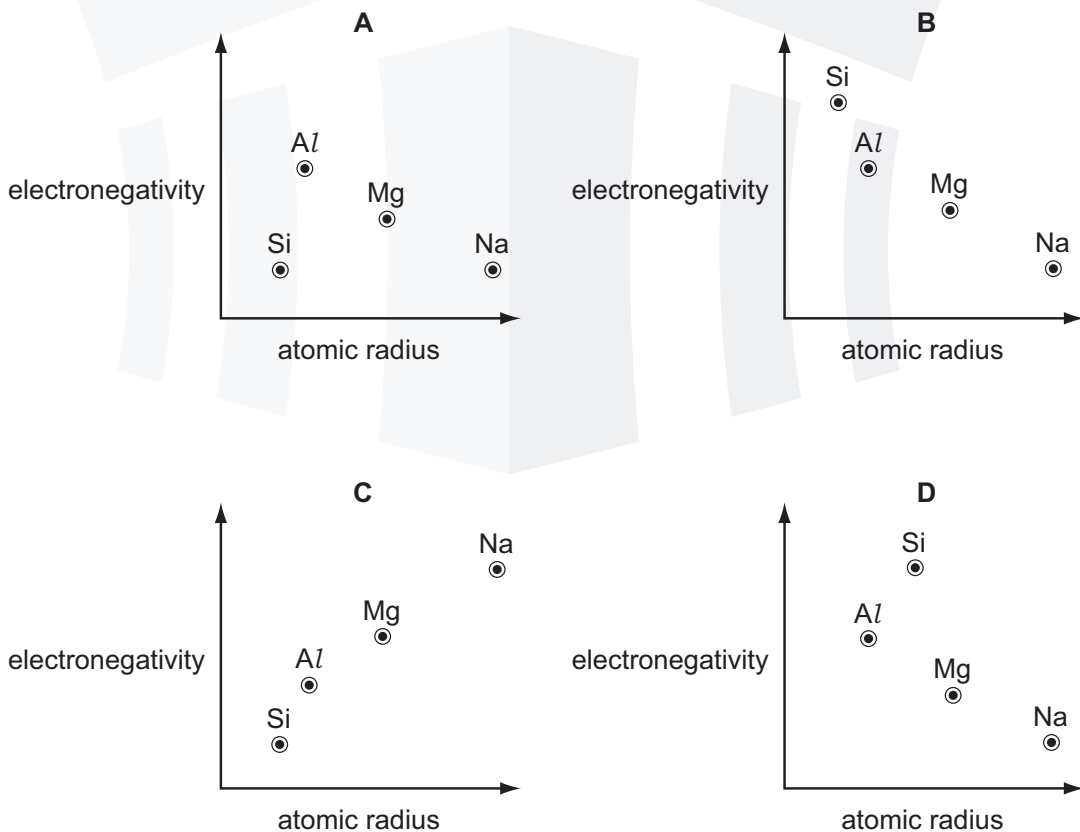
Which type of elements are labelled X and Y?

- A Group I metals
- B Group II metals
- C halogens
- D noble gases

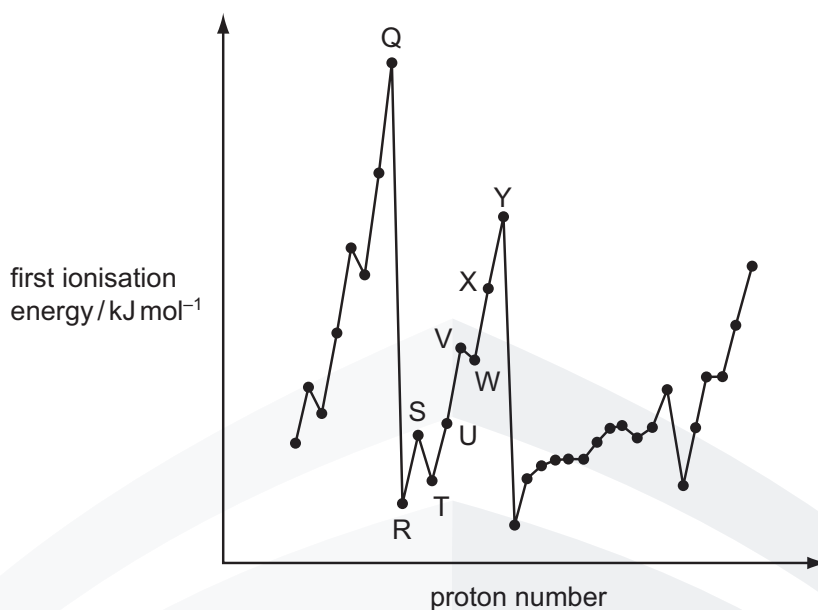
[S'11 12 Q15]

16 Use of the Data Booklet is relevant to this question.

Which graph correctly shows relative electronegativity plotted against relative atomic radius for the elements Na, Mg, Al and Si?



- 17 The graph below shows the variation of the first ionisation energy with the number of protons for some elements.



Which statement is correct?

- A Elements Q and Y are in the same period in the Periodic Table.
- B The general increase from elements R to Y is due to increasing atomic radius.
- C The small decrease between elements S and T is due to decreased shielding.
- D The small decrease between elements V and W is due to repulsion between paired electrons.

[W'13 3 Q18]

- 18 Which property **increases** in value going down Group II?

- A electronegativity
- B ionic radius
- C maximum oxidation number
- D second ionisation energy

[W'13 2 Q14]

- 19 Consecutive elements **X**, **Y** and **Z** are in Period 3 of the Periodic Table. Element **Y** has the highest first ionisation energy and the lowest melting point of these three elements.

What are the identities of **X**, **Y** and **Z**?

- A sodium, magnesium, aluminium
- B magnesium, aluminium, silicon
- C aluminium, silicon, phosphorus
- D silicon, phosphorus, sulfur

[M'16 Q12]

- 20 Why is the ionic radius of a chloride ion larger than the ionic radius of a sodium ion?
- A A chloride ion has one more occupied electron shell than a sodium ion.
 - B Chlorine has a higher proton number than sodium.
 - C Ionic radius increases regularly across the third period.
 - D Sodium is a metal, chlorine is a non-metal.

[W'12 1 Q13]

- 21 Why is the ionic radius of a chloride ion larger than the ionic radius of a sodium ion?
- A A chloride ion has one more occupied electron shell than a sodium ion.
 - B Chlorine has a higher proton number than sodium.
 - C Ionic radius increases regularly across the third period.
 - D Sodium is a metal, chlorine is a non-metal.

[S'12 1 Q13]

- 22 Sodium and sulfur react together to form sodium sulfide, Na₂S.

How do the atomic radius and ionic radius of sodium compare with those of sulfur?

	atomic radius	ionic radius
A	sodium < sulfur	sodium > sulfur
B	sodium < sulfur	sodium < sulfur
C	sodium > sulfur	sodium > sulfur
D	sodium > sulfur	sodium < sulfur

[S'16 2 Q12]

- 23 Which element has the **second** smallest atomic radius in its group and the **third** lowest first ionisation energy in its period?
- A boron
 - B calcium
 - C magnesium
 - D sodium

[S'18 1 Q13]

- 24 Element X has a higher first ionisation energy than element Y.

Two students state what they believe is one factor that helps to explain this.

student 1 "X has a higher first ionisation energy than Y because an atom of X has more protons in its nucleus than an atom of Y."

student 2 "X has a higher first ionisation energy than Y because X has a smaller atomic radius than Y."

Only **one** of the two students is correct.

What could X and Y be?

	X	Y
A	carbon	boron
B	magnesium	aluminium
C	oxygen	nitrogen
D	oxygen	sulfur

[S'18 1 Q10]

SECTION B

For each of the questions in this section, one or more of the three numbered statements 1 to 3 may be correct.

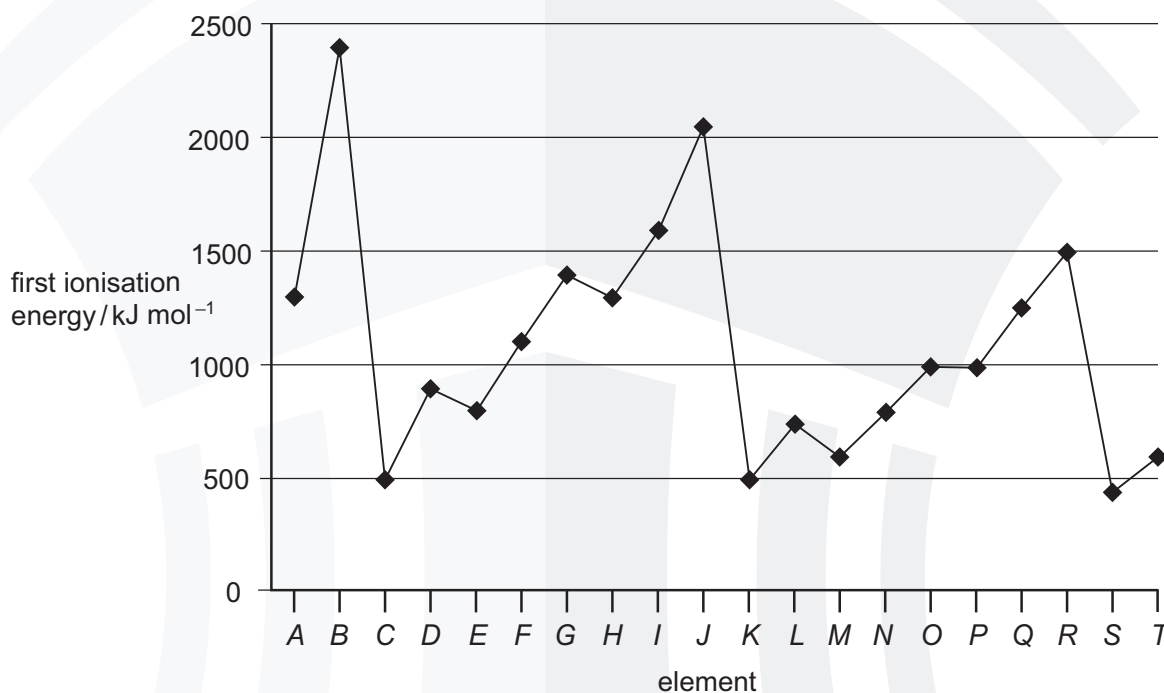
Decide whether each of the statements is or is not correct (you may find it helpful to put a tick against the statements that you consider to be correct).

The responses **A** to **D** should be selected on the basis of

A	B	C	D
1, 2 and 3 are correct	1 and 2 only are correct	2 and 3 only are correct	1 only is correct

No other combination of statements is used as a correct response.

- 1 The first ionisation energies of successive elements in the Periodic Table are represented in the graph.



Which of these statements about this graph are correct?

- Elements B, J and R are in Group 0 of the Periodic Table.
- Atoms of elements D and L contain 2 electrons in their outer shells.
- Atoms of elements G and O contain half-filled p orbitals.

2 Which of the following influence the size of the ionisation energy of an atom?

- 1 the amount of shielding by the inner electrons
- 2 the charge on the nucleus
- 3 the distance between the outer electrons and the nucleus

3 Compound X is made from two elements. One element has the second highest value of first ionisation energy in its group and the other element has the third highest value of first ionisation energy in its group.

Which compounds could be compound X?

- 1 calcium chloride
- 2 magnesium bromide
- 3 potassium sulfide

4 Why is the first ionisation energy of aluminium less than that of magnesium?

- 1 The outer electron in the aluminium atom is more shielded from the nuclear charge.
- 2 The outer electron in the aluminium atom is in a higher energy orbital.
- 3 The outer electron in the aluminium atom is further from the nucleus.

5 Compound X is made from two elements. One element has the second highest value of first ionisation energy in its group and the other element has the third highest value of first ionisation energy in its group.

Which compounds could be compound X?

- 1 calcium chloride
- 2 magnesium bromide
- 3 potassium sulfide

[S'16 3 31]

6 **X** is an element that has

- its outer electrons in the 4th principal quantum shell,
- a higher 1st ionisation energy than calcium.

What could be the identity of **X**?

- 1 bromine
- 2 krypton
- 3 xenon

PERIODIC TRENDS WS 2

- 1 The first six ionisation energies of an element **X** are given below.

ionisation energy / kJ mol ⁻¹					
first	second	third	fourth	fifth	sixth
950	1800	2700	4800	6000	12300

- (a) Define the term *first ionisation energy*.

.....

 [3]

- (b) Write an equation, with state symbols, for the **second** ionisation energy of element **X**.

..... [2]

- (c) Use the data given above to deduce in which Group of the Periodic Table element **X** is placed. Explain your answer.

Group

explanation

.....

 [3]

The first ionisation energies (I.E.) for the elements of Group IV are given below.

element	C	Si	Ge	Sn	Pb
1st I.E. / kJ mol ⁻¹	1090	786	762	707	716

- (d) Explain the trend shown by these values in terms of the atomic structure of the elements.

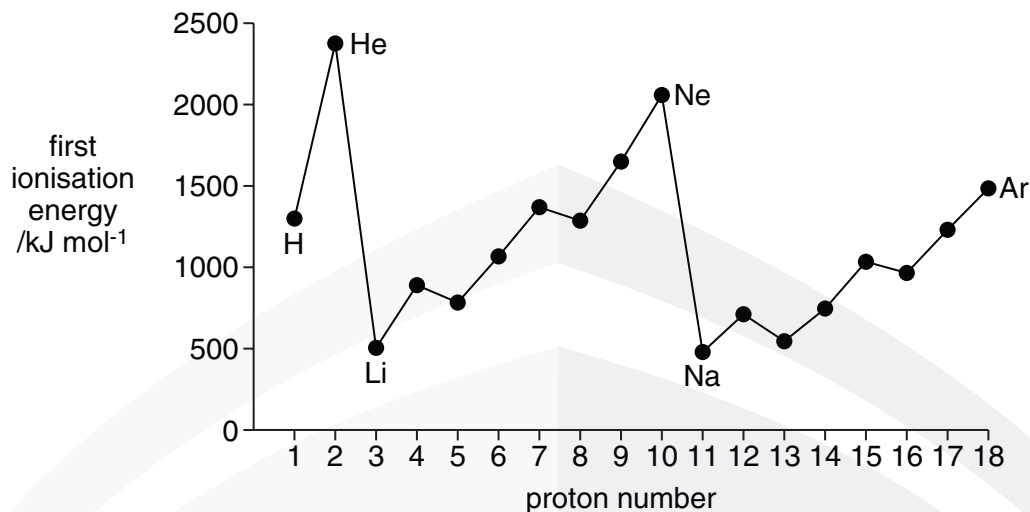
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 [4]

[Total: 12]

- 2 The Periodic Table we currently use is derived directly from that proposed by Mendeleev in 1869 after he had noticed patterns in the chemical properties of the elements he had studied.

The diagram below shows the first ionisation energies of the first 18 elements of the Periodic Table as we know it today.



- (a) Give the equation, including state symbols, for the first ionisation energy of fluorine.

..... [2]

- (b) Explain why there is a general increase in first ionisation energies from sodium to argon.

.....

 [3]

- (c) (i) Explain why the first ionisation energy of aluminium is less than that of magnesium.

.....

- (ii) Explain why the first ionisation energy of sulphur is less than that of phosphorus.

.....
.....
.....

[4]

- 3 Magnesium will react on heating with chlorine, or oxygen, or nitrogen to give the chloride, or oxide, or nitride respectively. Each of these compounds is ionic and in them magnesium has the same +2 oxidation state.

- (a) (i) Write an equation, with state symbols, for the **second** ionisation energy of magnesium.

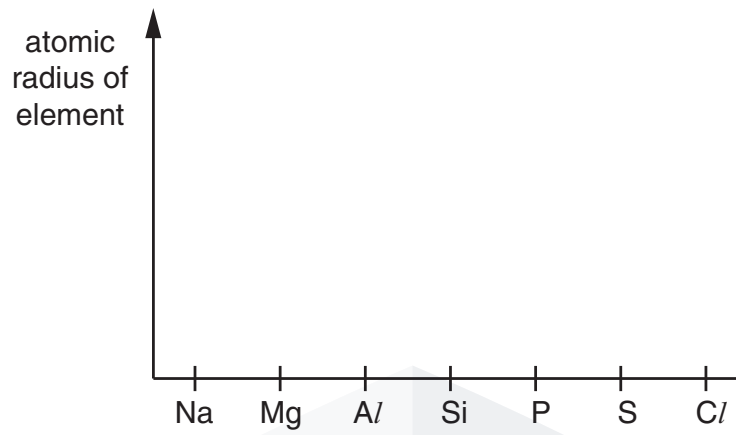
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- (ii) Use the *Data Booklet* to calculate the enthalpy change that occurs when one mole of gaseous magnesium ions, Mg^{2+} , is formed from one mole of gaseous magnesium atoms.

Include a sign in your answer.

enthalpy change = kJ mol^{-1}
[3]

- 4 Elements in the same period of the Periodic Table show trends in physical and chemical properties.
On the grid below, draw a clear sketch to show the variation of the stated property.
Below the grid, briefly explain the variation you have described in your sketch.
You should refer to the important factors that cause the differences in the property you are describing.



explanation

.....

.....

.....

[3]

5 Barium, Ba, was discovered by Davy in 1808. The element gets its name from the Greek 'barys' meaning 'heavy'.

(a) The table below compares some properties of barium with caesium.

element	Cs	Ba
group	1	2
atomic number	55	56
atomic radius/pm	531	435

(i) Why do caesium and barium have different atomic numbers?

..... [1]

(ii) State the block in the Periodic Table in which caesium and barium are found.

..... [1]

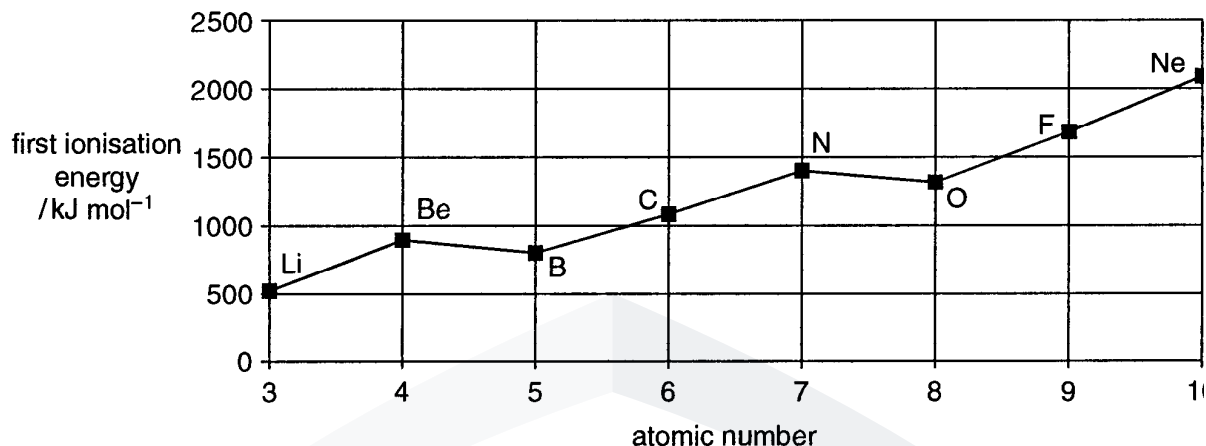
(iii) Explain why the atomic radius of barium is **less** than the atomic radius of caesium.

.....
.....
.....
..... [3]

(iv) Predict and explain whether a barium **ion** is *larger*, *smaller* or the *same size* as a barium **atom**.

.....
.....
.....
..... [2]

- 6 (b) The diagram below shows the variation in the first ionisation energies of elements across Period 2 of the Periodic Table.



- (i) Define the term *first ionisation energy*.

.....

 [3]

- (ii) Explain why the first ionisation energies show a **general** increase across Period 2.

.....

 [2]

- (iii) Explain why the first ionisation energy of B is **less** than that of Be.

.....

 [2]

- (iv) Estimate a value for the first ionisation energy of the element with atomic number 11. Explain how you made your choice.

First ionisation energy = kJ mol⁻¹

.....

 [2]

7 This question is about the elements in Group II of the Periodic Table, magnesium to barium.

- (a) Complete the table below to show the electronic configuration of calcium atoms and of strontium ions, Sr^{2+} .

	1s	2s	2p	3s	3p	3d	4s	4p	4d
Ca	2	2	6						
Sr^{2+}	2	2	6						

[2]

- (b) Explain the following observations.

- (i) The atomic radii of Group II elements increase down the Group.

.....

- (ii) The strontium ion is smaller than the strontium atom.

.....

- (iii) The first ionisation energies of the elements of Group II decrease with increasing proton number.

.....

[4]

- 8 The alkali metals are a series of six elements in Group I of the Periodic Table. The first ionisation energy of these elements shows a marked trend as the Group is descended.

(a) Define the term *first ionisation energy*.

.....
.....
..... [2]

(b) (i) State and explain the trend in first ionisation energy as Group I is descended.

.....
.....
.....

(ii) Suggest how this trend helps to explain the increase in the reactivity of the elements as the Group is descended.

.....
..... [3]

- 9 Although the actual size of an atom cannot be measured exactly, it is possible to measure the distance between the nuclei of two atoms. For example, the 'covalent radius' of the Cl atom is assumed to be half of the distance between the nuclei in a Cl_2 molecule. Similarly, the 'metallic radius' is half of the distance between two metal atoms in the crystal lattice of a metal. These two types of radius are generally known as 'atomic radii'. The table below contains the resulting atomic radii for the elements of period three of the Periodic Table, Na to Cl .

element	Na	Mg	Al	Si	P	S	Cl
atomic radius/nm	0.186	0.160	0.143	0.117	0.110	0.104	0.099

- (a) (i) Explain qualitatively this variation in atomic radius.

.....

.....

.....

.....

.....

- (ii) Suggest why it is not possible to use the same type of measurement for argon, Ar.

.....

.....

[4]

- (b) (i) Use the *Data Booklet* to complete the following table of radii of the cations and anions formed by some of the period three elements.

radius of cation/nm			radius of anion/nm		
Na ⁺	Mg ²⁺	Al ³⁺	P ³⁻	S ²⁻	Cl ⁻

(ii) Explain the differences in size between the cations and the corresponding atoms.

.....

.....

.....

(iii) Explain the differences in size between the anions and the corresponding atoms.

.....

.....

.....

[5]



10 The alkali metals are a series of six elements in Group I of the Periodic Table. The first ionisation energy of these elements shows a marked trend as the Group is descended.

(a) Define the term *first ionisation energy*.

.....
.....
..... [2]

(b) (i) State and explain the trend in first ionisation energy as Group I is descended.

.....
.....
.....

(ii) Suggest how this trend helps to explain the increase in the reactivity of the elements as the Group is descended.

.....
..... [3]

(c) In a redox reaction, 0.83 g of lithium reacted with water to form 0.50 dm³ of aqueous lithium hydroxide.



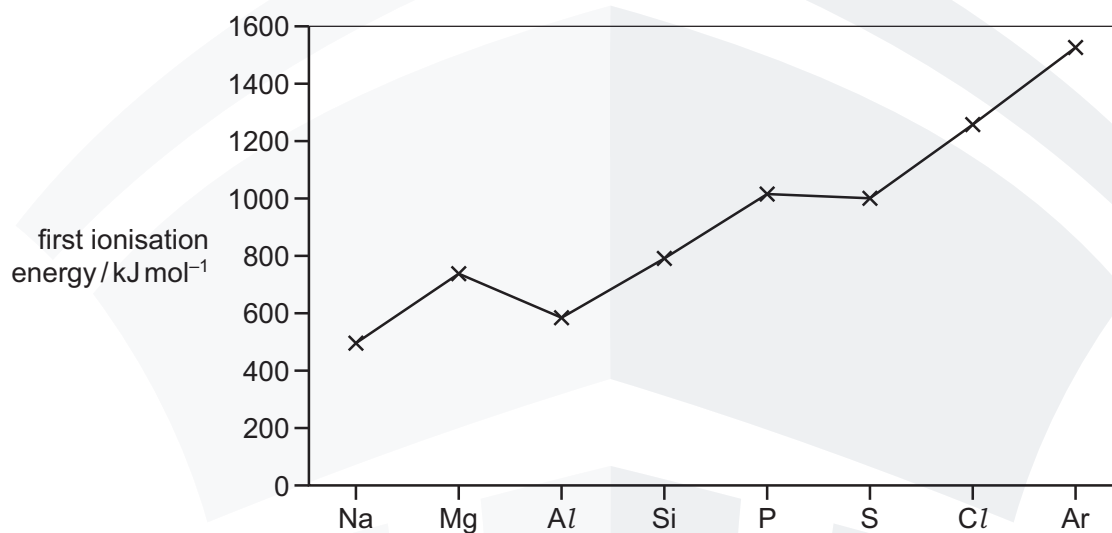
(i) Calculate the amount, in moles, of lithium that reacted.

