

Structure of Elements and Compounds

To succeed with this topic you need to:

- Understand what is meant by ionic, covalent and metallic bonding (covered in Factsheet 5 - Bonding)
- Understand the different types of intermolecular forces
- Know how to work out the sort of bonding in a compound from the elements in it

After working through this Factsheet you will:

- understand how bonding determines the structure and properties of compounds
- be able to deduce bonding from structure, or structure and properties from bonding, for unfamiliar substances
- know the structures and properties of elements and compounds specifically mentioned at AS level

Exam hint:- Questions will often use "unfamiliar" compounds. However, they will fit into the general pattern outlined in this sheet, so will be effectively the same as the specific examples you have learnt. For example, potassium bromide (KBr) is similar to sodium chloride (NaCl) because sodium and potassium are in the same group, and bromine and chlorine are in the same group.

Bonding

There are three main types of bonding between atoms - ionic, covalent and metallic (Factsheet 5 - Bonding). The key characteristics of these are summarised in Table 1.

However, in most compounds the bonding is not really pure ionic or pure covalent - it is somewhere in between. Such types of bonding are known as **intermediate**. This affects the structure and physical and chemical properties.

In an ionic compound, if the positive ion (cation) is very small, it has a high **charge density** - which means it has a lot of charge in a small volume! This high charge density attracts the electron cloud on the negative ion (anion) and tends to pull it out of shape. This is particularly likely if the anion is big - since then the electron cloud is a long way away from the nucleus, and so it is not so tightly held by the nucleus. Ionic compounds in which this occurs are said to be **polarised**, or **ionic with covalent character**.

In covalent compounds, sometimes one atom (the more **electronegative** element) exerts a greater "pull" on the electrons; if this happens, the electron cloud is pulled out of shape towards this atom. Such a bond is known as **covalent with ionic character**, or **polar covalent**.

Fig 1. Ionic, covalent and intermediate bonding

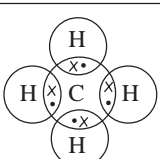
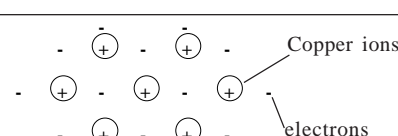
Pure ionic - ions are spherical

Ionic, with covalent character - the cation has pulled the electron cloud out of shape on the anion. This is called *polarisation*.

Covalent, with ionic character - the molecular orbital is shifted towards the more electronegative atom causing dipoles (small charges, δ^+ and δ^-). These are the cause of polar molecules ie. molecules with charges on certain atoms.

Pure covalent - equal distribution of the electron cloud (molecular orbital) between the two nuclei.

Table 1. The three main types of bonding

Type of bonding	Involves	Occurs in	Example
Ionic	Electrons being transferred from one atom to another so that positive and negative ions are formed. Each atom then (usually) ends up with a full outer shell of electrons.	Compounds of metals and non-metals	Sodium chloride (NaCl) $\text{Na} + \text{Cl} \rightarrow \text{Na}^+ + \text{Cl}^-$ $1s^2 2s^2 2p^6 3s^1 \quad 1s^2 2s^2 2p^6 3s^2 3p^5 \quad 1s^2 2s^2 2p^6 \quad 1s^2 2s^2 2p^6 3s^2 3p^6$
Covalent	Atoms sharing electrons, so that each atom (usually) ends up with a full outer shell of electrons	Compounds of two (or more) non-metals. Non-metal elements, except noble gases	Methane (CH ₄) 
Metallic	Metal atoms in a lattice losing their outer electrons, which become delocalised - free to move from place to place.	Metal elements	Copper (Cu) 

Intermolecular forces

These are the forces attracting molecules to each other. They are important because the stronger they are, the more energy is required to separate the molecules from each other. Since melting a solid, or boiling a liquid, requires separating the molecules, this means that the stronger the intermolecular forces, the higher the melting/boiling point of the substance.

All types of intermolecular force rely on **dipoles** - this is when one end of a molecule is slightly positive and one is slightly negative. The positive end of one molecule is attracted to the negative end of another (unlike charges attract) Table 2 summarises the three types of intermolecular forces.