(ii) Calculate the volume of hydrogen produced at room temperature and pressure.

(iii) Calculate the concentration, in mol dm^{-3} , of the LiOH(aq) formed.

[5]

11 (b) The graph below shows the variation of the first ionisation energies across Period 3.



(i) Explain why the first ionisation energy of Ar is greater than that of Cl.

.....
 [1]

(ii) Explain why the first ionisation energy of Al is less than that of Mg.

.....
 [1]

(iii) Explain why the first ionisation energy of S is less than that of P.

.....
 [1]

12 (a) Complete the full electronic configuration of neon.

1s² [1]

(b) (i) Explain what is meant by the term *first ionisation energy*.

.....
.....
..... [3]

(ii) Explain why the first ionisation energy of neon is greater than that of fluorine.

.....
..... [2]

- 13 (a) Successive ionisation energies for the elements magnesium to barium are given in the table.

element	1st ionisation energy / kJ mol ⁻¹	2nd ionisation energy / kJ mol ⁻¹	3rd ionisation energy / kJ mol ⁻¹
Mg	736	1450	7740
Ca	590	1150	4940
Sr	548	1060	4120
Ba	502	966	3390

- (i) Explain why the first ionisation energies decrease down the group.

.....

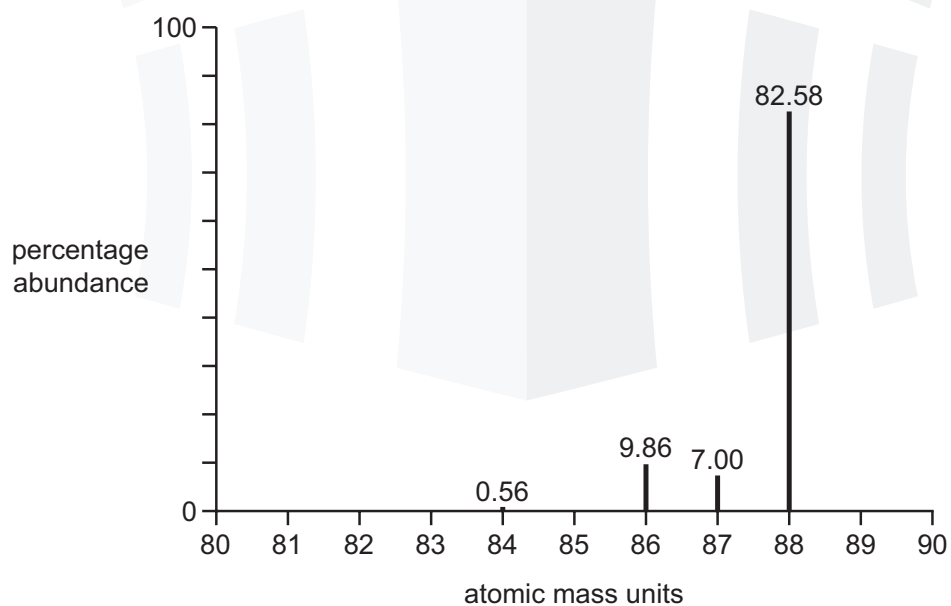
 [3]

- (ii) Explain why, for each element, there is a large increase between the 2nd and 3rd ionisation energies.

.....

 [2]

- (b) A sample of strontium, atomic number 38, gave the mass spectrum shown. The percentage abundances are given above each peak.



(i) Complete the full electronic configuration of strontium.

$1s^2 2s^2 2p^6$ [1]

(ii) Explain why there are four different peaks in the mass spectrum of strontium.

.....
 [1]

(iii) Calculate the atomic mass, A_r , of this sample of strontium.
 Give your answer to **three** significant figures.

$A_r =$ [2]

(c) A compound of barium, **A**, is used in fireworks as an oxidising agent and to produce a green colour.

(i) Explain, in terms of electron transfer, what is meant by the term *oxidising agent*.

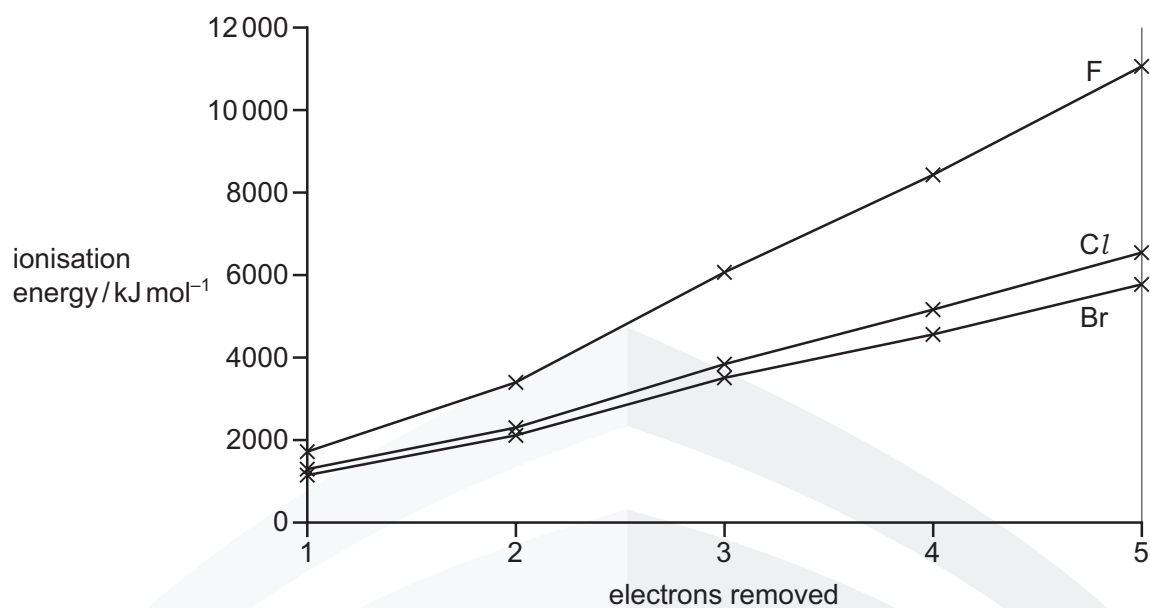
.....
 [1]

(ii) **A** has the following percentage composition by mass: Ba, 45.1; Cl, 23.4; O, 31.5.

Calculate the empirical formula of **A**.

empirical formula of **A** [3]

- 14 (a) Successive ionisation energies for the elements fluorine, F, to bromine, Br, are shown on the graph.



- (i) Explain why the first ionisation energies decrease down the group.

.....

.....

.....

.....

..... [3]

- (ii) Explain why there is an increase in the successive ionisation energies of fluorine.

.....

.....

..... [2]

- 15 The fifth to eighth ionisation energies of three elements in the third period of the Periodic Table are given. The symbols used for reference are **not** the actual symbols of the elements.

	ionisation energies, kJ mol ⁻¹			
	fifth	sixth	seventh	eighth
X	6274	21 269	25 398	29 855
Y	7012	8496	27 107	31 671
Z	6542	9362	11 018	33 606

- (i) State and explain the group number of element **Y**.

group number

explanation

[1]

- (ii) State and explain the general trend in **first** ionisation energies across the third period.

.....

.....

..... [2]

- (iii) Explain why the **first** ionisation energy of element **Y** is less than that of element **X**.

.....

.....

.....

..... [2]

- (iv) Complete the electronic configuration of element **Z**.

1s²

[1]

- 16 The fifth to eighth ionisation energies of three elements in the third period of the Periodic Table are given. The symbols used for reference are **not** the actual symbols of the elements.

	ionisation energies, kJ mol ⁻¹			
	fifth	sixth	seventh	eighth
X	7012	8496	27 107	31 671
Y	6542	9362	11 018	33 606
Z	7238	8781	11 996	13 842

- (i) State and explain the group number of element **Y**.

group number

explanation

[1]

- (ii) State and explain the general trend in **first** ionisation energies across the third period.

.....

.....

..... [2]

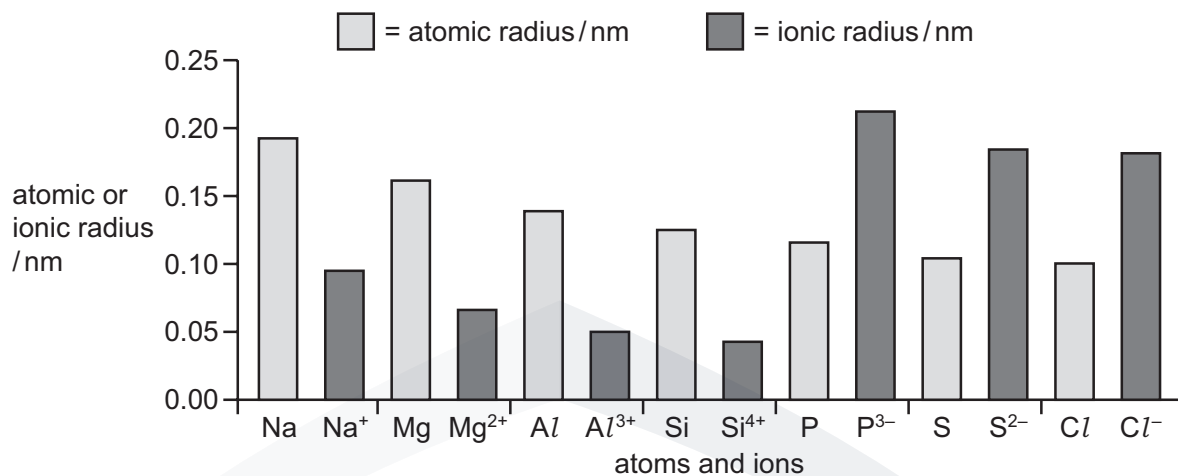
- (iii) Complete the electronic configuration of element **X**.

1s²

[1]

17 The elements in the third period exhibit periodicity in both their chemical and physical properties.

(a) A graph of the atomic and ionic radii across the third period is shown.



(i) Explain the decrease in atomic radius across the third period.

.....

.....

.....

..... [2]

(ii) Explain why, for sodium to silicon, the ionic radii are less than the atomic radii.

.....

..... [1]

(iii) Explain why, for phosphorus to chlorine, the ionic radii are greater than the atomic radii.

.....

.....

..... [2]

(b) The first ionisation energies of the elements across the third period show a general increase.

Aluminium and sulfur do **not** follow this general trend.

(i) Explain why aluminium has a lower first ionisation energy than magnesium.

.....

.....

..... [2]

[S'18 1 Q3]

18

The first six successive ionisation energies of an element **D** are shown in Table 4.1 below.

Table 4.1

element	ionisation energy / kJ mol^{-1}					
	1st	2nd	3rd	4th	5th	6th
D	1086	2353	4621	6223	37832	47278

(a) Define the term **first ionisation energy**.

.....

.....

.....

..... [3]

(b) Write an equation, with state symbols, to represent the **third** ionisation energy of element **D**.

..... [2]

(c) Use Table 4.1 to deduce which group of the Periodic Table contains element **D**. Explain your answer.

group

explanation

.....

..... [3]

- 19 Sir James Jeans, who was a great populariser of science, once described an atom of carbon as being like six bees buzzing around a space the size of a football stadium.

(a) (i) Suggest what were represented by the six bees in this description.

.....

(ii) Explain (in terms of an atom of carbon) what stopped the bees from flying away from the space of the football stadium.

.....

.....

(iii) What is missing from Jeans' description when applied to an atom of carbon?

.....

.....

[3]

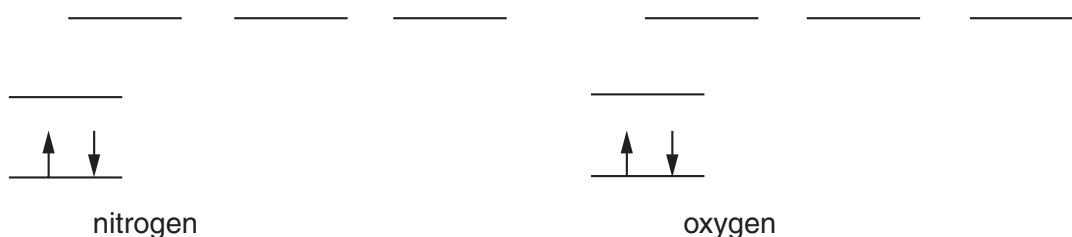
(b) The diagram below represents the energy levels of the orbitals in atoms of the second period, lithium to neon.

(i) Label the energy levels to indicate the principal quantum number and the type of orbital at each energy level.



(ii) In the space below, sketch the shapes of the two types of orbital.

- (iii) Complete the electron configurations of nitrogen and oxygen on the energy level diagrams below, using arrows to represent electrons.



- (iv) Explain, with reference to your answer to (iii), the relative values of the first ionisation energies of nitrogen and oxygen. The values are given in the *Data Booklet* and should be quoted in your answer.

.....

.....

.....

.....

[6]

- (c) (i) State the formulae of the negatively charged ions formed by these elements in simple binary compounds (nitrides and oxides).

.....

- (ii) Why do nitrogen and oxygen form negative ions, but not positive ions, in simple binary compounds?

.....

.....

.....

[2]

[Total : 11]

3 Chemical bonding

This topic introduces the different ways by which chemical bonding occurs and the effect this can have on physical properties.

3.2 Covalent bonding and co-ordinate (dative covalent) bonding



COVALENT BONDING

3 Chemical bonding

This topic introduces the different ways by which chemical bonding occurs and the effect this can have on physical properties.

Learning outcomes

Candidates should be able to:

3.2 Covalent bonding and co-ordinate (dative covalent) bonding including shapes of simple molecules

- a) describe, including the use of 'dot-and-cross' diagrams:
 - (i) covalent bonding, in molecules such as hydrogen, oxygen, chlorine, hydrogen chloride, carbon dioxide, methane, ethene
 - (ii) co-ordinate (dative covalent) bonding, such as in the formation of the ammonium ion and in the Al_2Cl_6 molecule
- b) describe covalent bonding in terms of orbital overlap, giving σ and π bonds, including the concept of hybridisation to form sp , sp^2 and sp^3 orbitals (see also Section 14.3)
- c) explain the shapes of, and bond angles in, molecules by using the qualitative model of electron-pair repulsion (including lone pairs), using as simple examples: BF_3 (trigonal), CO_2 (linear), CH_4 (tetrahedral), NH_3 (pyramidal), H_2O (non-linear), SF_6 (octahedral), PF_5 (trigonal bipyramidal)
- d) predict the shapes of, and bond angles in, molecules and ions analogous to those specified in 3.2(b) (see also Section 14.3)

CHEMICAL BONDING

When two or more atoms form a chemical compound, the atoms are held together in a characteristic arrangement by attractive forces.

The chemical bond is the force of attraction between any two atoms in a compound. The attraction is the force that overcomes the repulsion of the positively charged nuclei of the two atoms.

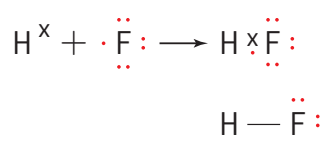
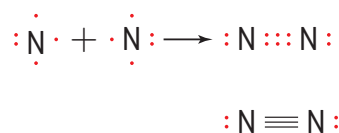
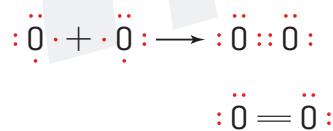
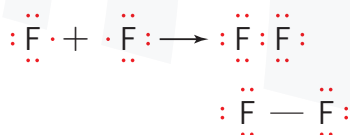
Interactions involving valence electrons are responsible for the chemical bond. We shall focus our attention on these electrons and the electron arrangement of atoms both before and after bond formation.

1

COVALENT BONDING

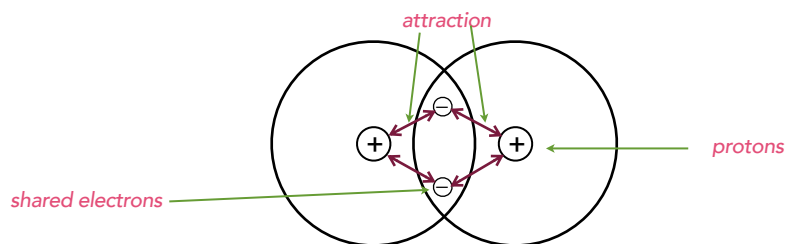
When electrons are shared rather than transferred, the shared electron pair is referred to as a covalent bond.

Covalent bonds tend to form between atoms with similar tendencies to gain or lose electrons. The most obvious examples are the diatomic molecules H_2 , N_2 , O_2 , F_2 , Cl_2 , Br_2 , and I_2 .

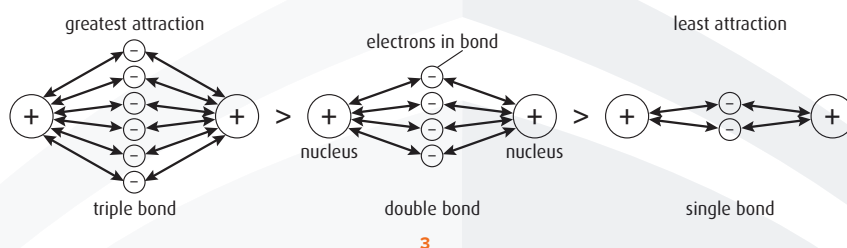


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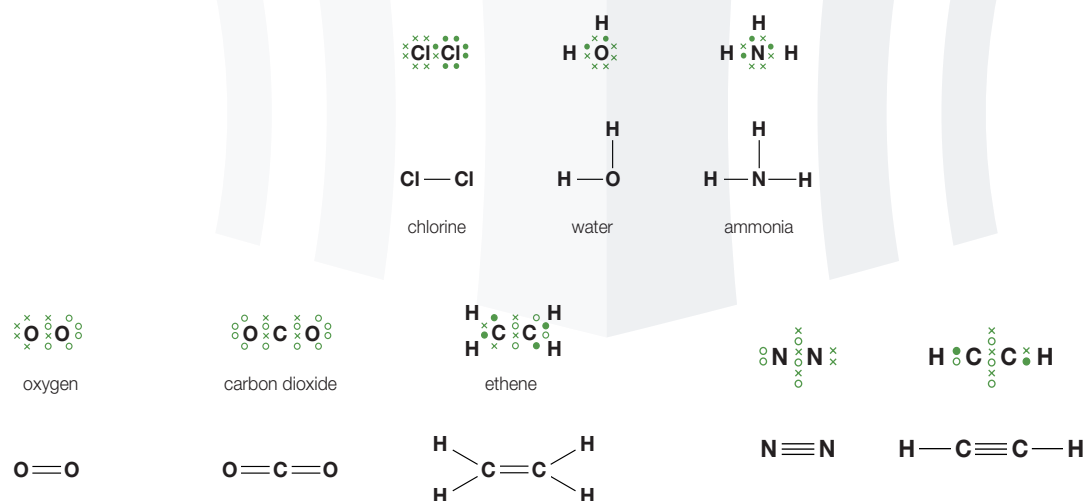
COVALENT BONDING



A covalent bond is the electrostatic force of attraction between the positively charged nuclei of both atoms and their shared pair(s) of electrons.



'DOT - AND - CROSS' DIAGRAMS



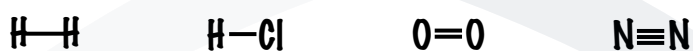
4

COVALENT BONDING

The bond is the force of attraction between the pair of electrons and the two positive nuclei of the atoms.

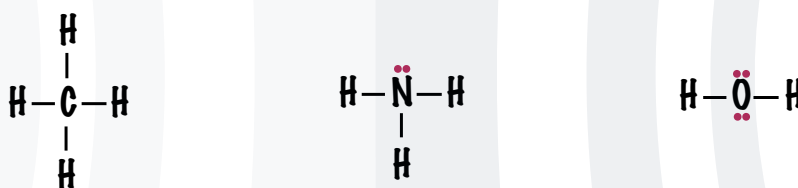
This increased negative charge in the centre holds the two positively charged nuclei together, thus forming the bond.

Depending on the number of electrons involved, the bonding is classified as single double and triple.



5

COVALENT COMPOUNDS



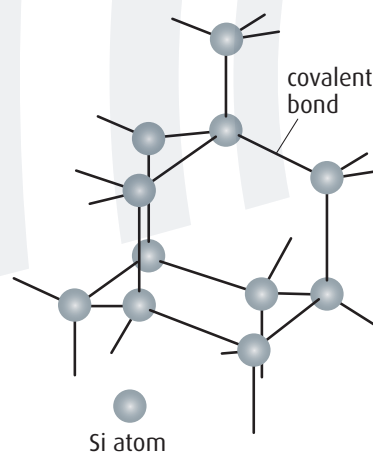
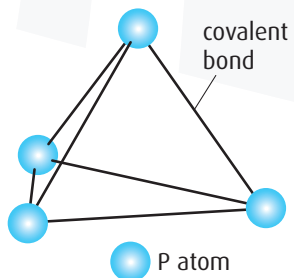
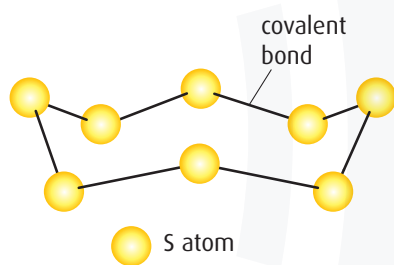
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SKILL CHECK 1

Draw dot and cross diagrams of PCl_3 , N_2 , CS_2 , C_2H_4 , NH_3 , H_2O_2 , N_2H_4 , SO_3

7

EXAMPLES OF MOLECULES

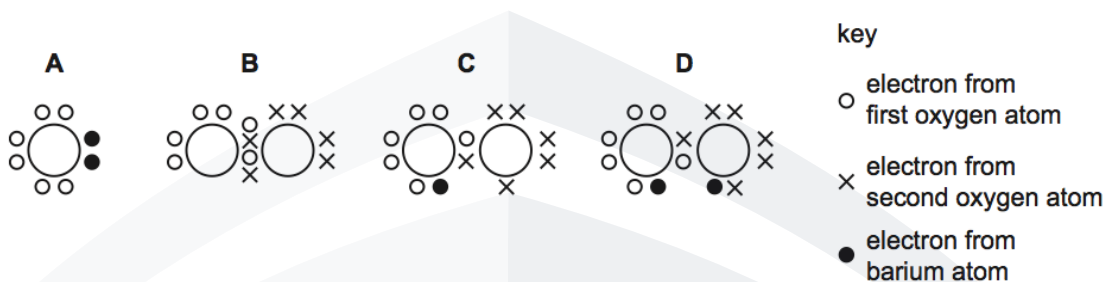


8

SKILL CHECK 2

When barium metal burns in oxygen, the ionic compound barium peroxide, BaO_2 , is formed.

Which dot-and-cross diagram represents the electronic structure of the peroxide anion in BaO_2 ?



9

SKILL CHECK 3

Dicarbon monoxide, C_2O , is found in dust clouds in space. Analysis of it shows that the sequence of atoms in this molecules is C-C-O. All bonds are double bonds and there are no unpaired electrons.

How many lone pairs of electrons are present in a molecule of C_2O ?

- A 1 B 2 C 3 D 4

10

COVALENT BONDING

Atoms share electrons to get the nearest noble gas electronic configuration

Some don't achieve an "octet" as they haven't got enough electrons

e.g. Al in AlCl_3

Others share only some — if they share all they will exceed their "octet"

e.g. NH_3 and H_2O

Atoms of elements in the 3rd period onwards can exceed their "octet" if they wish as they are not restricted to eight electrons in their "outer shell"

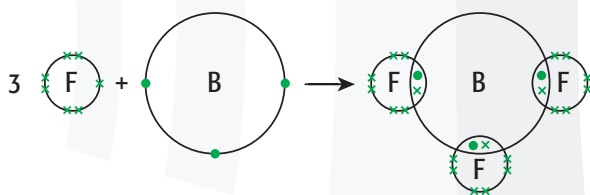
e.g. PCl_5 , SO_2 , SO_3 and SF_6

Only in period 2 are the elements restricted to form an octet. However, in period 3, more than 8 electrons can be taken in the outermost shell due to the s, p and d orbitals which take up 2, 6 and 10 electrons respectively.

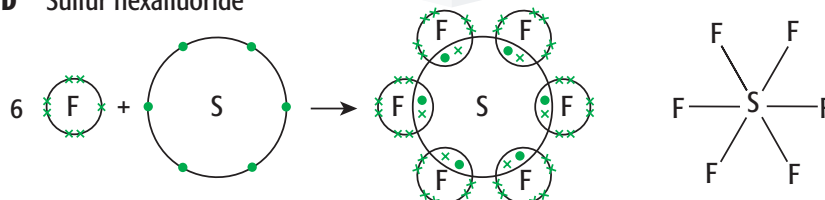
11

DEFYING OCTET

a Boron trifluoride

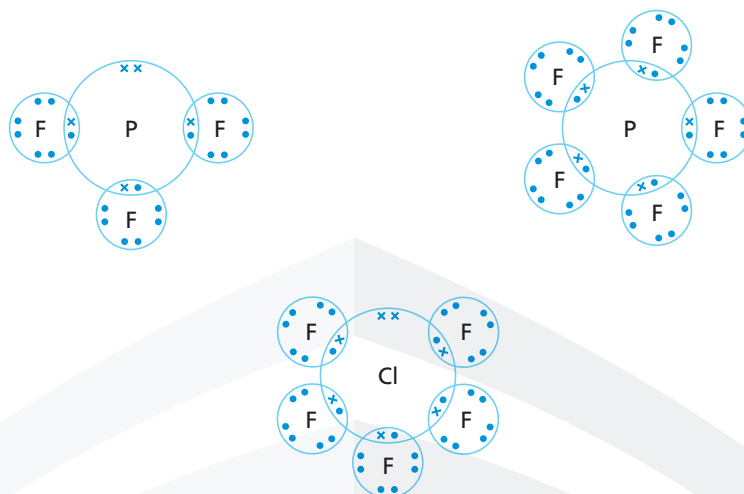


b Sulfur hexafluoride



12

DEFYING OCTET

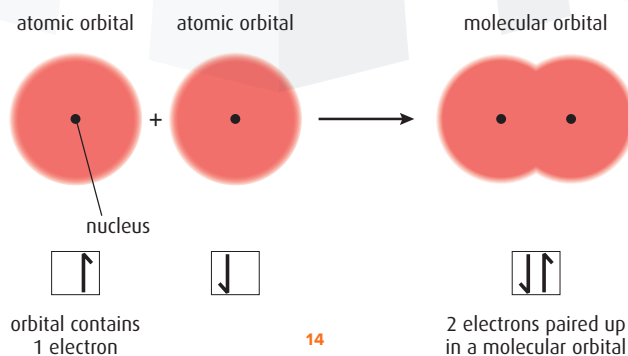


13

MOLECULAR ORBITALS

Covalent bonding is brought about by the atomic orbitals of each atom overlapping with each other, coalescing and forming a molecular orbital.

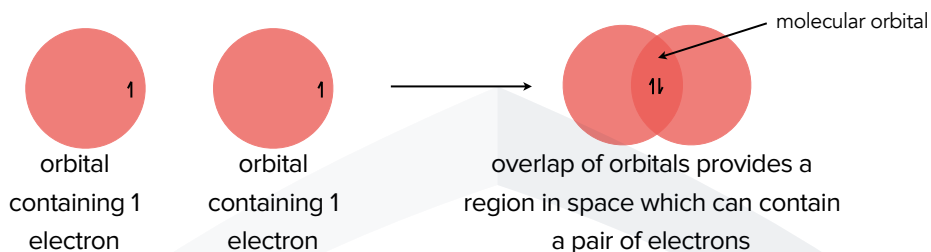
Only individually filled orbitals take part in such bonding, so that the resultant molecular orbital has only two electrons. In the molecular orbital the two electrons circulate around and are attracted to two nuclei of the two bonded atoms.



14

ORBITAL OVERLAP

Covalent bonds are formed when orbitals, each containing one electron, overlap. This forms a region in space where an electron pair can be found; new molecular orbitals are formed.



The space that these shared electrons move within is called a molecular orbital. A molecular orbital is made when two atomic orbitals overlap.

15

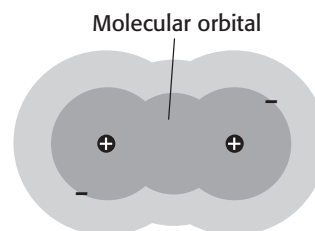
SIGMA BONDS

A Sigma bond (σ bond) is formed when orbitals overlap head-on in a covalent bond.

In a sigma bond, the electron density is concentrated in the orbital overlap volume between the two nuclei.

A sigma bond can be rotated without breaking the bond.

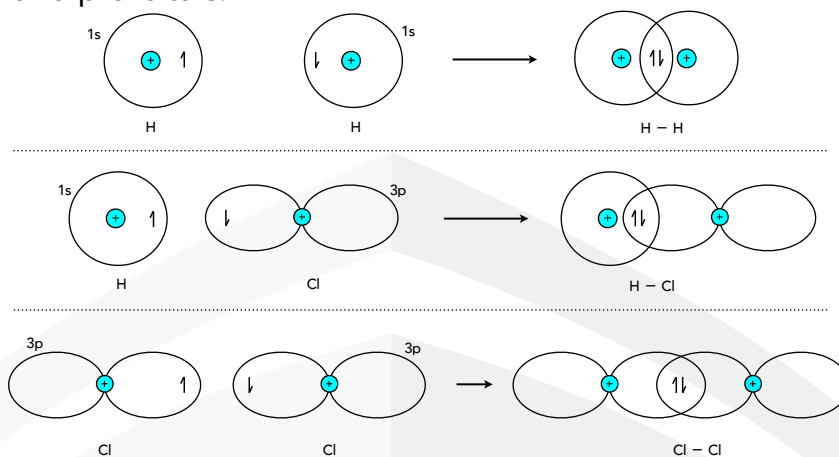
The region where the the two orbitals overlap is the molecular orbital which contains electrons of the sigma bond.



16

SIGMA BONDS

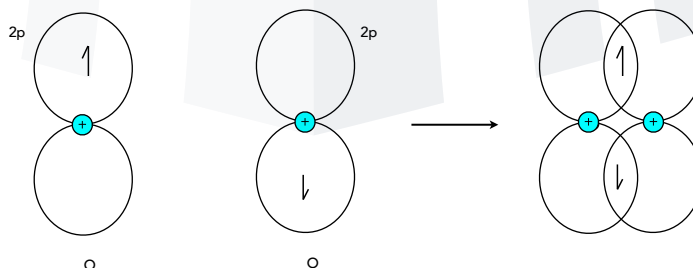
Sigma bonds can form by overlap of two s-orbitals, and s-orbital and p-orbital or two p-orbitals.



17

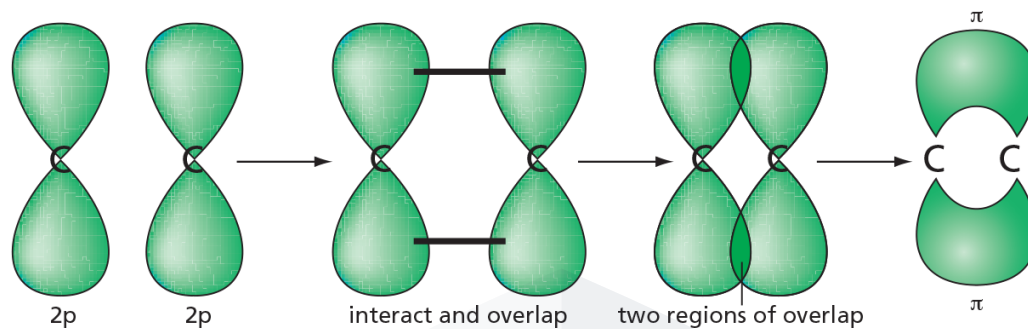
PI BONDS

A pi bond (π bond) is formed when orbitals overlap sideways in a covalent bond. Pi bonds are found in molecules with double and triple bonds.



18

PI BONDS

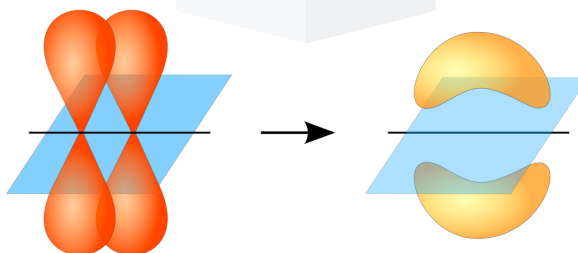
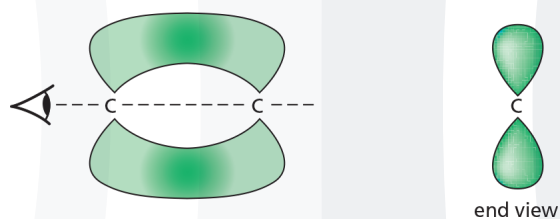


A single π bond is drawn as two electron clouds, one arising from each lobe of the p orbitals.

The two clouds of electrons in a π bond represent one bond consisting of a total of two electrons.

19

PI BONDS

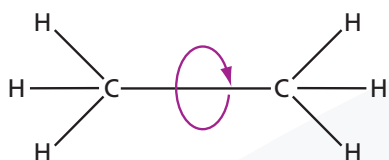


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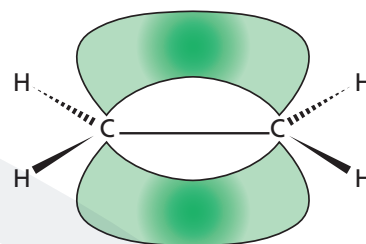
PI BONDS

In a pi bond, the electron density is concentrated in the orbital overlap volumes above and below the line joining the two nuclei.

A pi bond cannot be rotated without breaking the bond.



rotation possible around
the single bond



no rotation possible

21

SKILL CHECK 4

What is always involved in a carbon-carbon π bond?

- A a shared pair of electrons
- B a sideways overlap of p orbitals
- C delocalized electrons

22

DOUBLE BONDS

A double bond consists of one sigma bond and one pi bond, for example the C=C double bond in ethene and the O=O double bond in oxygen.

A typical triple bond, for example in nitrogen, consists of one sigma bond and two pi bonds in two mutually perpendicular planes.

Pi bonds are weaker than sigma bonds.

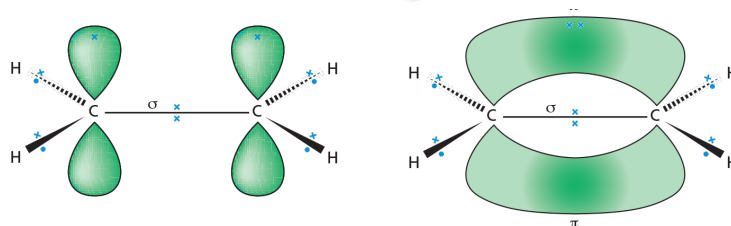
23

MULTIPLE BONDS - ETHENE

An example of a pi bond is the C=C bond in ethene. This bond consists of two parts.

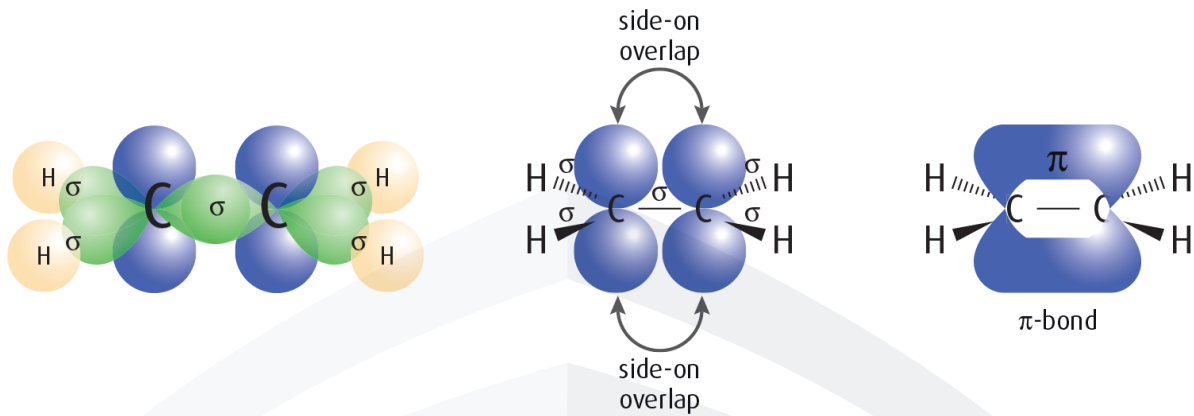
One part consists of two p orbitals of carbon overlapping in a sigma bond.

In the other part of the bond, two p orbitals overlap in a pi bond



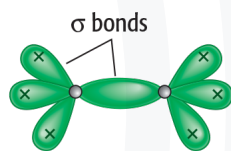
24

MULTIPLE BONDS - ETHENE

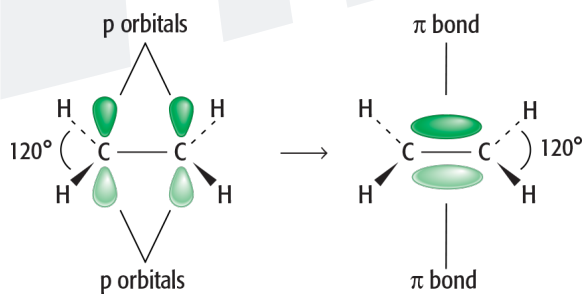
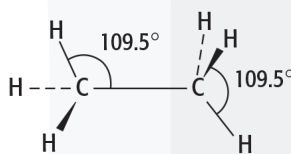


25

ETHANE AND ETHENE

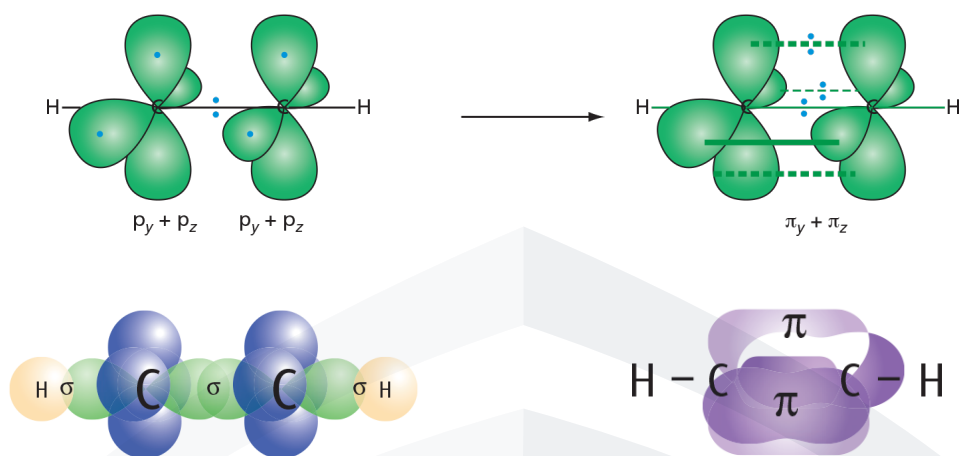


- carbon nucleus
- × hydrogen nucleus



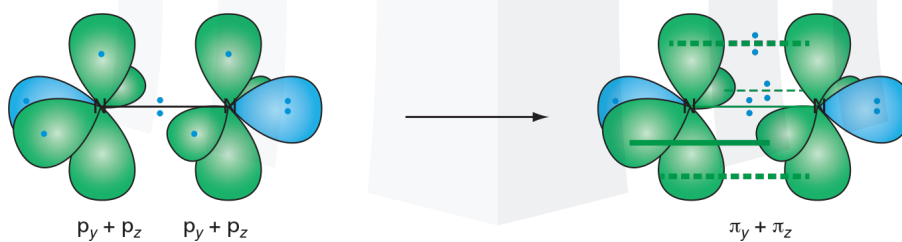
26

TRIPLE BOND - ETHYNE



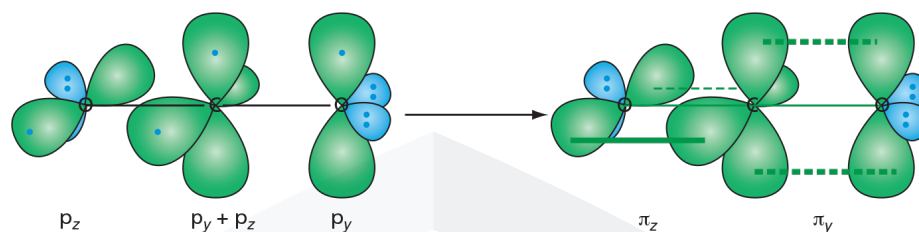
27

TRIPLE BOND - NITROGEN



28

TWO DOUBLES - CARBON DIOXIDE



29

SKILL CHECK 5

Which statements about covalent bonds are correct?

- A** A triple bond consists of one π bond and two σ bonds.
- B** The electron density in a σ bond is highest along the axis between the two bonded atoms.
- C** A π bond restricts rotation about the σ bond axis.

30

DATIVE COVALENT BONDING

A dative covalent bond (or coordinate covalent bond) is a covalent bond between two atoms in which the shared electrons are contributed by only one of the atoms.

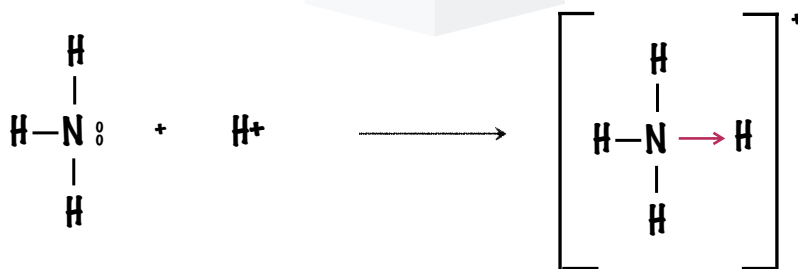
e.g. Boron trifluoride & ammonia NH_3BF_3

Boron has an incomplete shell in BF_3 and can accept/share a pair of electrons donated by ammonia.



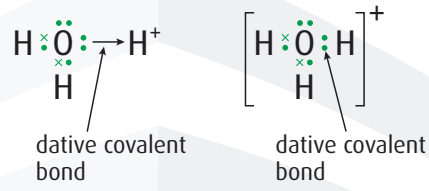
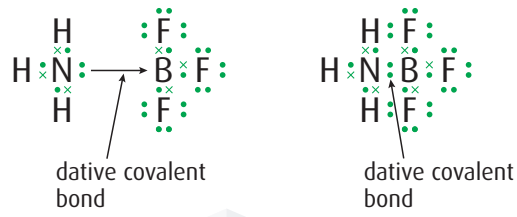
31

DATIVE COVALENT BONDING



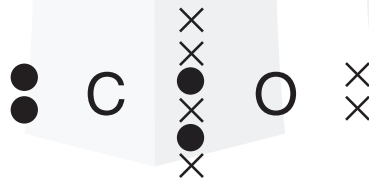
32

DATIVE COVALENT BONDING



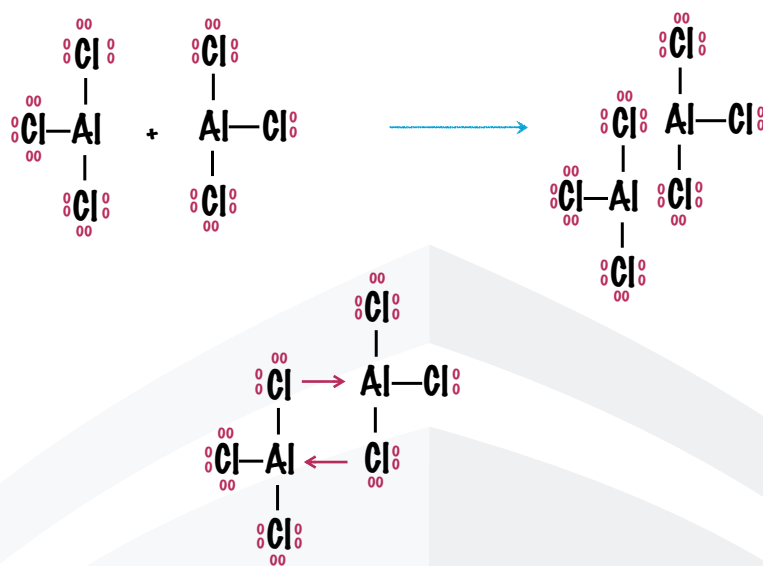
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DATIVE COVALENT BONDING

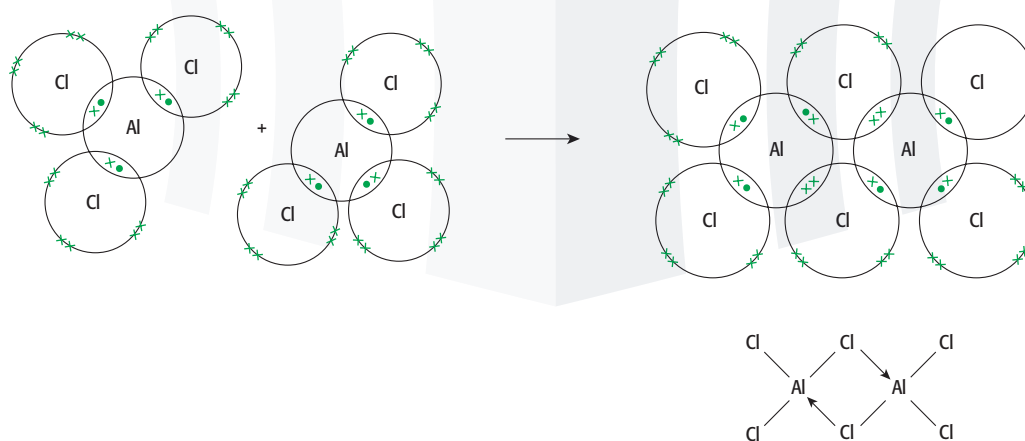


34

AL₂CL₆



AL₂CL₆



DATIVE COVALENT BONDING

A dative covalent bond differs from covalent bond only in its formation

Both electrons of the shared pair are provided by one species (donor) and it shares the electrons with the acceptor

Donor species will have lone pairs in their outer shells

Acceptor species will be short of their “octet” or maximum.

Chemists call it a dative covalent bond because the word dative means ‘giving’ and one atom gives both the electrons to make the bond. Once formed, there is no difference between a dative bond and any other covalent bond.

37

BOND ENERGY

The strength of a covalent bond is measured by the bond energy.

The bond energy is the amount of energy required to break a covalent bond, per mole of bonds. The greater the bond energy, the stronger the bond.

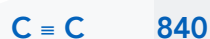
Very large bond energies can make molecules unreactive. The nitrogen molecule (N_2) is unreactive because of the very large $\text{N}\equiv\text{N}$ bond energy of 944 KJ mol^{-1} .

38

BOND ENERGY

Bond forming releases energy, and is therefore exothermic.

Bond breaking requires energy, and is therefore endothermic. For the same two atoms, triple bonds are stronger than double bonds which in turn are stronger than single bonds.



39

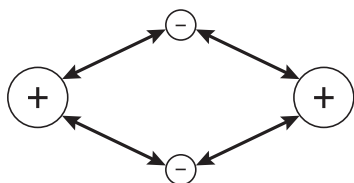
BOND LENGTH

The covalent bond length is the distance between the nuclei of the two atoms linked by one or more covalent bonds

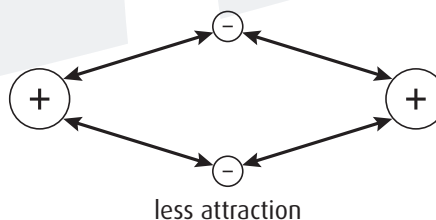
For the same two atoms, triple bonds are shorter than double bonds which in turn are shorter than single bonds.

a

greater attraction



b



less attraction

40

COVALENT BONDING WS 1

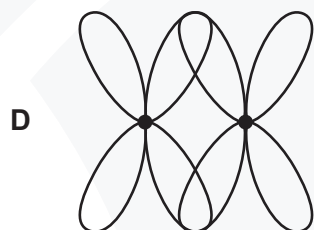
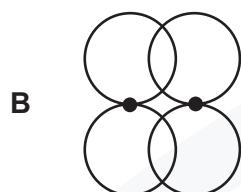
SECTION A

1 Which molecule contains only six bonding electrons?

- A C_2H_4 B C_2F_6 C H_2O D NF_3

[W'03 Q6]

2 Which diagram describes the formation of a π bond from the overlap of its orbitals?



[W'06 Q5]

3 The CN^- ion is widely used in the synthesis of organic compounds.

What is the pattern of electron pairs in this ion?

	bonding pairs of electrons	lone pairs on carbon atom	lone pairs on nitrogen atom
A	2	1	1
B	2	2	1
C	3	1	1
D	3	1	2

4 In which species does the underlined atom have an incomplete outer shell?

- A \underline{Al}_2Cl_6 B $\underline{C}H_3^+$ C $Cl_2\underline{O}$ D $H_2\underline{Cl}C\cdot$

[J'12 1 Q11]

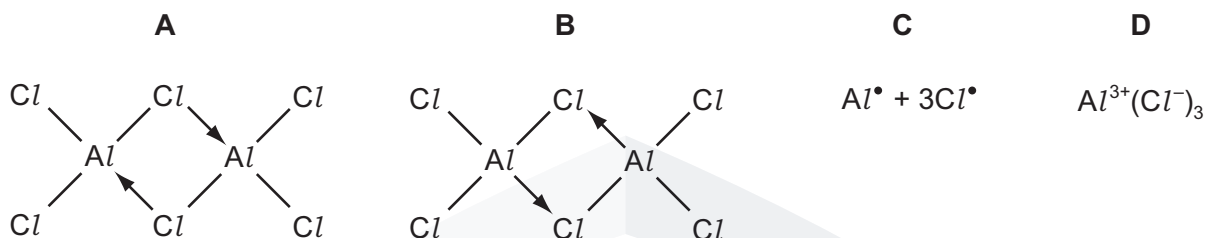
5 In which species does the underlined atom have an incomplete outer shell?

- A $\underline{\text{B}}\text{F}_3$ B $\underline{\text{C}}\text{H}_3^-$ C $\text{F}_2\underline{\text{O}}$ D $\text{H}_3\underline{\text{O}}^+$

[M'1 Q12]

6 Aluminium chloride sublimes at 178°C .

Which structure best represents the species in the vapour at this temperature?



[S'06 Q15]

7 Which element is expected to show the greatest tendency to form some covalent compounds?

- A aluminium
B calcium
C magnesium
D sodium

[S'13 Q17]

8 What is the correct number of bonds of each type in the Al_2Cl_6 molecule?

	covalent	co-ordinate (dative covalent)
A	6	1
B	6	2
C	7	0
D	7	1

[S'16 Q2]

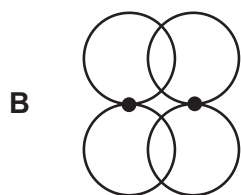
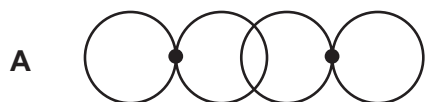
9 When solid aluminium chloride is heated, Al_2Cl_6 is formed.

Which bonding is present in Al_2Cl_6 ?

- A covalent and co-ordinate (dative covalent)
B covalent only
C ionic and co-ordinate (dative covalent)
D ionic only

[W'16 2 Q6]

10 Which diagram represents the overlap of two orbitals which will form a π bond?



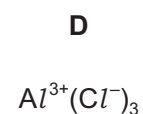
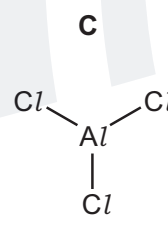
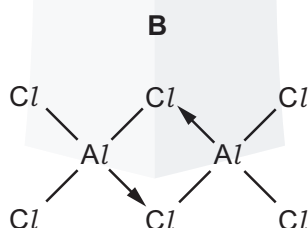
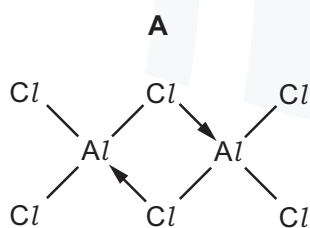
[W'15 1 Q4]

11 What is the correct number of bonds of each type in the Al_2Cl_6 molecule?

	covalent	co-ordinate (dative covalent)
A	6	1
B	6	2
C	7	0
D	7	1

12 Solid aluminium chloride sublimes at 178°C .

Which structure best represents the species in the vapour at this temperature?



[S'06 Q15]

13 Carbon and silicon have the same outer electronic structure.

Why is a Si–Si bond weaker than a C–C bond?

- A Silicon atoms have a larger atomic radius than carbon atoms.
- B Silicon has a greater nuclear charge than carbon.
- C Silicon has a smaller first ionisation energy than carbon.
- D Silicon is more metallic than carbon.

[S'16 2 6]



SECTION B

For each of the questions in this section, one or more of the three numbered statements 1 to 3 may be correct.

Decide whether each of the statements is or is not correct (you may find it helpful to put a tick against the statements that you consider to be correct).

The responses **A** to **D** should be selected on the basis of

A	B	C	D
1, 2 and 3 are correct	1 and 2 only are correct	2 and 3 only are correct	1 only is correct

No other combination of statements is used as a correct response.

- 1 Which of the following statements are correct for the sequence of compounds below considered from left to right?

NaF MgO AlN SiC

- The electronegativity difference between the elements in each compound increases.
- The formula-units of these compounds are isoelectronic (have the same number of electrons).
- The bonding becomes increasingly covalent.

[W'03 1 Q34]

- 2 Sodium hydrosulfide, NaSH, is used to remove hair from animal hides.

Which statements about the SH⁻ ion are correct?

- It contains 18 electrons.
- Three lone pairs of electrons surround the sulfur atom.
- Sulfur has an oxidation state of +2.

[S'10 3 Q32]

- 3 Which elements have atoms which can form π bonds with atoms of other elements?

- oxygen
- nitrogen
- fluorine

4 Which elements can form π bonds in their compounds?

- 1 carbon
- 2 oxygen
- 3 nitrogen

[M'16 2 Q31]

5 In the gas phase, aluminium chloride exists as the dimer, Al_2Cl_6 .

By using this information, which of the following are structural features of the Al_2Cl_6 molecule?

- 1 Each aluminium atom is surrounded by four chlorine atoms.
- 2 There are twelve non-bonded electron pairs in the molecule.
- 3 Each aluminium atom contributes electrons to four covalent bonds.

COVALENT BONDS WS 2

- 1 Ethyne is a linear molecule with a triple bond, $C\equiv C$, between the two carbon atoms.

Draw a 'dot-and-cross' diagram of an ethyne molecule.

[1]

- 2 At low temperatures, aluminium chloride vapour has the formula Al_2Cl_6 . Draw a 'dot-and-cross' diagram to show the bonding in Al_2Cl_6 . Show outer electrons only. Represent the aluminium electrons by ●. Represent the chlorine electrons by x.

[6]



3 Chemical bonding

This topic introduces the different ways by which chemical bonding occurs and the effect this can have on physical properties.

3.2 shapes of simple molecules



SHAPES OF MOLECULES

3 Chemical bonding

This topic introduces the different ways by which chemical bonding occurs and the effect this can have on physical properties.

Learning outcomes

Candidates should be able to:

3.2 Covalent bonding and co-ordinate (dative covalent) bonding including shapes of simple molecules

- a) describe, including the use of 'dot-and-cross' diagrams:
 - (i) covalent bonding, in molecules such as hydrogen, oxygen, chlorine, hydrogen chloride, carbon dioxide, methane, ethene
 - (ii) co-ordinate (dative covalent) bonding, such as in the formation of the ammonium ion and in the Al_2Cl_6 molecule
- b) describe covalent bonding in terms of orbital overlap, giving σ and π bonds, including the concept of hybridisation to form sp , sp^2 and sp^3 orbitals (see also Section 14.3)
- c) explain the shapes of, and bond angles in, molecules by using the qualitative model of electron-pair repulsion (including lone pairs), using as simple examples: BF_3 (trigonal), CO_2 (linear), CH_4 (tetrahedral), NH_3 (pyramidal), H_2O (non-linear), SF_6 (octahedral), PF_5 (trigonal bipyramidal)
- d) predict the shapes of, and bond angles in, molecules and ions analogous to those specified in 3.2(b) (see also Section 14.3)

SHAPES OF MOLECULES

The shape of a molecule plays a large part in determining its properties and reactivity.

The specific orientation of electron pairs in covalent molecules imparts a characteristic shape to the molecules.

The shape of a molecule made of only two atoms, such as H_2 or CO , is easy to determine. Only a linear shape is possible when there are two atoms. Determining the shapes of molecules made of more than two atoms is more complicated.

Using **Valence Shell Electron Pair Repulsion (VSEPR)** theory one can predict the shape of a molecule by examining the Lewis structure of the molecule.

1

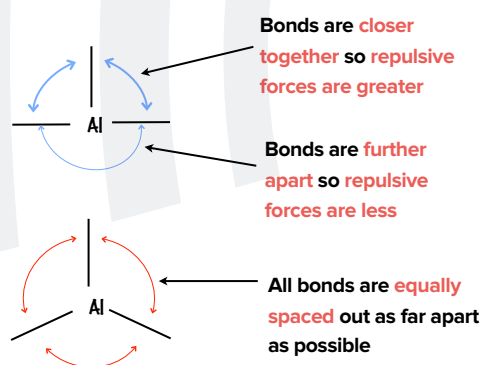
VSEPR THEORY

The electron pairs around the central atom of the molecule arrange themselves to minimise electronic repulsion and so that they can be as far away as possible from each other.

This fact is used to predict molecular shape.

Molecules contain covalent bonds.

As covalent bonds consist of a pair of electrons, each bond will repel other bonds.

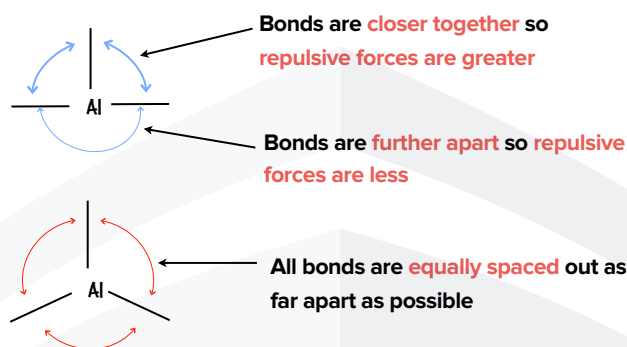


2

VSEPR THEORY

Bonds will therefore push each other as far apart as possible to reduce the repulsive forces.

Because the repulsions are equal, the bonds will also be equally spaced.



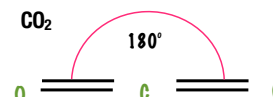
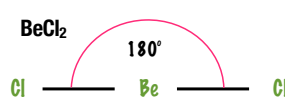
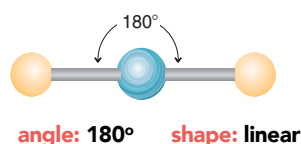
3

LINEAR

Beryllium chloride has two shared electron pairs around the beryllium atom.

These electron pairs have minimum repulsion if they are located as far apart as possible while still bonding the chlorine to the central atom.

This condition is met if the electron pairs are located on opposite sides of the molecule, resulting in a linear structure, 180° apart:



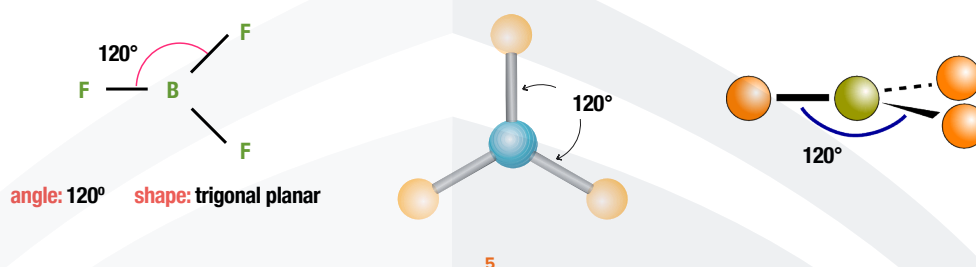
4

TRIGONAL PLANAR

Now think about what happens when the central atom is surrounded by three shared pairs. Look at BF_3 .

Boron trifluoride has three shared electron pairs around the central atom.

Placing the electron pairs in a plane, forming a triangle, minimizes the electron pair repulsion in this molecule.



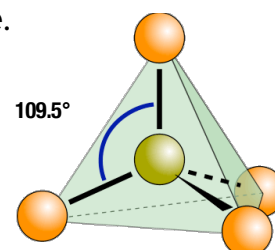
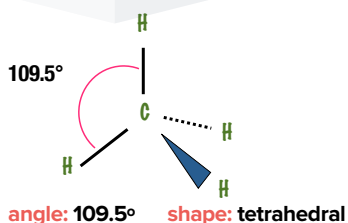
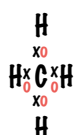
TETRAHEDRAL

Methane has four shared pairs of electrons.

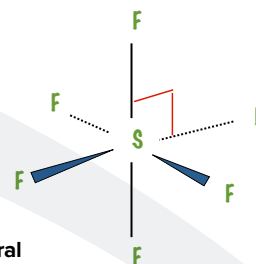
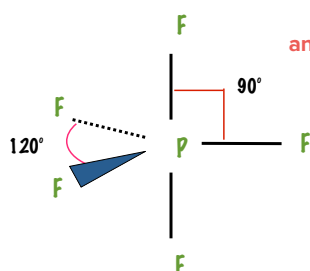
Here, minimum electron repulsion is achieved by arranging the electrons at the corners of a tetrahedron.

Each $\text{H}-\text{C}-\text{H}$ bond angle is 109.5° .

Methane has a three – dimensional tetrahedral structure.



5 AND 6 BONDS



7

IRREGULAR SHAPES

NH_3 also has four electron pairs about the central atom. In contrast to CH_4 , in which all four pairs are bonding, ammonia has three pairs of bonding electrons and one nonbonding lone pair of electrons.



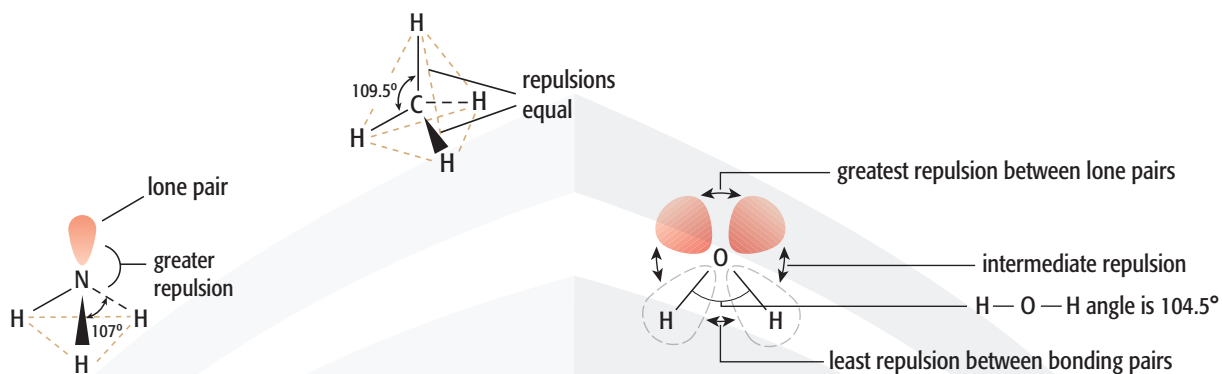
The lone pair in ammonia is closer to the central atom, N, than the bonding pairs and has greater repulsion.

Thus the arrangement of electron pairs in ammonia is distorted.

8

IRREGULAR SHAPES

The **H** atoms in NH_3 are pushed closer together than in CH_4 . The bond angle is 107° because lone pair–bond pair repulsions are greater than bond pair–bond pair repulsions.



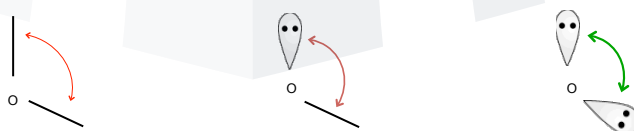
9

IRREGULAR SHAPES

If a molecule, or ion, has lone pairs on the central atom, the shapes are slightly distorted away from the regular shapes.

This is because of the extra repulsion caused by the lone pairs.

BOND PAIR – BOND PAIR < LONE PAIR – BOND PAIR < LONE PAIR – LONE PAIR

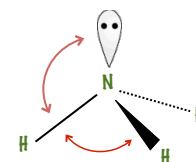
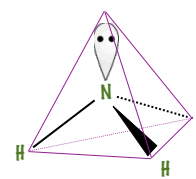


As a result of the extra repulsion, bond angles tend to be slightly less as the bonds are squeezed together.

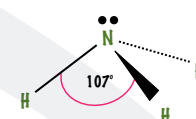
10

AMMONIA

- Nitrogen has five electrons in its outer shell
- 3 covalent bonds are formed and a pair of non-bonded electrons is left
- As the total number of electron pairs is 4, the shape is BASED on four bond tetrahedral shape
- Not all the repulsions are the same.
Repulsions: **LONE PAIR - BOND PAIR** > **BOND PAIR - BOND PAIR**
- The N-H bonds are pushed closer together
- Lone pairs are not included in the shape



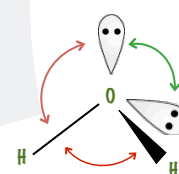
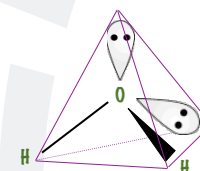
angle: 107° shape: trigonal pyramidal



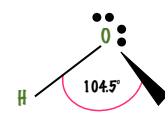
11

WATER

- Oxygen has six electrons in its outer shell
- 2 covalent bonds are formed and 2 pairs of non-bonded electrons are left
- As the total number of electron pairs is 4, the shape is BASED on the four bond tetrahedral shape.
- Not all the repulsions are the same.
Repulsions: **LONE PAIR - LONE PAIR** > **LONE PAIR - BOND PAIR** > **BOND PAIR - BOND PAIR**
- The O-H bonds are pushed even closer together
- Lone pairs are not included in the shape



angle: 104.5° shape: angular / bent



12

SUMMARY OF SHAPES

bonds	lone pairs	shape	angle	example
2	0	linear	180°	BeCl ₂ CO ₂
3	0	trigonal planar	120°	BF ₃ AlCl ₃
2	1	bent / angular	117°	SO ₂
4	0	tetrahedral	109.5°	SiCl ₄ CH ₄
3	1	trigonal pyramidal	107°	NH ₃ PCl ₃
2	2	bent / angular	104.5°	H ₂ O
5	0	trigonal bipyramidal	90° & 120°	PCl ₅
6	0	octahedral	90°	SF ₆

13

CALCULATING SHAPES

The shape of a molecule or a complex ion is calculated by:

1. Calculating the number of electrons in the outer shell of the central species
2. Pairing up electrons, making sure the outer shell maximum is not exceeded
3. Calculating the number of bond pairs and lone pairs
4. Using VSEPR to calculate shape and bond angle(s)

14

CALCULATING SHAPES

For IONS:

The number of electrons in the outer shell depends on the charge on the ion

- if the ion is positive you remove as many electrons as there are positive charges
- if the ion is negative you add as many electrons as there are negative charges

e.g. for PF_6^- add one electron to the outer shell of P

for PCl_4^+ remove one electron from the outer shell of P

15

EXAMPLES

NH_3 **BOND PAIRS** 3 **PYRAMIDAL**
LONE PAIRS 1 **H-N-H 107°**

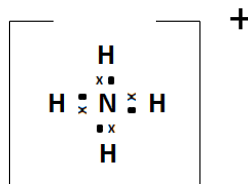
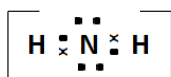
NH_4^+ **BOND PAIRS** 4 **TETRAHEDRAL**
LONE PAIRS 0 **H-N-H 109.5°**

NH_2^- **BOND PAIRS** 2 **ANGULAR**
LONE PAIRS 2 **H-N-H 104.5°**

A compound with an overall charge may not be ionic, it can also be covalent.

e.g: NH_4^+

Number of valence electrons = 5
 But due to "+" it loses 1e- ∴ = 4



16

SKILL CHECK 1

Determine the number, and type, of electron pairs around the central atom(s) in each of the following. Predict the shape and bond angles of each. (Hint: it may help to draw 'dot-and-cross' diagrams)

- (a) phosphine, PH_3
- (b) sulfur dichloride, SCl_2
- (c) dichloromethane, CH_2Cl_2
- (d) cobalt(II) chloride, CoCl_2
- (e) xenon tetrafluoride, XeF_4

17

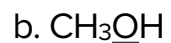
MORE

BF_3	3 bp 0 lp	120°	trigonal planar	boron pairs up all 3 electrons in its outer shell
SiCl_4	4 bp 0 lp	109.5°	tetrahedral	silicon pairs up all 4 electrons in its outer shell
PCl_4^+	4 bp 0 lp	109.5°	tetrahedral	as ion is +, remove an electron in the outer shell then pair up
PCl_6^-	6 bp 0 lp	90°	octahedral	as the ion is -, add one electron to the 5 in the outer shell then pair up
SiCl_6^{2-}	6 bp 0 lp	90°	octahedral	as the ion is $2-$, add two electrons to the outer shell then pair up

18

SKILL CHECK 2

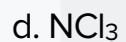
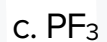
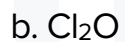
Draw the shapes for the following molecules. The underlined atom is the central atom



19

SKILL CHECK 3

Draw the shapes of the following molecules



20

SKILL CHECK 4

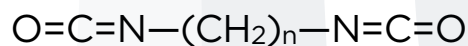
Deduce the shapes of the following ions:

- a. NH_4^+ b. CH_3^+ c. CH_3^- d. CO_3^{2-} e. SO_4^{2-} f. AlH_4^- g. AlF_6^{3-}

21

SKILL CHECK 5

Lycra[®] is a polyurethane fibre used in the fashion industry. It is a polymer made from two monomers, one of which has the following formula.



What is the O-C-N bond angle in this molecule?

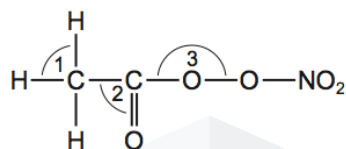
- A** 90° **B** 109° **C** 120° **D** 180°

22

SKILL CHECK 6

Organic nitrates in photochemical smog can cause breathing difficulties.

The diagram shows an example of an organic nitrate molecule.



What is the correct order of the bond angles shown in ascending order (smallest first)?

- A** 1 → 2 → 3 **B** 2 → 1 → 3 **C** 3 → 1 → 2 **D** 3 → 2 → 1

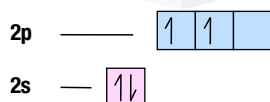
23

HYBRIDISATION

Hybridisation is the mixing of atomic orbitals to produce a new set of orbitals (the same number as originally) that have characteristics of the original orbitals and are better arranged spatially for covalent bonding.

To form a covalent bond, an orbital containing one electron is required. These orbitals overlap to form a covalent bond.

Carbon has six electrons and the outer shell electronic configuration $2s^2 2p^2$:



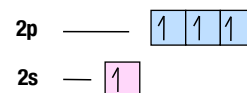
As it has only two unpaired electrons, carbon should form two covalent bonds.

24

HYBRIDISATION

However, it is well known that carbon virtually always forms four covalent bonds.

One of the electrons in the 2s orbital must then be promoted to the 2p sub-shell to give four unpaired electrons. This requires energy.



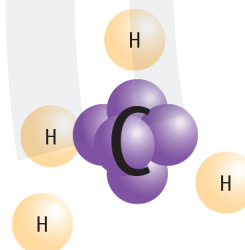
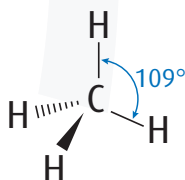
However, bond formation releases energy and the formation of four bonds instead of two more than pays back the energy needed to promote an electron to a higher sub-shell.

Carbon now has four unpaired electrons and can form four covalent bonds, but the atomic orbitals do not point in the correct direction for bonding.

25

HYBRIDISATION

CH₄ is tetrahedral with bond angles of 109.5° but the p orbitals are at 90° to each other.



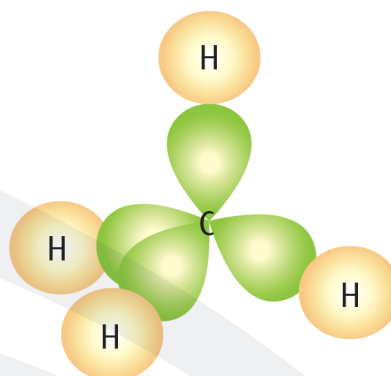
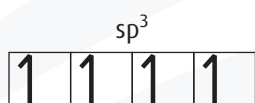
26

SP³ HYBRIDISATION

When carbon forms methane, the four atomic orbitals on carbon, one s and three p, then mix to give four sp³ hybrid orbitals, which point to the vertices of a tetrahedron.

This is the process of hybridisation.

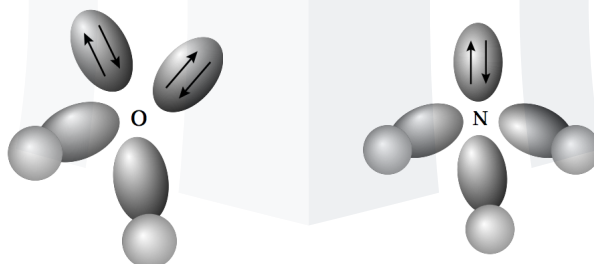
The four sp³ hybrid orbitals all have the same energy



27

SP³ HYBRIDISATION

Should only three atoms bond to the sp³ hybridised atom, then the molecular geometry is trigonal pyramidal. Ammonia is an example of this.



In water the oxygen is sp³ hybridised but because only two atoms have bonded to the oxygen, the molecular geometry is bent.

28

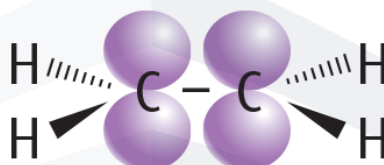
SP² HYBRIDISATION

In an sp² hybridisation one 2s and two 2p orbitals combine to form a new hybrid shape.

In this hybridised state the carbon will make two single bonds and one double bond.

Of the three p orbitals on each C atom, one of them is not in the same plane as the H atoms or the other C atom.

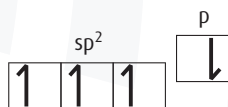
This p orbital is not involved in hybridisation.



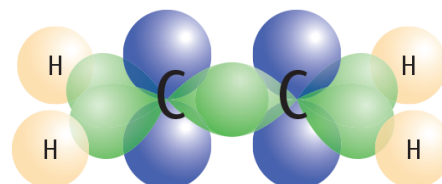
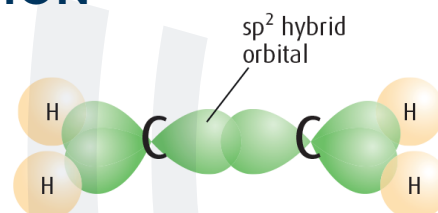
29

SP² HYBRIDISATION

Mixing the two p orbitals and one s orbital all in the same plane produces three sp² orbitals pointing towards the corners of an equilateral triangle:



This leaves one p orbital, containing one electron, perpendicular to the single bond () framework on each C atom:



30

HYBRIDISATION

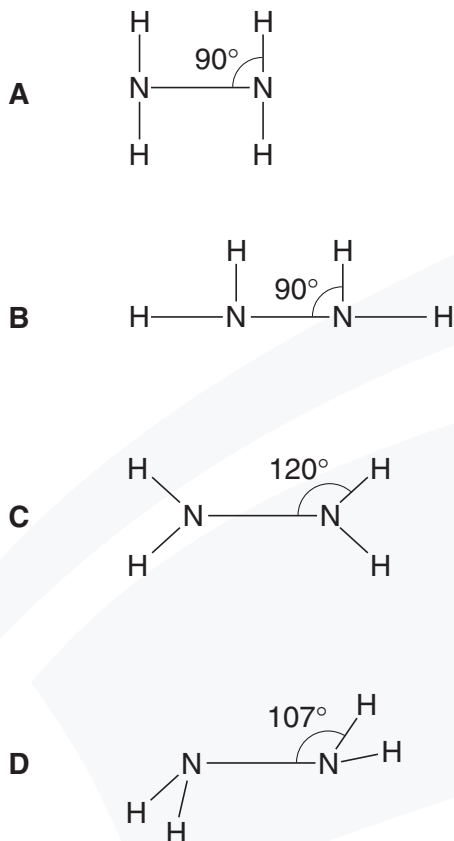
	sp^3 hybridisation	sp^2 hybridisation	sp hybridisation
Number of Atoms Bonded to the Central Atom	4	3	2
Angle between Atoms Bonded to Central Atom	109.5°	120°	180°
Molecular Geometry	Tetrahedral with four atoms bonded. Trigonal pyramidal with three atoms bonded. Bent with two atoms bonded.	Trigonal planar with three atoms bonded.	Linear with two atoms bonded.
Types of Bonds Found	Four single bonds.	One double bond and two single bonds.	One single and one triple bond. (Or) Two double bonds.

31

SHAPES OF MOLECULES WS 1

SECTION A

1 Which is the most likely shape of a molecule of hydrazine, N_2H_4 ?



[W'02 Q6]

2 Chemists have been interested in the properties of hydrogen selenide, H_2Se , to compare it with 'bad egg' gas hydrogen sulphide, H_2S .

Which set of data would the hydrogen selenide molecule be expected to have?

	number of lone pairs on Se atom	bond angle
A	1	104°
B	2	104°
C	2	109°
D	2	180°

[W'03 Q7]

3 Which molecule is planar?

- A NF_3
 B C_2Cl_4
 C C_3H_6
 D C_3H_8

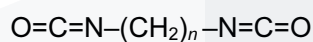
[S'04 Q20]

4 What are the bond angles in the PH_3 molecule likely to be?

- A 90° B 104° C 109° D 120°

[W'04 Q7]

5 *Lycra*[®] is a polyurethane fibre used in the fashion industry. It is a polymer made from two monomers, one of which has the following formula.



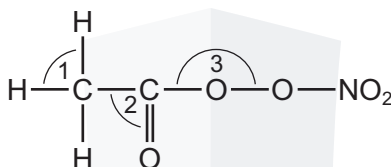
What is the O–C–N bond angle in this molecule?

- A 90° B 109° C 120° D 180°

[W'07 Q6]

6 Organic nitrates in photochemical smog can cause breathing difficulties.

The diagram shows an example of an organic nitrate molecule.



What is the correct order of the bond angles shown in ascending order (smallest first)?

- A $1 \rightarrow 2 \rightarrow 3$ B $2 \rightarrow 1 \rightarrow 3$ C $3 \rightarrow 1 \rightarrow 2$ D $3 \rightarrow 2 \rightarrow 1$

[W'10 Q7]

- 7 Methyl isocyanate, CH_3NCO , is a toxic liquid which is used in the manufacture of some pesticides.

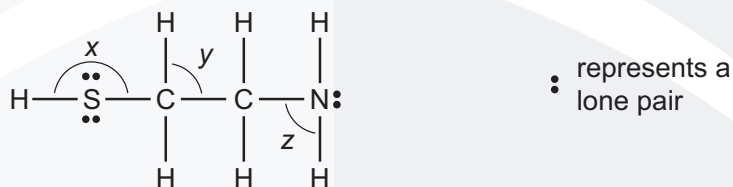
In the methyl isocyanate molecule, the sequence of atoms is $\text{H}_3\text{C}-\text{N}=\text{C}=\text{O}$.

What is the approximate angle between the bonds formed by the N atom?

A	B	C	D
104°	109°	120°	180°

[W'11 1 Q4]

- 8 The antidote molecule shown can help to prevent liver damage if someone takes too many paracetamol tablets.



What is the order of **decreasing** size of the bond angles x , y and z ?

	largest	→	smallest
A	x		z
B	x		y
C	y		x
D	z		x

[W'09 1 Q4]

- 9 Which molecule or structure does **not** contain three atoms bonded at an angle between 109° and 110° ?
- A ethanoic acid
 B graphite
 C propane
 D silicon(IV) oxide

[1 Q]

10 In which pair do the molecules have the same shape as each other?

- A H_2O and CO_2
 B H_2O and SCl_2
 C NH_3 and BH_3
 D SCl_2 and BeCl_2

[W'12 1 Q12]

11 X is an element in Period 2.

In which fluoride is the F-X-F angle the largest?

- A BF_3 B CF_4 C NF_3 D OF_2

12 Which series shows molecules in order of increasing bond angle?

- A $\text{CH}_4 \rightarrow \text{BF}_3 \rightarrow \text{NH}_3$
 B $\text{H}_2\text{O} \rightarrow \text{CO}_2 \rightarrow \text{BF}_3$
 C $\text{NH}_3 \rightarrow \text{CH}_4 \rightarrow \text{CO}_2$
 D $\text{NH}_3 \rightarrow \text{CH}_4 \rightarrow \text{H}_2\text{O}$

[M'16 Q6]

13 Which row of the table is correct?

	shape		bonds present	
	ammonia molecule	ammonium ion	ammonia molecule	ammonium ion
A	pyramidal	regular tetrahedral	σ	σ
B	pyramidal	regular tetrahedral	σ	π
C	regular tetrahedral	pyramidal	σ	σ
D	regular tetrahedral	pyramidal	π	σ

14 Dicarbon monoxide, C_2O , is found in dust clouds in space. The structure of this molecule is $\text{C}=\text{C}=\text{O}$. The molecule contains no unpaired electrons.

How many lone pairs of electrons are present in a molecule of C_2O ?

- A 1 B 2 C 3 D 4

[S'13 2 Q9]

15 $AlCl_3$ vapour forms molecules with formula Al_2Cl_6 as it is cooled.

What happens to the bond angles during the change from $AlCl_3$ to Al_2Cl_6 ?

- A Some decrease, some remain the same.
- B Some increase, some remain the same.
- C They all decrease.
- D They all increase.

[S'14 1 Q6]

16 Which pair has species with different shapes?

- A $BeCl_2$ and CO_2
- B CH_4 and NH_4^+
- C NH_3 and BF_3
- D SCl_2 and H_2O

[S'15 3 Q4]

17 Each of the four species in this question are isolated and gaseous.

Which species is **not** planar?

- A BF_3
- B CH_3^+
- C C_2H_4
- D NH_3

[S'16 2 Q5]

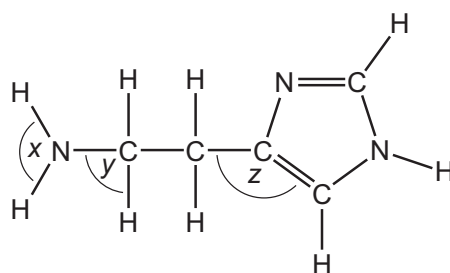
18 Sodium borohydride, $NaBH_4$, and boron trifluoride, BF_3 , are compounds of boron.

What are the shapes around boron in the borohydride ion and in boron trifluoride?

	borohydride ion	boron trifluoride
A	square planar	pyramidal
B	square planar	trigonal planar
C	tetrahedral	pyramidal
D	tetrahedral	trigonal planar

[W'12 2 Q3]

- 19 Histamine is produced in the body to help fight infection. Its shape allows it to fit into receptors which expand blood vessels.



histamine

What are the bond angles x , y and z in histamine, from the smallest to the largest?

	smallest bond angle	→	largest bond angle
A	x		z
B	y		z
C	y		x
D	z		x

[W'16 1 Q6]

- 20 Which molecule is planar?

A C₂Cl₄ **B** C₃H₆ **C** C₃H₈ **D** NF₃

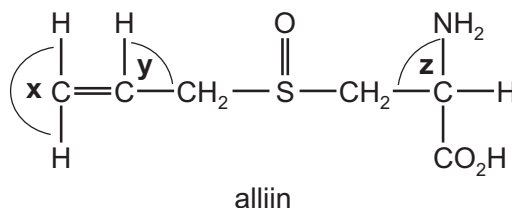
[S'04 Q20]

- 21 In which hydride is the H-X-H bond angle the smallest?

A BH₃ **B** CH₄ **C** C₂H₆ **D** NH₃

[W'16 2 Q7]

22 The characteristic smell of garlic is due to alliin.



What are the approximate bond angles **x**, **y** and **z** in a molecule of alliin?

	x	y	z
A	90°	90°	109°
B	120°	109°	90°
C	120°	120°	109°
D	180°	109°	109°

[M'17 Q5]

23 Which feature is present in both ethene and poly(ethene)?

- A** bond angles of 109°
- B** π covalent bonds
- C** σ covalent bonds
- D** sp^3 orbitals

[S'18 2 Q1]

24 Which statement describes the bond between carbon and hydrogen in an ethene molecule?

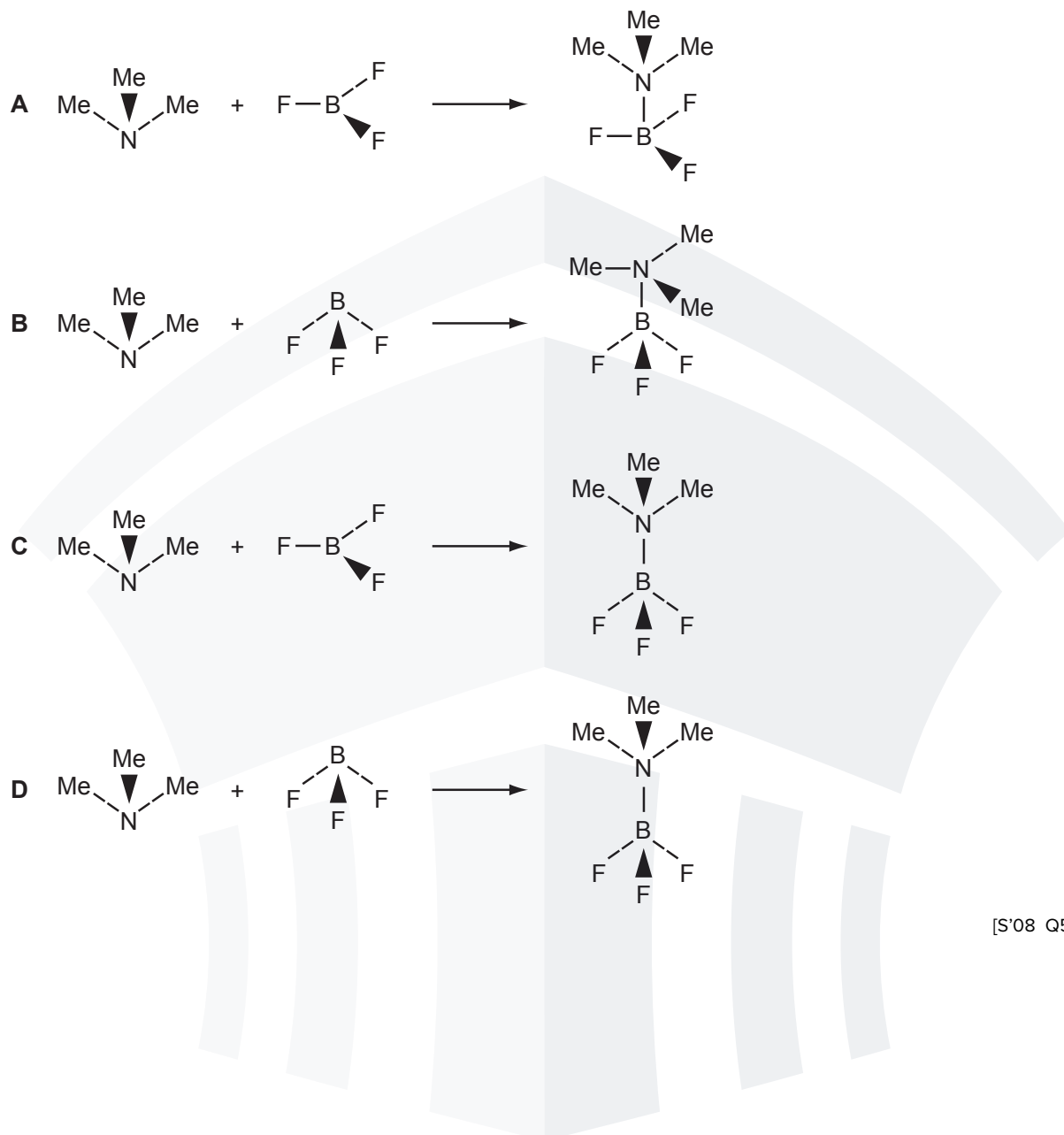
- A** a π bond between an s orbital and an sp^2 orbital
- B** a π bond between an s orbital and an sp^3 orbital
- C** a σ bond between an s orbital and an sp^2 orbital
- D** a σ bond between an s orbital and an sp^3 orbital

[S'18 3 Q4]

25 In this question, the methyl group, CH_3 , is represented by Me.

Trimethylamine, Me_3N , reacts with boron trifluoride, BF_3 , to form a compound of formula $\text{Me}_3\text{N}\cdot\text{BF}_3$.

How may this reaction be written in terms of the shapes of the reactants and products?



SECTION B

For each of the questions in this section, one or more of the three numbered statements 1 to 3 may be correct.

Decide whether each of the statements is or is not correct (you may find it helpful to put a tick against the statements that you consider to be correct).

The responses **A** to **D** should be selected on the basis of

A	B	C	D
1, 2 and 3 are correct	1 and 2 only are correct	2 and 3 only are correct	1 only is correct

No other combination of statements is used as a correct response.

1 Which of the following molecules and ions have a regular trigonal planar shape?

- 1 $AlCl_3$
- 2 CH_3^+
- 3 PH_3

[S'05 Q31]

2 Which molecules are planar?

- 1 BCl_3
- 2 NH_3
- 3 PH_3

[W'05 Q32]

3 In which sequences are the molecules quoted in order of increasing bond angle within the molecule?

- 1 H_2O NH_3 CH_4
- 2 H_2O SF_6 BF_3
- 3 CH_4 CO_2 SF_6

[S'02 Q32]

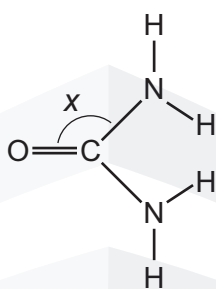
4 Which descriptions of the ammonium ion are correct?

- 1 It contains ten electrons.
- 2 It has a bond angle of 109.5° .
- 3 It has only three bonding pairs of electrons.

5 Which elements can form π bonds in their compounds?

- 1 carbon
- 2 oxygen
- 3 nitrogen

6 Urea is a product of animal metabolism. It can also be used as a fertiliser.



urea

The diagram shows angle x in this molecule.

Which statements about the structure of urea are correct?

- 1 Angle x is approximately 120° .
- 2 The molecule has two π bonds.
- 3 The molecule has only three lone pairs of electrons.

[S'15 1 Q32]

7 Which statements are correct?

- 1 The hydrogen bonds in ice are more regularly arranged than in water.
- 2 The solidification of water to form ice is exothermic.
- 3 Pure water is less dense than ice.

[S'18 1 Q32]

3 Chemical bonding

This topic introduces the different ways by which chemical bonding occurs and the effect this can have on physical properties.

3.3 Intermolecular forces, electronegativity and bond properties



INTERMOLECULAR FORCES

3 Chemical bonding

This topic introduces the different ways by which chemical bonding occurs and the effect this can have on physical properties.

Learning outcomes

Candidates should be able to:

3.3 Intermolecular forces, electronegativity and bond properties

- describe hydrogen bonding, using ammonia and water as simple examples of molecules containing N–H and O–H groups
- understand, in simple terms, the concept of electronegativity and apply it to explain the properties of molecules such as bond polarity (see also Section 3.3(c)), the dipole moments of molecules (3.3(d)) and the behaviour of oxides with water (9.2(c))
- explain the terms *bond energy*, *bond length* and *bond polarity* and use them to compare the reactivities of covalent bonds (see also Section 5.1(b)(ii))
- describe intermolecular forces (van der Waals' forces), based on permanent and induced dipoles, as in, for example, $\text{CHCl}_3(\text{l})$; $\text{Br}_2(\text{l})$ and the liquid Group 18 elements

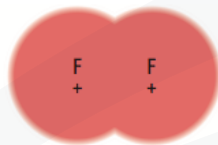
BOND POLARITIES

The example in which two hydrogen atoms bond is simple because both atoms are the same.

Also, each one has a single proton and a single electron, so the attractions are easy to identify.

However, many covalent bonds form between two different atoms.

These atoms often have different attractions for shared electrons.



electrons symmetrically distributed in covalent bond

1

BOND POLARITIES

Now consider a diatomic molecule composed of two different elements; HF is a common example.

It has been experimentally shown that the electrons in the H—F bond are not equally shared; the electrons spend more time in the vicinity of the fluorine atom.

This is because fluorine is a more electronegative element than hydrogen.



electrons lie, on average, closer to F



2

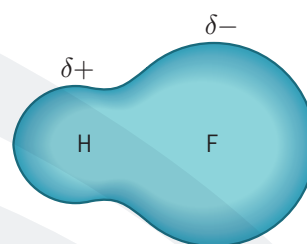
POLAR BONDS

Polar covalent bond is the preferred term for a bond made up of unequally shared electron pairs.

One end of the bond (in this case, the F atom) is more electron rich (higher electron density), hence, more negative.

The other end of the bond (in this case, the H atom) is less electron rich (lower electron density), hence, more positive.

These two ends, one somewhat positive and the other somewhat negative may be described as electronic poles, hence the term polar covalent bonds.



3

POLAR BONDS

In a polar covalent bond, the shared electrons, which are in a molecular orbital, are more likely to be found nearer to the atom whose electronegativity is higher.

This unequal distribution of charge makes the bond polar covalent.

To emphasize the dipole nature of the HF molecule, the formula can be written as $H^{\delta+} F^{\delta-}$. The symbol δ means partial.

With polar molecules, such as HF, the symbol $\delta+$ is used to show a partial positive charge on one end of the molecule.

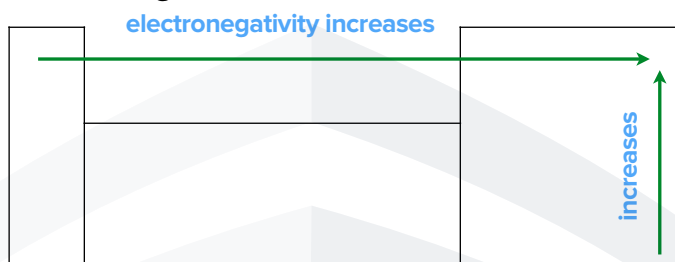
Likewise, the symbol $\delta-$ is used to show a partial negative charge on the other end.

4

ELECTRONEGATIVITY

Electronegativity is a measure of the ability of an atom to attract electrons in a chemical bond. Elements with high electronegativity have a greater ability to attract electrons than do elements with low electronegativity.

The four most electronegative elements are F, O, N, Cl.



Electronegativity increases across a period and decreases down a group

5

BOND POLARITIES

Non-polar bond

- Similar atoms have the same electronegativity
- They will both pull on the electrons to the same extent
- The electrons will be equally shared

Polar bond

- Different atoms have different electronegativities
- One will pull the electron pair closer to its end
- It will be slightly more negative than average, δ^-
- The other will be slightly less negative, or more positive, δ^+
- A dipole is formed and the bond is said to be polar
- Greater electronegativity difference = greater polarity

6

MOLECULAR POLARITY

The electronegativity difference between two atoms covalently bonded together results in the electrons lying more towards one atom than the other. We call such a bond polar.

However, whether an overall molecule is polar also depends on the shape of the molecule.

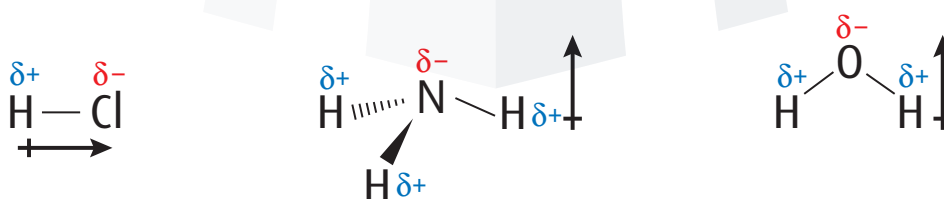
The polarity of molecules is distinct from the polarity of individual bonds; a non-polar molecule may have polar bonds.

7

POLAR MOLECULES

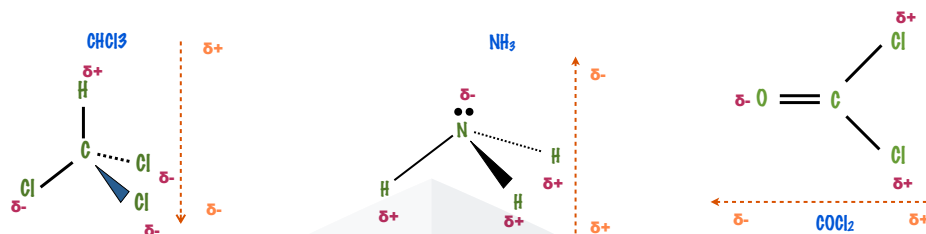
For a molecule to be polar it must have a positive end to the molecule and a negative end. For instance, HCl, NH₃ and H₂O are all polar.

These molecules all have an overall dipole moment, and the arrow indicates the direction of the dipole moment.



8

POLAR MOLECULES

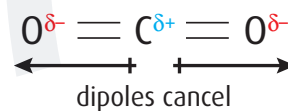


9

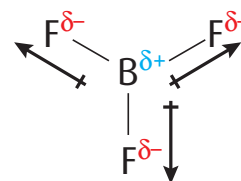
NON-POLAR MOLECULES

Although individual bonds may be polar, the overall molecule may be non-polar if, owing to the symmetry of the molecule, the dipole moments of the individual bonds cancel out.

CO₂ is a non-polar molecule. Each C–O bond is polar, because oxygen is more electronegative than carbon, but overall the dipoles cancel so that there is no overall dipole moment and the molecule is non-polar.



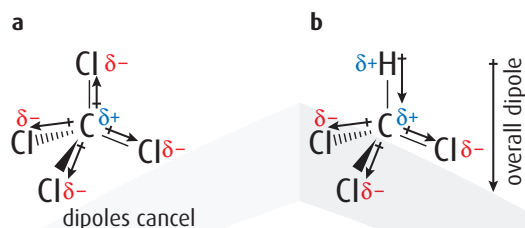
BF₃ is also non-polar. Again, each individual bond is polar but the dipoles cancel.



10

NON-POLAR MOLECULES

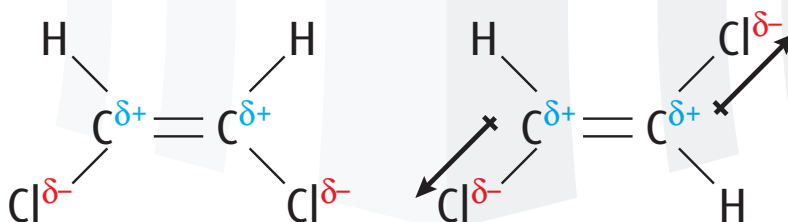
In contrast, a molecule containing polar bonds may be either polar or non-polar depending on the relative arrangement of the bonds and any lone pairs of electrons, e.g. CCl_4 is non-polar, but CHCl_3 is polar.



a CCl_4 is non-polar because the individual dipoles cancel. **b** CHCl_3 is polar because the dipoles do not cancel; there is a positive end to the molecule and a negative end. Although the C in CHCl_3 is shown as δ^+ , it is not as positive as the H (as C is more electronegative than H); therefore, the C is slightly negative compared with the H, although it is positive overall in the molecule.

11

DIPOLE MOMENTS



12

SKILL CHECK 1

Decide whether the following bonds are polar or non-polar. If the bond is polar, state which is the δ^+ atom, and explain whether or not the molecule is polar:

A C-O as in CO_2

B C-I as in CH_3I

13

SKILL CHECK 2

Predict which of the following bonds are polar, and, if polar, in which direction the electrons are pulled:

a. O—S

b. Cl—Cl

c. C—N

d. I—Cl

Predict whether each of the following molecules is polar:

a. BCl_3

b. HCl

c. NH_3

d. SiCl_4

14

SKILL CHECK 3

Predict whether each of the following molecules is polar:



Using the shapes drawn on slide 48 to 51, predict whether each of the following molecules is polar:



15

INTERMOLECULAR FORCES

Intermolecular forces are weak attractive forces between molecules.

These forces determine such properties as the solubility of one substance in another and the freezing and boiling points of liquids.

Without intermolecular forces there could be no molecular liquids or solids.

16

INTERMOLECULAR FORCES

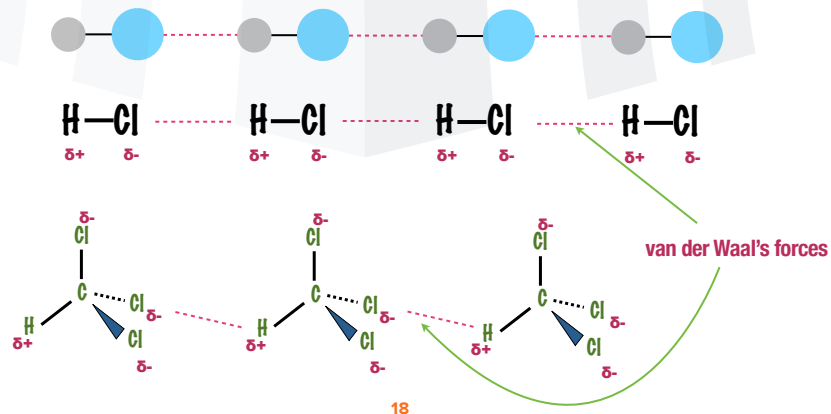
Weak intermolecular forces arise from electrostatic attractions between dipoles, including attractions between:

- Molecules with permanent dipoles such as hydrogen chloride
- A permanent dipole in one molecule and a dipole induced in a neighbouring molecule, such as the attraction between iodine and water
- Temporary dipoles are created fleetingly in non-polar atoms or molecules

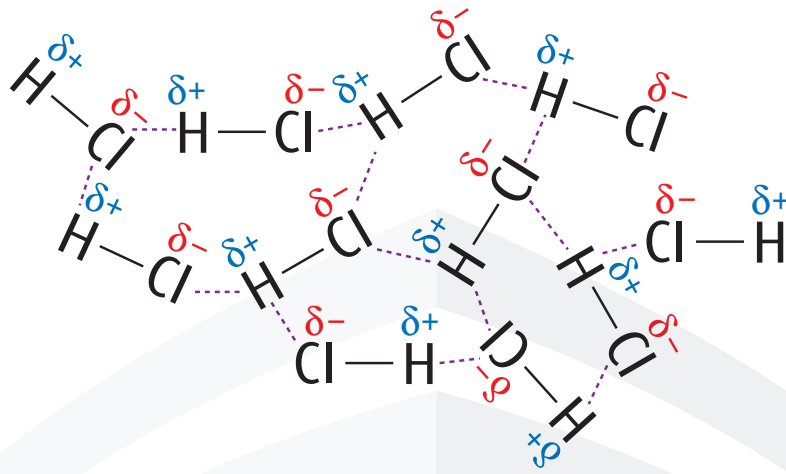
17

VAN DER WAALS' FORCES DUE TO PERMANENT DIPOLES

Van der Waal's forces due to permanent dipoles are interactions between polar molecules - the positive end of one molecule attracts the negative end of a neighbouring molecule.



VAN DER WAALS' FORCES DUE TO PERMANENT DIPOLES



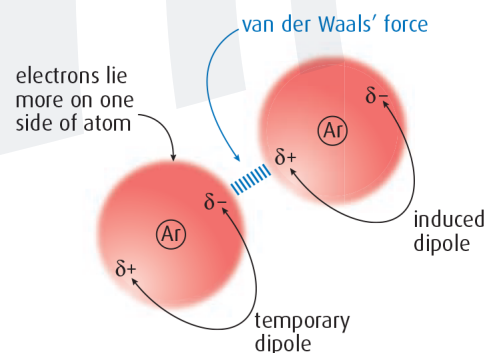
19

VAN DER WAALS' FORCES IN NON-POLAR MOLECULES

Intermolecular forces also exist in non-polar molecules. Van der Waal's forces due to induced dipoles are the intermolecular attraction resulting from the uneven distribution of electrons and the creation of temporary dipoles. Because electrons move quickly in orbitals, their position is constantly changing; at any given instant they could be anywhere in an atom.

The possibility will exist that one side will have more electrons than the other.

This will give rise to a dipole.



20

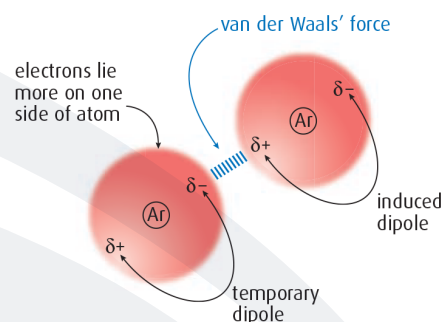
VAN DER WAALS' FORCES DUE TO INDUCED DIPOLES

Consider liquid argon. The electrons in an atom are in constant motion, and at any one time the electrons will not be symmetrically distributed about the nucleus.

This results in a temporary (instantaneous) dipole in the atom, which will induce an opposite dipole in a neighbouring atom.

These dipoles will attract each other so that there is an attractive force between atoms.

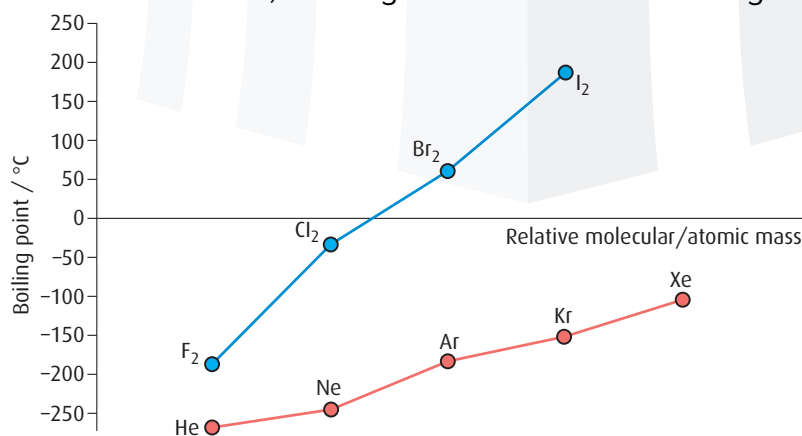
Although the dipoles are constantly disappearing and reappearing, the overall force between the argon atoms is always attractive, because a dipole always induces an opposite one.



21

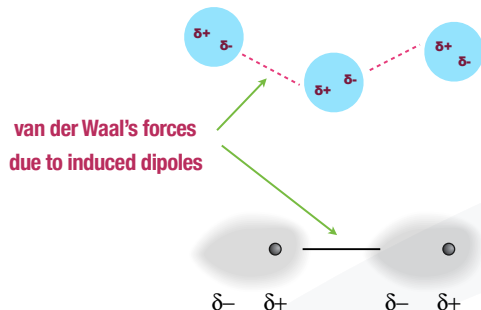
VAN DER WAALS' FORCES DUE TO INDUCED DIPOLES

In general, van der Waals' forces get stronger as the number of electrons in a molecule increases. As the number of electrons increases, the relative molecular mass also increases, resulting in an increase in the strength of van der Waals' forces.



22

VAN DER WAALS' FORCES DUE TO INDUCED DIPOLES

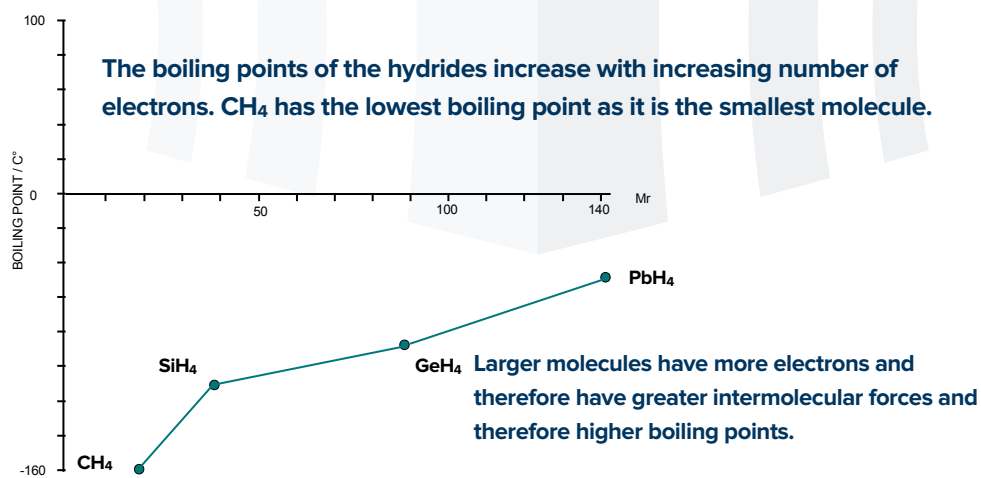


	Electrons	b.p. / °C
NOBLE GASES		
He	2	-269
Ne	10	-246
Ar	18	-186
Kr	36	-152
ALKANES		
CH ₄	10	-161
C ₂ H ₆	18	-88
C ₃ H ₈	26	-42

23

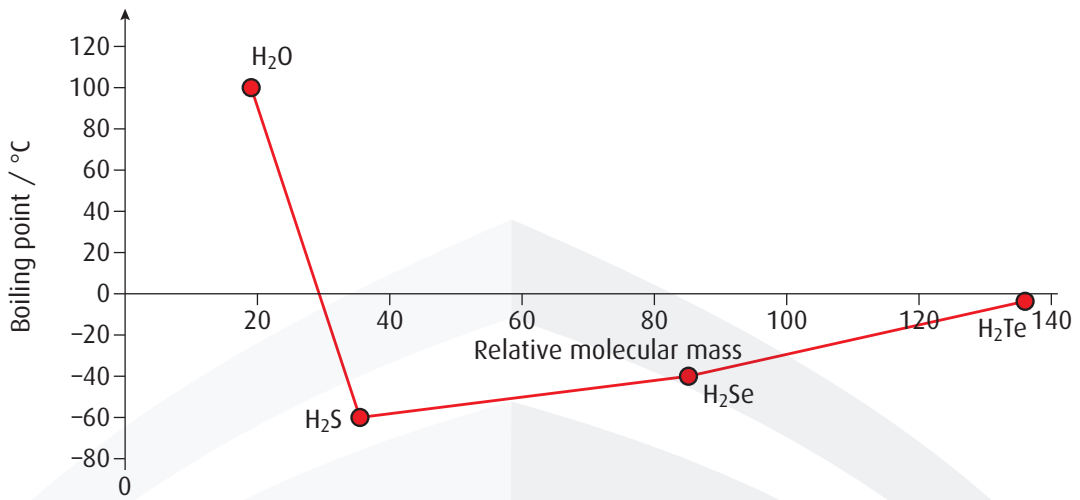
EXAMPLES OF VAN DER WAAL'S

BOILING POINTS OF HYDRIDES OF GROUP 14



24

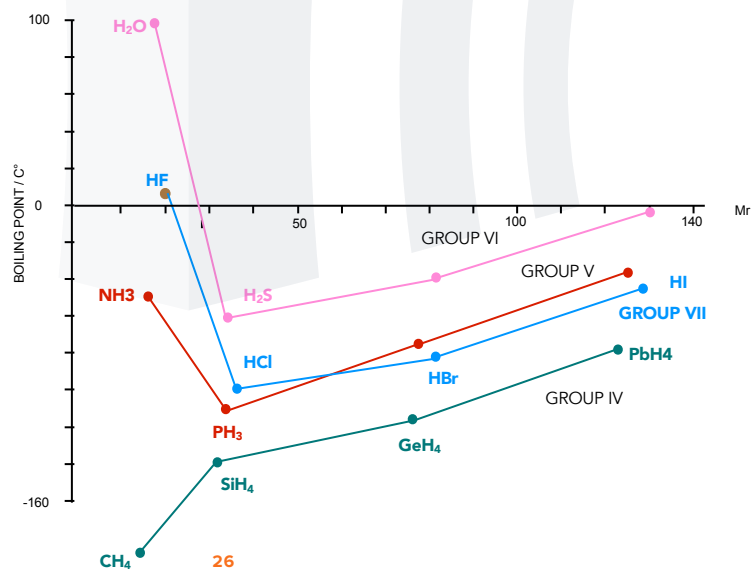
HYDRIDES OF GROUP 16



25

HYDROGEN BONDING

The higher than expected boiling points of NH₃, H₂O and HF are due to intermolecular **HYDROGEN BONDING**



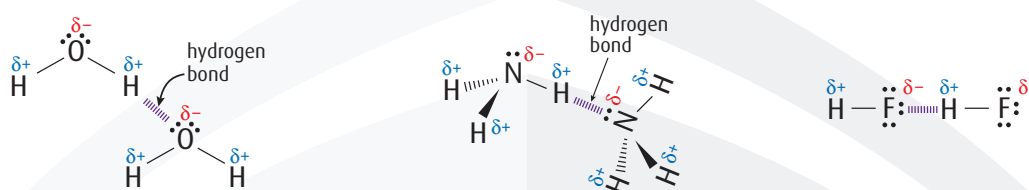
26

HYDROGEN BONDING

Strong hydrogen bonds can form with a hydrogen atom that is covalently bonded to very electronegative atoms in the upper-right part of the periodic table: nitrogen, oxygen, and fluorine.

When a hydrogen atom bonds to an atom of N, O, or F, the hydrogen atom has a large, partially positive charge.

The partially positive hydrogen atom of polar molecules can be attracted to the unshared pairs of electrons of neighbouring molecules.



27

HYDROGEN BONDING

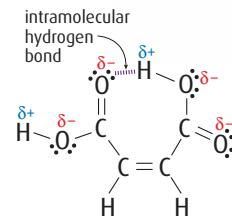
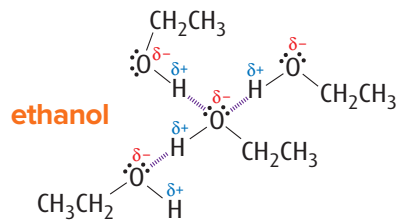
One reason that hydrogen bonds are such strong forces is because the hydrogen atom is small and has only one electron.

When that electron is pulled away by a highly electronegative atom, there are no more electrons under it. Thus, the single proton of the hydrogen nucleus is partially exposed.

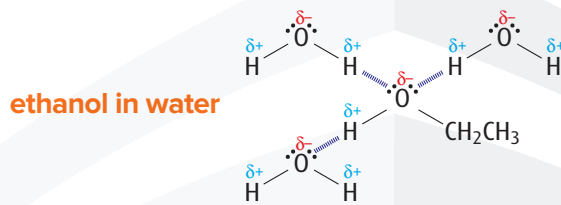
As a result, hydrogen's proton is strongly attracted to the lone pair of electrons of other molecules. The combination of the large electronegative difference (high polarity) and hydrogen's small size accounts for the strength of the hydrogen bond.

28

EXAMPLES OF HYDROGEN BONDING



but-2-ene-1,4-dioic acid

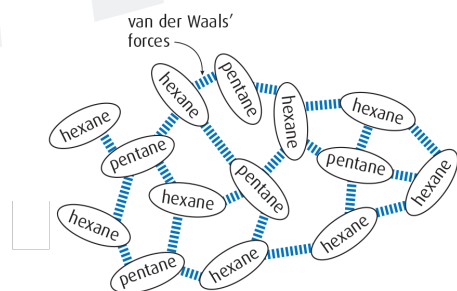
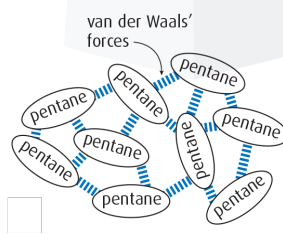
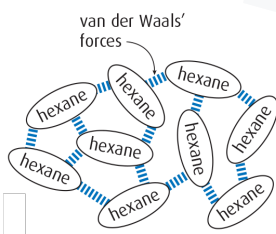


29

SOLUBILITY

Generally a substance will dissolve in a solvent if the intermolecular forces in the solute and solvent are similar. E.g. pentane is readily soluble in hexane but not in water.

The amount of energy required to break the van der Waals' forces in pure hexane and pure pentane is paid back when van der Waals' forces are formed between the molecules of hexane and pentane

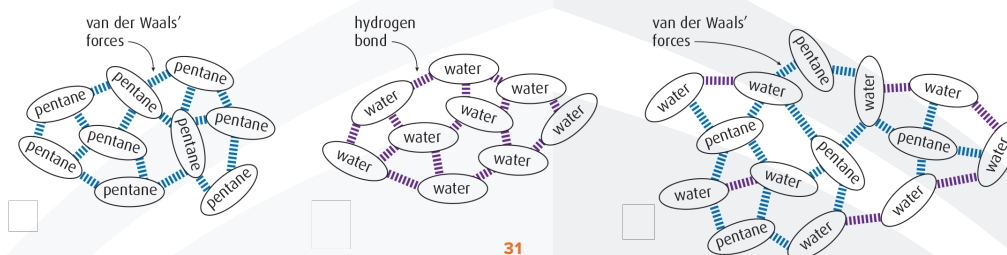


30

SOLUBILITY

Pentane does not dissolve in water because there is hydrogen bonding between water molecules.

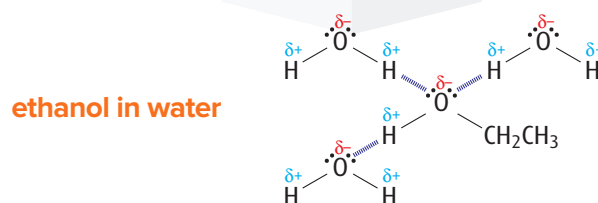
If pentane were to dissolve in water there would be van der Waals' forces between water molecules and pentane. The energy released if van der Waals' forces were to form between water molecules and pentane molecules would not pay back the energy required to break the hydrogen bonds between water molecules, as hydrogen bonds are stronger than van der Waals' forces



SOLUBILITY

Ethanol (C_2H_5OH) is very soluble in water, because ethanol is able to form hydrogen bonds with the water.

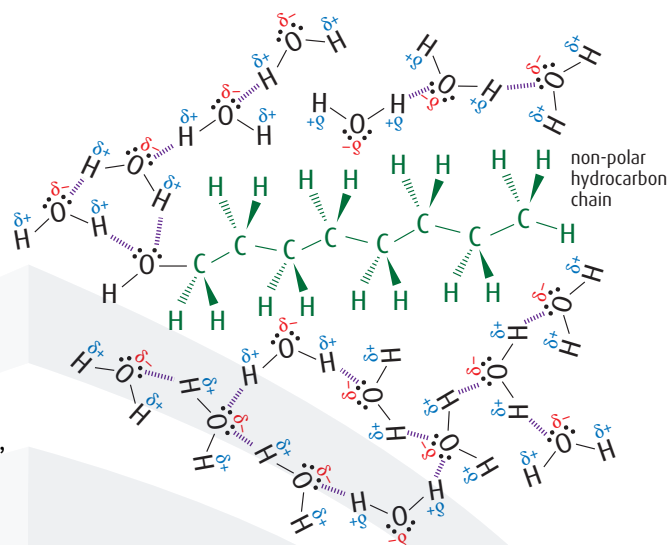
The hydrogen bonding between water and ethanol molecules in the solution releases energy and pays back the energy to break the hydrogen bonds in pure water and pure ethanol.



SOLUBILITY

Octan-1-ol is insoluble in water. Although there is some hydrogen bonding between the O–H group of the alcohol and the water molecules, the long hydrocarbon chain prevents water molecules on either side from hydrogen bonding to each other.

Energy is needed to break the hydrogen bonds between the water molecules, but this is not paid back as only van der Waals' forces form between the water molecules and the hydrocarbon part of the molecule.



33

SKILL CHECK 4

Explain why, in comparison with the other group 6 hydrides, water has an anomalous boiling temperature.

34

SKILL CHECK 5

State all the forces operating between molecules of:

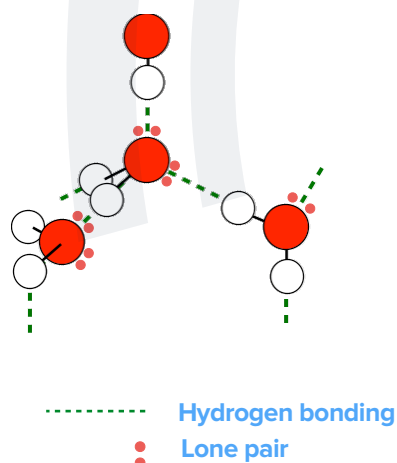
- (a) ammonia, NH_3
- (b) methane, CH_4
- (c) oxygen fluoride, OF_2

35

HYDROGEN BONDING IN ICE

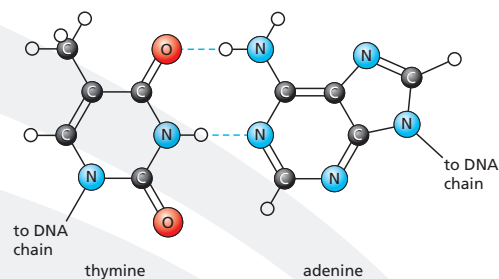
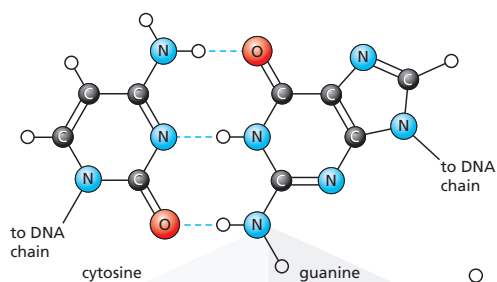
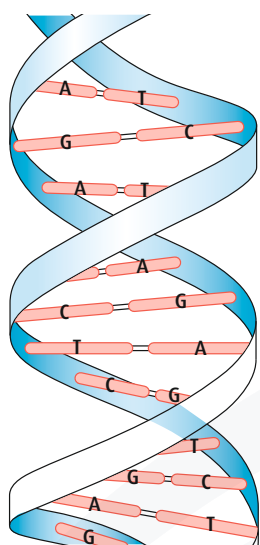
- Each water molecule is hydrogen-bonded to 4 others in a tetrahedral formation
- Ice has a “diamond-like” structure
- Volume is larger than the liquid making it less dense
- When ice melts, the structure collapses slightly and the molecules come closer; they then move a little further apart as they get more energy as they warm up

This is why water has a maximum density at 4°C and ice floats.



36

HYDROGEN BONDING IN DNA



37

SKILL CHECK 6

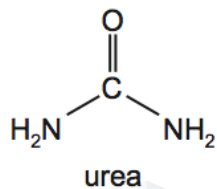
What is involved when a hydrogen bond is formed between two molecules?

- A** a hydrogen atom bonded to an atom less electronegative than itself
- B** a lone pair of electrons
- C** an electrostatic attraction between opposite charges

38

SKILL CHECK 7

Which types of intermolecular forces can exist between adjacent urea molecules?

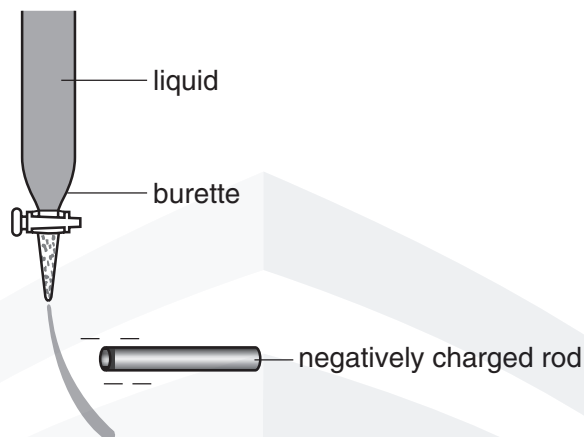


- A** hydrogen bonding
- B** permanent dipole-dipole forces
- C** temporary induced dipole-dipole forces

INTERMOLECULAR FORCES

SECTION A

- 1 A slow stream of water from a tap can be deflected by an electrostatically charged plastic rod because water is a polar molecule.



Why is a water molecule polar?

- A Molecules are bonded together by hydrogen bonds.
- B The oxygen and hydrogen atoms have different electronegativities.
- C The oxygen atom has two lone pairs of electrons.
- D Water is able to dissociate into ions.

[S'02 Q4]

- 2 When heated, solid iodine readily forms iodine vapour.

What does this information suggest about the nature of the particles in these two physical states of iodine?

- | | <i>solid</i> | <i>vapour</i> |
|---|--------------|---------------|
| A | ionic | atomic |
| B | ionic | molecular |
| C | molecular | atomic |
| D | molecular | molecular |

[S'02 Q7]

- 3 The African weaver ant defends its territory by spraying an intruder with a mixture of compounds. The ease by which these compounds are detected by other ants depends upon the volatility, which decreases as the strength of the intermolecular forces in the compound increases.

Which compound would be the most volatile?

- A $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$
 B $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO}$
 C $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$
 D $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$

[W'02 Q4]

- 4 The gecko, a small lizard, can climb up a smooth glass window. The gecko has millions of microscopic hairs on its toes and each hair has thousands of pads at its tip. The result is that the molecules in the pads are extremely close to the glass surface on which the gecko is climbing.

What is the attraction between the gecko's toe pads and the glass surface?

- A co-ordinate bonds
 B covalent bonds
 C ionic bonds
 D van der Waals' forces

[W'04 Q6]

- 5 In which process are hydrogen bonds broken?

- A $\text{H}_2(\text{l}) \rightarrow \text{H}_2(\text{g})$
 B $\text{NH}_3(\text{l}) \rightarrow \text{NH}_3(\text{g})$
 C $2\text{HI}(\text{g}) \rightarrow \text{H}_2(\text{g}) + \text{I}_2(\text{g})$
 D $\text{CH}_4(\text{g}) \rightarrow \text{C}(\text{g}) + 4\text{H}(\text{g})$

[S'06 Q5]

- 6 A crystal of iodine produces a purple vapour when gently heated.

Which pair of statements correctly describes this process?

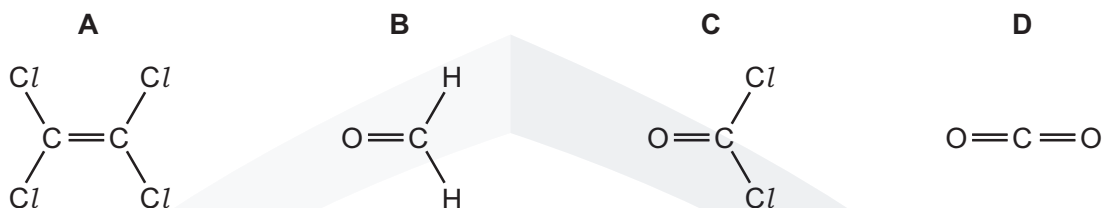
	type of bond broken	formula of purple species
A	covalent	I
B	covalent	I_2
C	induced dipole-dipole	I_2
D	permanent dipole-dipole	I_2

[S'09 1 Q7]

- 7 Why is the boiling point of ammonia, NH_3 , higher than the boiling point of phosphine, PH_3 ?
- A** Ammonia molecules are polar; phosphine molecules are not.
- B** Ammonia molecules have significant hydrogen bonding; phosphine molecules do not.
- C** N–H covalent bonds are stronger than P–H covalent bonds.
- D** There is one lone pair in each ammonia molecule but no lone pair in each phosphine molecule.

[S'18 3 Q1]

- 8 Which molecule has the largest overall dipole?



[W'09 1 Q5]

- 9 Which statement explains why the boiling point of methane is higher than that of neon?
[Ar: H, 1; C, 12; Ne, 20]

- A** A molecule of methane has a greater mass than a molecule of neon.
- B** Molecules of methane form hydrogen bonds, but those of neon do not.
- C** Molecules of methane have stronger intermolecular forces than those of neon.
- D** The molecule of methane is polar, but that of neon is not.

[S'09 1 Q5]

- 10 The boiling points of methane, ethane, propane and butane are given.

compound	CH_4	CH_3CH_3	$\text{CH}_3\text{CH}_2\text{CH}_3$	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$
boiling point/K	112	185	231	273

Which statement explains the increase in boiling point from methane to butane?

- A** Closer packing of molecules results in stronger van der Waals' forces.
- B** More covalent bonds are present and therefore more energy is required to break the bonds.
- C** More electrons in the molecules results in stronger van der Waals' forces.
- D** More hydrogen atoms in the molecules results in stronger hydrogen bonding.

[M'17 2 Q4]

- 11 The ability of an atom in a covalent bond to attract electrons to itself is called its electronegativity.

The greater the difference between the electronegativities of the two atoms in the bond, the more polar is the bond.

Which pair will form the most polar covalent bond between the atoms?

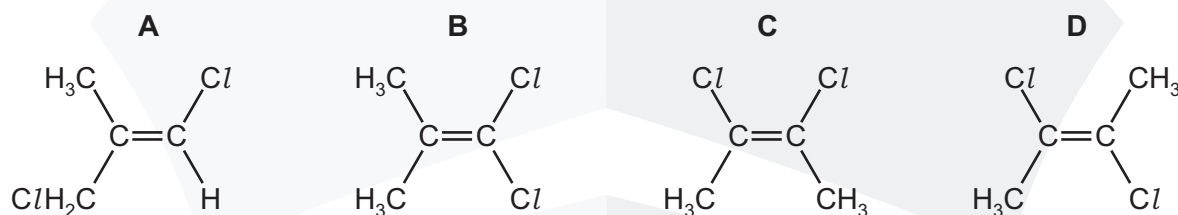
- A chlorine and bromine
- B chlorine and iodine
- C fluorine and chlorine
- D fluorine and iodine

[W'10 2 Q1]

- 12 In which change would only van der Waals' forces have to be overcome?

- A evaporation of ethanol $\text{C}_2\text{H}_5\text{OH}(\text{l}) \rightarrow \text{C}_2\text{H}_5\text{OH}(\text{g})$
- B melting of ice $\text{H}_2\text{O}(\text{s}) \rightarrow \text{H}_2\text{O}(\text{l})$
- C melting of solid carbon dioxide $\text{CO}_2(\text{s}) \rightarrow \text{CO}_2(\text{l})$
- D solidification of butane $\text{C}_4\text{H}_{10}(\text{l}) \rightarrow \text{C}_4\text{H}_{10}(\text{s})$

- 13 Which molecular structure will have the **smallest** overall dipole?



[W'09 2 Q4]

- 14 How do the strengths of the covalent bonds within molecules, and the van der Waals' forces between molecules, vary going down Group VII from chlorine to bromine to iodine?

	strength of covalent bonds	strength of van der Waals' forces
A	decrease	decrease
B	decrease	increase
C	increase	decrease
D	increase	increase

[S'13 3 Q16]

15 At room temperature and pressure, H_2O is a liquid and H_2S is a gas.

What is the reason for this difference?

- A O has higher first and second ionisation energies than S.
- B The covalent bond between O and H is stronger than the covalent bond between S and H.
- C There is significant hydrogen bonding between H_2O molecules but not between H_2S molecules.
- D The instantaneous dipole-induced dipole forces between H_2O molecules are stronger than the instantaneous dipole-induced dipole forces between H_2S molecules.

[S'16 1 Q7]

16 The presence of dipoles helps to explain why the element Br_2 and the compound CHCl_3 exist as liquids at room temperature.

Which types of dipole are involved?

	Br_2	CHCl_3
A	induced dipoles and permanent dipoles	induced dipoles and permanent dipoles
B	induced dipoles and permanent dipoles	induced dipoles only
C	induced dipoles only	induced dipoles and permanent dipoles
D	induced dipoles only	induced dipoles only

[W'11 2 Q5]

17 Nitrogen, N_2 , and carbon monoxide, CO , both have $M_r = 28$.

The boiling point of N_2 is 77 K.

The boiling point of CO is 82 K.

What could be responsible for this difference in boiling points?

- A CO molecules have a permanent dipole, the N_2 molecules are not polar.
- B N_2 has σ and π bonding, CO has σ bonding only.
- C N_2 has a strong $\text{N}\equiv\text{N}$ bond, CO has a $\text{C}=\text{O}$ bond.
- D The CO molecule has more electrons than the N_2 molecule.

[W'15 1 Q4]

18 The boiling points of methane, ethane, propane and butane are given.

compound	CH ₄	CH ₃ CH ₃	CH ₃ CH ₂ CH ₃	CH ₃ CH ₂ CH ₂ CH ₃
boiling point/K	112	185	231	273

Which statement explains the increase in boiling point from methane to butane?

- A Closer packing of molecules results in stronger van der Waals' forces.
- B More covalent bonds are present and therefore more energy is required to break the bonds.
- C More electrons in the molecules results in stronger van der Waals' forces.
- D More hydrogen atoms in the molecules results in stronger hydrogen bonding.

[M'17 2 Q4]

19 Which statement can be explained by intermolecular hydrogen bonding?

- A Ethanol has a higher boiling point than propane.
- B Hydrogen chloride has a higher boiling point than silane, SiH₄.
- C Hydrogen iodide forms an acidic solution when dissolved in water.
- D Propanone has a higher boiling point than propane.

[W'12 3 Q2]

20 The boiling points of methane, ethane, propane and butane are given.

compound	CH ₄	CH ₃ CH ₃	CH ₃ CH ₂ CH ₃	CH ₃ CH ₂ CH ₂ CH ₃
boiling point/K	112	185	231	273

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- D More hydrogen atoms in the molecules results in stronger hydrogen bonding.

[M'17 2 Q4]

SECTION B

For each of the questions in this section, one or more of the three numbered statements 1 to 3 may be correct.

Decide whether each of the statements is or is not correct (you may find it helpful to put a tick against the statements that you consider to be correct).

The responses **A** to **D** should be selected on the basis of

A	B	C	D
1, 2 and 3 are correct	1 and 2 only are correct	2 and 3 only are correct	1 only is correct

No other combination of statements is used as a correct response.

- 1 Boron is a non-metallic element which is placed above aluminium in Group III of the Periodic Table. It forms a compound with nitrogen known as boron nitride which has a graphite structure.

Which of the following conclusions can be drawn from this information?

- The empirical formula of boron nitride is BN.
- The boron and nitride atoms are likely to be arranged alternately in a hexagonal pattern.
- Boron nitride has a layer structure with van der Waals' forces between the layers.

[W'05 Q33]

- 2 What is involved when a hydrogen bond is formed between two molecules?

- a hydrogen atom bonded to an atom less electronegative than itself
- a lone pair of electrons
- an electrostatic attraction between opposite charges

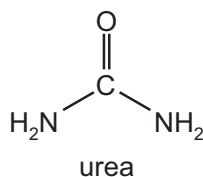
[S'11 2 Q34]

- 3 Which physical properties are due to hydrogen bonding between water molecules?

- Water has a higher boiling point than H₂S.
- Ice floats on water.
- The H–O–H bond angle in water is approximately 104°.

[W'09 Q32]

- 4 Which types of intermolecular forces can exist between adjacent urea molecules?



- hydrogen bonding
- permanent dipole-dipole forces
- temporary induced dipole-dipole forces

[W'10 1 Q33]

- 5 The concepts of bond energy, bond length and bond polarity are useful when comparing the behaviour of similar molecules, e.g. thermal stability.

For example, it could be said

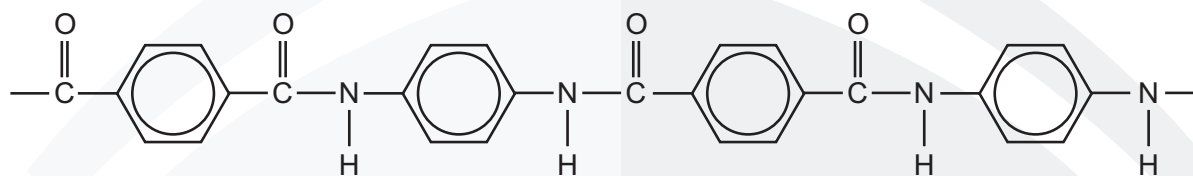
“Compared with the HCl molecule, the bondX..... of the HI molecule isY.....”

Which pairs of words correctly complete the above sentence?

	X	Y
1	energy	greater
2	length	greater
3	polarity	less

[S'02 Q33]

- 6 Kevlar has the structure below.



Compared to a steel rope of similar dimensions, a Kevlar rope is both lighter and stronger.

Which properties of Kevlar help to explain these facts?

- 1 The fibres of Kevlar align due to hydrogen bonding.
- 2 The mass per unit length is less in a Kevlar rope than in a steel rope.
- 3 The Kevlar molecule has no permanent dipole.

[W'08 Q31]

- 7 Water has some unusual physical properties compared to other hydrides of Group 16 elements. Some of these properties are due to hydrogen bonds. These intermolecular forces are much stronger in water than they are in H₂S, for example.

Which statements are correct?

- 1 Hydrogen bonds cause the melting point of ice to be higher than expected.
- 2 Hydrogen bonds cause the surface tension of water to be higher than expected.
- 3 Hydrogen bonds cause the viscosity of water to be higher than expected.

[S'16 3 Q32]

- 8 The three statements that follow are all true.

Which of these can be explained, at least in part, by reference to hydrogen bonding?

- 1 At 0 °C ice floats on water.
- 2 The boiling point of propan-2-ol is 82 °C. The boiling point of propanone is 56 °C.
- 3 At 20 °C propanone and propanal mix completely.

[W'11 3 Q32]

- 9 The intermolecular forces between iodine molecules are instantaneous dipole-induced dipole forces.

Which statements explain why iodine has these intermolecular forces?

- 1 An iodine molecule is polar and experiences an attraction from a lone pair of electrons on an adjacent molecule.
- 2 An iodine molecule has a fluctuating dipole because the electrons in a molecule are more mobile than the nuclei.
- 3 The electron charge cloud within an I_2 molecule may become unsymmetrical and may then attract other I_2 molecules.

[S'14 3 Q36]

- 10 Which molecules have an overall dipole moment?

- 1 carbon monoxide, CO
- 2 phosphine, PH_3
- 3 carbon dioxide, CO_2

INTERMOLECULAR FORCES WS 2

SECTION A

- 1 Ethene, C_2H_4 , and hydrazine, N_2H_4 , are hydrides of elements which are adjacent in the Periodic Table. Data about ethene and hydrazine are given in the table below.

	C_2H_4	N_2H_4
melting point/ $^{\circ}C$	-169	+2
boiling point/ $^{\circ}C$	-104	+114
solubility in water	insoluble	high
solubility in ethanol	high	high

- (a) Ethene and hydrazine have a similar arrangement of atoms but differently shaped molecules.

(i) What is the H-C-H bond angle in ethene?

.....

(ii) Draw a 'dot-and-cross' diagram for hydrazine.

(iii) What is the H-N-H bond angle in hydrazine?

.....

[4]

- (b) The melting and boiling points of hydrazine are much higher than those of ethene. Suggest reasons for these differences in terms of the intermolecular forces **each** compound possesses.

.....

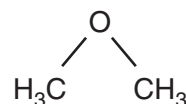
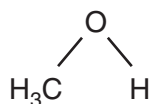
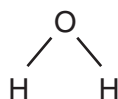
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.....

.....

.....[3]

- 5 The structural formulae of water, methanol and methoxymethane, CH_3OCH_3 , are given below.



- (a) (i) How many lone pairs of electrons are there around the oxygen atom in methoxymethane?

.....

- (ii) Suggest the size of the C–O–C bond angle in methoxymethane.

.....

[2]

The physical properties of a covalent compound, such as its melting point, boiling point, vapour pressure, or solubility, are related to the strength of attractive forces between the molecules of that compound.

These relatively weak attractive forces are called intermolecular forces. They differ in their strength and include the following.

- A interactions involving permanent dipoles
- B interactions involving temporary or induced dipoles
- C hydrogen bonds

- (b) By using the letters **A**, **B**, or **C**, state the **strongest** intermolecular force present in **each** of the following compounds.

For each compound, write the answer on the dotted line.

ethanal CH_3CHO

ethanol $\text{CH}_3\text{CH}_2\text{OH}$

methoxymethane CH_3OCH_3

2-methylpropane $(\text{CH}_3)_2\text{CHCH}_3$

[4]

(c) Methanol and water are completely soluble in each other.

(i) Which intermolecular force exists between methanol molecules and water molecules that makes these two liquids soluble in each other?

.....

(ii) Draw a diagram that clearly shows this intermolecular force. Your diagram should show any lone pairs or dipoles present on either molecule that you consider to be important.

[4]

6 Neon and argon can both be obtained by fractional distillation of liquid air as they have different boiling points.

Neon has a boiling point of 27.3 K. The boiling point of argon is 87.4 K.

(i) Name the force that has to be overcome in order to boil neon or argon and explain what causes it.

.....
.....
..... [3]

(ii) Explain why argon has a higher boiling point than neon.

.....
.....
..... [2]

7 Carbon disulphide, CS_2 , is a volatile, stinking liquid which is used to manufacture viscose rayon and cellophane.

(a) The carbon atom is in the centre of the CS_2 molecule.

Draw a 'dot-and-cross' diagram of the carbon disulphide molecule.

Show outer electrons only.

[2]

(b) Suggest the shape of the molecule and give its bond angle.

shape

bond angle

[2]

Hydrogen sulphide, H_2S , is a foul-smelling compound found in the gases from volcanoes. Hydrogen sulphide is covalent, melting at -85°C and boiling at -60°C .

(c) (i) Draw a 'dot-and-cross' diagram to show the structure of the H_2S molecule.

(ii) Predict the shape of the H_2S molecule.

.....

(iii) Oxygen and sulphur are both in Group VI of the Periodic Table.

Suggest why the melting and boiling points of water, H_2O , are much higher than those of H_2S .

.....

.....

..... [4]

- 8 (a) Fill the gaps in the table for each of the given particles.

name of isotope	type of particle	charge	symbol	electron configuration
carbon-13				$1s^2 2s^2 2p^2$
		-1	${}^{37}_{17}\text{Cl}^-$	
sulfur-34	atom	0		
iron-54	cation			$1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$

[5]

- (b) One of the factors that determines the type of bonding present between the particles of a substance is the relative electronegativities of the bonded particles.

- (i) Explain the meaning of the term *electronegativity*.

.....

 [2]

- (ii) Name and describe the type of bonding you would expect to find between particles with equal electronegativities.

.....

 [2]

- (iii) Name and describe the type of bonding you would expect to find between particles with very different electronegativities.

.....

 [2]

(c) The boiling points of some molecules with equal numbers of electrons are given.

substance	fluorine	argon	hydrogen chloride	methanol
formula	F_2	Ar	HCl	CH_3OH
boiling point/K	85	87	188	338

(i) Explain why the boiling points of fluorine and argon are so similar.

.....
.....
..... [2]

(ii) Explain why the boiling point of hydrogen chloride is higher than that of fluorine.

.....
.....
..... [2]

(iii) Explain why methanol has the highest boiling point of all these molecules.

.....
.....
..... [2]

9 Elements and compounds which have small molecules usually exist as gases or liquids.

- (a) Chlorine, Cl_2 , is a gas at room temperature whereas bromine, Br_2 , is a liquid under the same conditions.

Explain these observations.

.....

 [2]

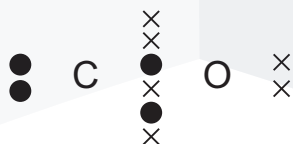
- (b) The gases nitrogen, N_2 , and carbon monoxide, CO , are isoelectronic, that is they have the same number of electrons in their molecules.

Suggest why N_2 has a lower boiling point than CO .

.....

 [2]

- (c) A 'dot-and-cross' diagram of a CO molecule is shown below. Only electrons from outer shells are represented.



In the table below, there are three copies of this structure.

On the structures, draw a circle around a pair of electrons that is associated with **each** of the following.

a co-ordinate bond	a covalent bond	a lone pair
<pre> x x x x x ● ● C ● O x x x </pre>	<pre> x x x x x ● ● C ● O x x x </pre>	<pre> x x x x x ● ● C ● O x x x </pre>

[3]

DATA BOOKLET

1 Important values, constants and standards

molar gas constant	$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
the Faraday constant	$F = 9.65 \times 10^4 \text{ C mol}^{-1}$
the Avogadro constant	$L = 6.02 \times 10^{23} \text{ mol}^{-1}$
the Planck constant	$h = 6.63 \times 10^{-34} \text{ J s}$
speed of light in a vacuum	$c = 3.00 \times 10^8 \text{ m s}^{-1}$
rest mass of proton, ${}_1^1\text{H}$	$m_p = 1.67 \times 10^{-27} \text{ kg}$
rest mass of neutron, ${}_0^1\text{n}$	$m_n = 1.67 \times 10^{-27} \text{ kg}$
rest mass of electron, ${}_{-1}^0\text{e}$	$m_e = 9.11 \times 10^{-31} \text{ kg}$
electronic charge	$e = -1.60 \times 10^{-19} \text{ C}$
molar volume of gas	$V_m = 22.4 \text{ dm}^3 \text{ mol}^{-1}$ at s.t.p. $V_m = 24.0 \text{ dm}^3 \text{ mol}^{-1}$ under room conditions (where s.t.p. is expressed as 101 kPa, approximately, and 273 K (0 °C))
ionic product of water	$K_w = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$ (at 298 K (25 °C))
specific heat capacity of water	$= 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ ($= 4.18 \text{ J g}^{-1} \text{ K}^{-1}$)

2 Ionisation energies (1st, 2nd, 3rd and 4th) of selected elements,
in kJ mol^{-1}

	Proton number	First	Second	Third	Fourth
H	1	1310	–	–	–
He	2	2370	5250	–	–
Li	3	519	7300	11800	–
Be	4	900	1760	14800	21000
B	5	799	2420	3660	25000
C	6	1090	2350	4610	6220
N	7	1400	2860	4590	7480
O	8	1310	3390	5320	7450
F	9	1680	3370	6040	8410
Ne	10	2080	3950	6150	9290
Na	11	494	4560	6940	9540
Mg	12	736	1450	7740	10500
Al	13	577	1820	2740	11600
Si	14	786	1580	3230	4360
P	15	1060	1900	2920	4960
S	16	1000	2260	3390	4540
Cl	17	1260	2300	3850	5150
Ar	18	1520	2660	3950	5770
K	19	418	3070	4600	5860
Ca	20	590	1150	4940	6480
Sc	21	632	1240	2390	7110
Ti	22	661	1310	2720	4170
V	23	648	1370	2870	4600
Cr	24	653	1590	2990	4770
Mn	25	716	1510	3250	5190
Fe	26	762	1560	2960	5400
Co	27	757	1640	3230	5100
Ni	28	736	1750	3390	5400
Cu	29	745	1960	3350	5690
Zn	30	908	1730	3828	5980
Ga	31	577	1980	2960	6190

	Proton number	First	Second	Third	Fourth
Br	35	1140	2080	3460	4850
Rb	37	403	2632	3900	5080
Sr	38	548	1060	4120	5440
Ag	47	731	2074	3361	–
I	53	1010	1840	2040	4030
Cs	55	376	2420	3300	–
Ba	56	502	966	3390	–

3 Bond energies

3(a) Bond energies in diatomic molecules (these are exact values)

Homonuclear

Bond	Energy/kJ mol ⁻¹
H-H	436
D-D	442
N≡N	944
O=O	496
P≡P	485
S=S	425
F-F	158
Cl-Cl	242
Br-Br	193
I-I	151

Heteronuclear

Bond	Energy/kJ mol ⁻¹
H-F	562
H-Cl	431
H-Br	366
H-I	299
C≡O	1077

3(b) Bond energies in polyatomic molecules (these are average values)

Homonuclear

Bond	Energy/kJ mol ⁻¹
C–C	350
C=C	610
C≡C	840
C \cdots C (benzene)	520
N–N	160
N=N	410
O–O	150
Si–Si	222
P–P	200
S–S	264

Heteronuclear

Bond	Energy/kJ mol ⁻¹
C–H	410
C–Cl	340
C–Br	280
C–I	240
C–N	305
C=N	610
C≡N	890
C–O	360
C=O	740
C=O in CO ₂	805
N–H	390
N–Cl	310
O–H	460
Si–Cl	359
Si–H	320
Si–O (in SiO ₂ (s))	460
Si=O (in SiO ₂ (g))	640
P–H	320
P–Cl	330
P–O	340
P=O	540
S–H	347
S–Cl	250
S–O	360
S=O	500

4 Standard electrode potential and redox potentials, E^\ominus at 298 K (25 °C)

For ease of reference, two tables are given:

- (a) an extended list in alphabetical order
 (b) a shorter list in decreasing order of magnitude, i.e. a redox series.

(a) E^\ominus in alphabetical order

Electrode reaction	E^\ominus/V
$\text{Ag}^+ + \text{e}^- \rightleftharpoons \text{Ag}$	+0.80
$\text{Al}^{3+} + 3\text{e}^- \rightleftharpoons \text{Al}$	-1.66
$\text{Ba}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ba}$	-2.90
$\text{Br}_2 + 2\text{e}^- \rightleftharpoons 2\text{Br}^-$	+1.07
$\text{Ca}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ca}$	-2.87
$\text{Cl}_2 + 2\text{e}^- \rightleftharpoons 2\text{Cl}^-$	+1.36
$2\text{HOCl} + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Cl}_2 + 2\text{H}_2\text{O}$	+1.64
$\text{ClO}^- + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{Cl}^- + 2\text{OH}^-$	+0.89
$\text{Co}^{2+} + 2\text{e}^- \rightleftharpoons \text{Co}$	-0.28
$\text{Co}^{3+} + \text{e}^- \rightleftharpoons \text{Co}^{2+}$	+1.82
$[\text{Co}(\text{NH}_3)_6]^{2+} + 2\text{e}^- \rightleftharpoons \text{Co} + 6\text{NH}_3$	-0.43
$\text{Cr}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cr}$	-0.91
$\text{Cr}^{3+} + 3\text{e}^- \rightleftharpoons \text{Cr}$	-0.74
$\text{Cr}^{3+} + \text{e}^- \rightleftharpoons \text{Cr}^{2+}$	-0.41
$\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6\text{e}^- \rightleftharpoons 2\text{Cr}^{3+} + 7\text{H}_2\text{O}$	+1.33
$\text{Cu}^+ + \text{e}^- \rightleftharpoons \text{Cu}$	+0.52
$\text{Cu}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu}$	+0.34
$\text{Cu}^{2+} + \text{e}^- \rightleftharpoons \text{Cu}^+$	+0.15
$[\text{Cu}(\text{NH}_3)_4]^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu} + 4\text{NH}_3$	-0.05
$\text{F}_2 + 2\text{e}^- \rightleftharpoons 2\text{F}^-$	+2.87
$\text{Fe}^{2+} + 2\text{e}^- \rightleftharpoons \text{Fe}$	-0.44
$\text{Fe}^{3+} + 3\text{e}^- \rightleftharpoons \text{Fe}$	-0.04
$\text{Fe}^{3+} + \text{e}^- \rightleftharpoons \text{Fe}^{2+}$	+0.77
$[\text{Fe}(\text{CN})_6]^{3-} + \text{e}^- \rightleftharpoons [\text{Fe}(\text{CN})_6]^{4-}$	+0.36
$\text{Fe}(\text{OH})_3 + \text{e}^- \rightleftharpoons \text{Fe}(\text{OH})_2 + \text{OH}^-$	-0.56
$2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{H}_2$	0.00
$2\text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{H}_2 + 2\text{OH}^-$	-0.83
$\text{I}_2 + 2\text{e}^- \rightleftharpoons 2\text{I}^-$	+0.54

Electrode reaction	E^\ominus/V
$K^+ + e^- \rightleftharpoons K$	-2.92
$Li^+ + e^- \rightleftharpoons Li$	-3.04
$Mg^{2+} + 2e^- \rightleftharpoons Mg$	-2.38
$Mn^{2+} + 2e^- \rightleftharpoons Mn$	-1.18
$Mn^{3+} + e^- \rightleftharpoons Mn^{2+}$	+1.49
$MnO_2 + 4H^+ + 2e^- \rightleftharpoons Mn^{2+} + 2H_2O$	+1.23
$MnO_4^- + e^- \rightleftharpoons MnO_4^{2-}$	+0.56
$MnO_4^- + 4H^+ + 3e^- \rightleftharpoons MnO_2 + 2H_2O$	+1.67
$MnO_4^- + 8H^+ + 5e^- \rightleftharpoons Mn^{2+} + 4H_2O$	+1.52
$NO_3^- + 2H^+ + e^- \rightleftharpoons NO_2 + H_2O$	+0.81
$NO_3^- + 3H^+ + 2e^- \rightleftharpoons HNO_2 + H_2O$	+0.94
$NO_3^- + 10H^+ + 8e^- \rightleftharpoons NH_4^+ + 3H_2O$	+0.87
$Na^+ + e^- \rightleftharpoons Na$	-2.71
$Ni^{2+} + 2e^- \rightleftharpoons Ni$	-0.25
$[Ni(NH_3)_6]^{2+} + 2e^- \rightleftharpoons Ni + 6NH_3$	-0.51
$H_2O_2 + 2H^+ + 2e^- \rightleftharpoons 2H_2O$	+1.77
$HO_2^- + H_2O + 2e^- \rightleftharpoons 3OH^-$	+0.88
$O_2 + 4H^+ + 4e^- \rightleftharpoons 2H_2O$	+1.23
$O_2 + 2H_2O + 4e^- \rightleftharpoons 4OH^-$	+0.40
$O_2 + 2H^+ + 2e^- \rightleftharpoons H_2O_2$	+0.68
$O_2 + H_2O + 2e^- \rightleftharpoons HO_2^- + OH^-$	-0.08
$Pb^{2+} + 2e^- \rightleftharpoons Pb$	-0.13
$Pb^{4+} + 2e^- \rightleftharpoons Pb^{2+}$	+1.69
$PbO_2 + 4H^+ + 2e^- \rightleftharpoons Pb^{2+} + 2H_2O$	+1.47
$SO_4^{2-} + 4H^+ + 2e^- \rightleftharpoons SO_2 + 2H_2O$	+0.17
$S_2O_8^{2-} + 2e^- \rightleftharpoons 2SO_4^{2-}$	+2.01
$S_4O_6^{2-} + 2e^- \rightleftharpoons 2S_2O_3^{2-}$	+0.09
$Sn^{2+} + 2e^- \rightleftharpoons Sn$	-0.14
$Sn^{4+} + 2e^- \rightleftharpoons Sn^{2+}$	+0.15
$V^{2+} + 2e^- \rightleftharpoons V$	-1.20
$V^{3+} + e^- \rightleftharpoons V^{2+}$	-0.26
$VO^{2+} + 2H^+ + e^- \rightleftharpoons V^{3+} + H_2O$	+0.34
$VO_2^+ + 2H^+ + e^- \rightleftharpoons VO^{2+} + H_2O$	+1.00
$VO_3^- + 4H^+ + e^- \rightleftharpoons VO^{2+} + 2H_2O$	+1.00
$Zn^{2+} + 2e^- \rightleftharpoons Zn$	-0.76

(b) E^\ominus in decreasing order of oxidising power

(a selection only – see also the extended alphabetical list on the previous pages)

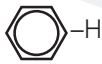
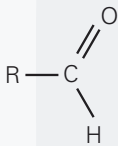
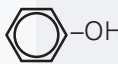
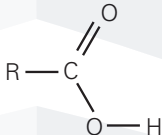

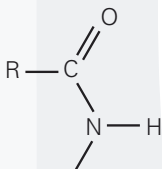
Electrode reaction	E^\ominus/V
$F_2 + 2e^- \rightleftharpoons 2F^-$	+2.87
$S_2O_8^{2-} + 2e^- \rightleftharpoons 2SO_4^{2-}$	+2.01
$H_2O_2 + 2H^+ + 2e^- \rightleftharpoons 2H_2O$	+1.77
$MnO_4^- + 8H^+ + 5e^- \rightleftharpoons Mn^{2+} + 4H_2O$	+1.52
$PbO_2 + 4H^+ + 2e^- \rightleftharpoons Pb^{2+} + 2H_2O$	+1.47
$Cl_2 + 2e^- \rightleftharpoons 2Cl^-$	+1.36
$Cr_2O_7^{2-} + 14H^+ + 6e^- \rightleftharpoons 2Cr^{3+} + 7H_2O$	+1.33
$O_2 + 4H^+ + 4e^- \rightleftharpoons 2H_2O$	+1.23
$Br_2 + 2e^- \rightleftharpoons 2Br^-$	+1.07
$ClO^- + H_2O + 2e^- \rightleftharpoons Cl^- + 2OH^-$	+0.89
$NO_3^- + 10H^+ + 8e^- \rightleftharpoons NH_4^+ + 3H_2O$	+0.87
$NO_3^- + 2H^+ + e^- \rightleftharpoons NO_2 + H_2O$	+0.81
$Ag^+ + e^- \rightleftharpoons Ag$	+0.80
$Fe^{3+} + e^- \rightleftharpoons Fe^{2+}$	+0.77
$I_2 + 2e^- \rightleftharpoons 2I^-$	+0.54
$O_2 + 2H_2O + 4e^- \rightleftharpoons 4OH^-$	+0.40
$Cu^{2+} + 2e^- \rightleftharpoons Cu$	+0.34
$SO_4^{2-} + 4H^+ + 2e^- \rightleftharpoons SO_2 + 2H_2O$	+0.17
$Sn^{4+} + 2e^- \rightleftharpoons Sn^{2+}$	+0.15
$S_4O_6^{2-} + 2e^- \rightleftharpoons 2S_2O_3^{2-}$	+0.09
$2H^+ + 2e^- \rightleftharpoons H_2$	0.00
$Pb^{2+} + 2e^- \rightleftharpoons Pb$	-0.13
$Sn^{2+} + 2e^- \rightleftharpoons Sn$	-0.14
$Fe^{2+} + 2e^- \rightleftharpoons Fe$	-0.44
$Zn^{2+} + 2e^- \rightleftharpoons Zn$	-0.76
$2H_2O + 2e^- \rightleftharpoons H_2 + 2OH^-$	-0.83
$V^{2+} + 2e^- \rightleftharpoons V$	-1.20
$Mg^{2+} + 2e^- \rightleftharpoons Mg$	-2.38
$Ca^{2+} + 2e^- \rightleftharpoons Ca$	-2.87
$K^+ + e^- \rightleftharpoons K$	-2.92

5 Atomic and ionic radii

(a) Period 1	atomic/nm		ionic/nm			
single covalent	H	0.037	H ⁺	0.208		
van der Waals	He	0.140				
(b) Period 2						
metallic	Li	0.152	Li ⁺	0.060		
	Be	0.112	Be ²⁺	0.031		
single covalent	B	0.080	B ³⁺	0.020		
	C	0.077	C ⁴⁺	0.015	C ⁴⁻	0.260
	N	0.074			N ³⁻	0.171
	O	0.073			O ²⁻	0.140
	F	0.072			F ⁻	0.136
van der Waals	Ne	0.160				
(c) Period 3						
metallic	Na	0.186	Na ⁺	0.095		
	Mg	0.160	Mg ²⁺	0.065		
	Al	0.143	Al ³⁺	0.050		
single covalent	Si	0.117	Si ⁴⁺	0.041		
	P	0.110			P ³⁻	0.212
	S	0.104			S ²⁻	0.184
	Cl	0.099			Cl ⁻	0.181
van der Waals	Ar	0.190				
(d) Group 2						
metallic	Be	0.112	Be ²⁺	0.031		
	Mg	0.160	Mg ²⁺	0.065		
	Ca	0.197	Ca ²⁺	0.099		
	Sr	0.215	Sr ²⁺	0.113		
	Ba	0.217	Ba ²⁺	0.135		
	Ra	0.220	Ra ²⁺	0.140		



(e) Group 14		atomic/nm		ionic/nm	
single covalent	C	0.077			
	Si	0.117	Si ⁴⁺	0.041	
	Ge	0.122	Ge ²⁺	0.093	
metallic	Sn	0.162	Sn ²⁺	0.112	
	Pb	0.175	Pb ²⁺	0.120	
(f) Group 17					
single covalent	F	0.072	F ⁻	0.136	
	Cl	0.099	Cl ⁻	0.181	
	Br	0.114	Br ⁻	0.195	
	I	0.133	I ⁻	0.216	
	At	0.140			
(g) First row transition elements					
metallic	Sc	0.164		Sc ³⁺	0.081
	Ti	0.146	Ti ²⁺	0.090	Ti ³⁺ 0.067
	V	0.135	V ²⁺	0.079	V ³⁺ 0.064
	Cr	0.129	Cr ²⁺	0.073	Cr ³⁺ 0.062
	Mn	0.132	Mn ²⁺	0.067	Mn ³⁺ 0.062
	Fe	0.126	Fe ²⁺	0.061	Fe ³⁺ 0.055
	Co	0.125	Co ²⁺	0.078	Co ³⁺ 0.053
	Ni	0.124	Ni ²⁺	0.070	Ni ³⁺ 0.056
	Cu	0.128	Cu ²⁺	0.073	
	Zn	0.135	Zn ²⁺	0.075	

6 Typical proton (^1H) chemical shift values (δ) relative to TMS = 0

Type of proton	Environment of proton	Example structures	Chemical shift range (δ)
C-H	alkane	$-\text{CH}_3, -\text{CH}_2-, >\text{CH}-$	0.9–1.7
	alkyl next to C=O	$\text{CH}_3-\text{C}=\text{O}, -\text{CH}_2-\text{C}=\text{O}, >\text{CH}-\text{C}=\text{O}$	2.2–3.0
	alkyl next to aromatic ring	$\text{CH}_3-\text{Ar}, -\text{CH}_2-\text{Ar}, >\text{CH}-\text{Ar}$	2.3–3.0
	alkyl next to electronegative atom	$\text{CH}_3-\text{O}, -\text{CH}_2-\text{O}, -\text{CH}_2-\text{Cl}, >\text{CH}-\text{Br}$	3.2–4.0
	attached to alkyne	$\equiv\text{C}-\text{H}$	1.8–3.1
	attached to alkene	$=\text{CH}_2, =\text{CH}-$	4.5–6.0
	attached to aromatic ring		6.0–9.0
O-H (see note below)	aldehyde		9.3–10.5
	alcohol	$\text{RO}-\text{H}$	0.5–6.0
	phenol		4.5–7.0
N-H (see note below)	carboxylic acid		9.0–13.0
	alkyl amine	$\text{R}-\text{NH}-$	1.0–5.0
	aryl amine		3.0–6.0
amide			5.0–12.0

Note: δ values for $-\text{O}-\text{H}$ and $-\text{N}-\text{H}$ protons can vary depending on solvent and concentration.

7 Typical carbon (^{13}C) chemical shift values (δ) relative to TMS = 0

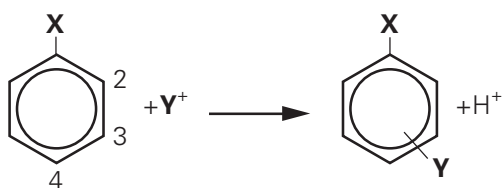
Hybridisation of the carbon atom	Environment of carbon atom	Example structures	Chemical shift range (δ)
sp^3	alkyl	CH_3- , CH_2- , $-\text{CH}<$	0–50
sp^3	next to alkene/arene	$-\text{CH}_2-\text{C}=\text{C}$, $-\text{CH}_2-$ 	10–40
sp^3	next to carbonyl/carboxyl	$-\text{CH}_2-\text{COR}$, $-\text{CH}_2-\text{CO}_2\text{R}$	25–50
sp^3	next to nitrogen	$-\text{CH}_2-\text{NH}_2$, $-\text{CH}_2-\text{NR}_2$, $-\text{CH}_2-\text{NHCO}$	30–65
sp^3	next to chlorine ($-\text{CH}_2-\text{Br}$ and $-\text{CH}_2-\text{I}$ are in the same range as alkyl)	$-\text{CH}_2-\text{Cl}$	30–60
sp^3	next to oxygen	$-\text{CH}_2-\text{OH}$, $-\text{CH}_2-\text{O}-\text{CO}-$	50–70
sp^2	alkene or arene	$>\text{C}=\text{C}<$, 	110–160
sp^2	carboxyl	$\text{R}-\text{CO}_2\text{H}$, $\text{R}-\text{CO}_2\text{R}$	160–185
sp^2	carbonyl	$\text{R}-\text{CHO}$, $\text{R}-\text{CO}-\text{R}$	190–220
sp	alkyne	$\text{R}-\text{C}\equiv\text{C}-$	65–85
sp	nitrile	$\text{R}-\text{C}\equiv\text{N}$	100–125

8 Characteristic infra-red absorption frequencies for some selected bonds

Bond	Functional groups containing the bond	Absorption range (in wavenumbers)/cm ⁻¹	Appearance of peak (<i>s</i> = strong, <i>w</i> = weak)
C–O	alcohols, ethers, esters	1040–1300	s
C=C	aromatic compounds, alkenes	1500–1680	w unless conjugated
C=O	amides	1640–1690	s
	ketones and aldehydes	1670–1740	s
	esters	1710–1750	s
C≡C	alkynes	2150–2250	w unless conjugated
C≡N	nitriles	2200–2250	w
C–H	alkanes, CH ₂ –H	2850–2950	s
	alkenes/arenes, =C–H	3000–3100	w
N–H	amines, amides	3300–3500	w
O–H	carboxylic acids, RCO ₂ –H	2500–3000	s and very broad
	H-bonded alcohol, RO–H	3200–3600	s
	free alcohol, RO–H	3580–3650	s and sharp

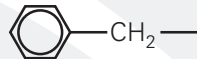
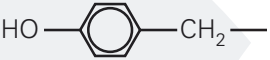
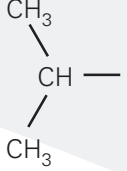
9 The orientating effect of groups in aromatic substitution reactions.

The position of the incoming group, **Y**, is determined by the nature of the group, **X**, already bonded to the ring, and not by the nature of the incoming group **Y**.



X- groups that direct the incoming Y group to the 2- or 4- positions	X- groups that direct the incoming Y group to the 3- position
$-\text{NH}_2$, $-\text{NHR}$ or $-\text{NR}_2$	$-\text{NO}_2$
$-\text{OH}$ or $-\text{OR}$	$-\text{NH}_3$
$-\text{NHCOR}$	$-\text{CN}$
$-\text{CH}_2$, -alkyl	$-\text{CHO}$, $-\text{COR}$
$-\text{Cl}$	$-\text{CO}_2\text{H}$, $-\text{CO}_2\text{R}$

10 Names, structures and abbreviations of some amino acids

Name	3-letter abbreviation	1-letter symbol	structure of side chain R- in $\begin{array}{c} \text{NH}_2 \\ \\ \text{R}-\text{CH} \\ \\ \text{CO}_2\text{H} \end{array}$
alanine	Ala	A	CH_3-
aspartic acid	Asp	D	HO_2CCH_2-
cysteine	Cys	C	HSCH_2-
glutamic acid	Glu	E	$\text{HO}_2\text{CCH}_2\text{CH}_2-$
glycine	Gly	G	$\text{H}-$
lysine	Lys	K	$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_2-$
phenylalanine	Phe	F	
serine	Ser	S	HOCH_2-
tyrosine	Tyr	Y	
valine	Val	V	

Group																																									
1	2	13	14	15	16	17	18																																		
3	4	<table border="1"> <thead> <tr> <th colspan="2">Key</th> </tr> <tr> <th>atomic number</th> <th>atomic symbol</th> </tr> <tr> <th>name</th> <th>relative atomic mass</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>H</td> </tr> <tr> <td>hydrogen</td> <td>1.0</td> </tr> </tbody> </table>																Key		atomic number	atomic symbol	name	relative atomic mass	1	H	hydrogen	1.0	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Key																																									
atomic number	atomic symbol																																								
name	relative atomic mass																																								
1	H																																								
hydrogen	1.0																																								
Li lithium 6.9	Be beryllium 9.0	B boron 10.8	C carbon 12.0	N nitrogen 14.0	O oxygen 16.0	F fluorine 19.0	Ne neon 20.2	Na sodium 23.0	Mg magnesium 24.3	Al aluminium 27.0	Si silicon 28.1	P phosphorus 31.0	S sulfur 32.1	Cl chlorine 35.5	Ar argon 39.9																										
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36																								
K potassium 39.1	Ca calcium 40.1	Sc scandium 45.0	Ti titanium 47.9	V vanadium 50.9	Cr chromium 52.0	Mn manganese 54.9	Fe iron 55.8	Co cobalt 58.9	Ni nickel 58.7	Cu copper 63.5	Zn zinc 65.4	Ga gallium 69.7	Ge germanium 72.6	As arsenic 74.9	Se selenium 79.0	Br bromine 79.9	Kr krypton 83.8																								
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54																								
Rb rubidium 85.5	Sr strontium 87.6	Y yttrium 88.9	Zr zirconium 91.2	Nb niobium 92.9	Mo molybdenum 95.9	Tc technetium —	Ru ruthenium 101.1	Rh rhodium 102.9	Pd palladium 106.4	Ag silver 107.9	Cd cadmium 112.4	In indium 114.8	Sn tin 118.7	Sb antimony 121.8	Te tellurium 127.6	I iodine 126.9	Xe xenon 131.3																								
55	56	57-71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86																								
Cs caesium 132.9	Ba barium 137.3	lanthanoids	Hf hafnium 178.5	Ta tantalum 180.9	W tungsten 183.8	Re rhenium 186.2	Os osmium 190.2	Ir iridium 192.2	Pt platinum 195.1	Au gold 197.0	Hg mercury 200.6	Tl thallium 204.4	Pb lead 207.2	Bi bismuth 209.0	Po polonium —	At astatine —	Rn radon —																								
87	88	89-103	104	105	106	107	108	109	110	111	112	114	116	116	116	116	116																								
Fr francium —	Ra radium —	actinoids	Rf rutherfordium —	Db dubnium —	Sg seaborgium —	Bh bohrium —	Hs hassium —	Mt meitnerium —	Ds darmstadtium —	Rg roentgenium —	Cn copernicium —	Fl flerovium —	Lv livermorium —	—	—	—	—																								

57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
La lanthanum 138.9	Ce cerium 140.1	Pr praseodymium 140.9	Nd neodymium 144.4	Pm promethium —	Sm samarium 150.4	Eu europium 152.0	Gd gadolinium 157.3	Tb terbium 158.9	Dy dysprosium 162.5	Ho holmium 164.9	Er erbium 167.3	Tm thulium 168.9	Yb ytterbium 173.1	Lu lutetium 175.0
89	90	91	92	93	94	95	96	97	98	99	100	101	102	103
Ac actinium —	Th thorium 232.0	Pa protactinium 231.0	U uranium 238.0	Np neptunium —	Pu plutonium —	Am americium —	Cm curium —	Bk berkelium —	Cf californium —	Es einsteinium —	Fm fermium —	Md mendelevium —	No nobelium —	Lr lawrencium —