Table 2. Intermolecular forces

Name	Relative strength	Occurs	Explanation	Examples
Hydrogen bond	Strongest	In molecules containing a nitrogen, oxygen or fluorine atom bonded to a hydrogen.	The highly electronegative N, O or F atom attracts most of the electron cloud away from the hydrogen, leaving the hydrogen slightly positive and the other atom slightly negative.	$\text{NH}_3, \text{H}_2\text{O}, \text{HF}$
Dipole-dipole (or permanent dipole)	Middle	In molecules containing atoms of differing electronegativity - arranged asymmetrically	The more electronegative atom attracts a greater "share" of the electrons, giving it a small negative charge, and the other atom a small positive charge. If the molecule is asymmetrically arranged, this leads to a negative "end" and a positive "end", giving the molecule itself an overall dipole . However, in molecules where the electronegative atoms are symmetrically arranged, like CCl_4 and CO_2 , (see Factsheet 4 - Shapes of Molecules and Ions) all "ends" of the molecule are equally charged.	$\text{HCl}, \text{CHCl}_3$
Van der Waals forces (or temporary dipoles)	Weakest	In any atoms or molecules	The position of electrons around the nucleus in an atom can be instantaneously unbalanced, leading to a negative region and a positive region in the atom This creates induced dipoles in neighbouring atoms - the electrons in atoms near the positive region will be attracted, and those in atoms near the negative region will be repelled, so creating an imbalance in neighbouring atoms	Any molecular substance, but they increase in strength as the number of electrons in the atom increases and the number of atoms in the molecule increases

The effect of bonding on structure and properties

Table 3 below shows how structure and bonding are related for "typical" substances with ionic, covalent and metallic bonding. These general 'rules' explain the behaviour of the vast majority of elements and compounds. However, there are other influences e.g. intermolecular forces and sizes of atoms and molecules that affect the **properties** of elements and compounds

e.g. H_2O is simple molecular with an RMM = 18 (i.e. it is a small light-weight molecule) so should be a gas at room temperature. It is, of course, a liquid and this is due to the presence of strong hydrogen-bonding because of the presence of the oxygen atom. These 'special cases' are quoted in the AS level Chemistry specification and are given in the tables of specific examples that follow.

Table 3. Bonding, structure and properties

Bonding type	Structure	Key Properties
ionic	Millions of ions arranged in a crystal lattice (a regular structure) so it is a giant ionic structure held together by electrostatic attraction (+/-)	<ul style="list-style-type: none"> Solids with very high mpts/bpts (a lot of energy needed to break up the millions of bonds in the lattice). Most are soluble in water because of the ions which are attracted to the polar water molecules. Conducts electricity when in solution or molten due to being made of ions which can move. Solids do not conduct, as ions cannot move.
covalent	(a) i) a small group of atoms joined together as ' simple ' molecular . ii) simple molecules arranged in a lattice to produce a molecular giant structure	<ul style="list-style-type: none"> i) are usually liquids or gases with low mpts/bpts. (easy to separate because intermolecular forces between are weak). ii) are solids with low mpts/bpts. (easy to separate because intermolecular forces between are weak). Polar molecules may dissolve in water, Non-polar molecules do not, but will dissolve in non-aqueous solvents. No electrical conductivity.
	(b) many atoms joined together to form a giant covalent structure.	<ul style="list-style-type: none"> Solids with very high mpts/bpts (a giant structure so a lot of energy needed to separate the millions of covalent bonds) which are insoluble in water No electrical conductivity (except graphite - see page 3)
metallic	Millions of cations in a 'sea of electrons' making a giant metallic structure .	<ul style="list-style-type: none"> Solids(except mercury) with high mpts/bpts (a lot of energy needed to break up the giant structure). Conduct electricity because of the delocalised electrons.

Table 4. Specific examples of giant structures

Name/ Formula	Structure	Description	Physical Properties
Sodium chloride NaCl(s)		Giant ionic lattice	<ul style="list-style-type: none"> • Solid at room temperature • High MPt/BPt • Soluble in water • Conducts electricity when molten or in solution • Crystalline
Diamond C(s)		Giant covalent molecule. Each carbon atom joined to 4 other carbon atoms in a tetrahedral arrangement – this makes a very strong and rigid structure.	<ul style="list-style-type: none"> • Solid at room temperature • High MPt/BPt • Insoluble in water and non-aqueous solvents • Does not conduct electricity • Crystalline – the hardest known natural material
Graphite C(s)		Giant covalent molecule. Arranged in layers held together by weak Van der Waals forces. The carbon atoms in the layers are arranged in hexagons (each connected to 3 others, the non-bonded electron from carbon joins with others.) These delocalised electrons flow along layers but not between them.	<ul style="list-style-type: none"> • Solid at room temperature • High MPt/BPt • Insoluble in water and non-aqueous solvents • Conducts electricity in one direction/plane only • Feels soft when rubbed (used as a lubricant) because pressure makes the layers move across each other as the weak bonding is broken
Iron Fe(s)		Giant structure of cations surrounded by a 'sea of delocalised electrons'.	<ul style="list-style-type: none"> • Solid at room temperature • High MPt/BPt • Conducts electricity in all directions • Insoluble in water and non-polar solvents • High density
Silicon dioxide (silica) SiO ₂ (s)		Giant covalent structure. Every Si atom is linked to 4 O atoms, and in turn every O atom is linked to 2 Si atoms.	<ul style="list-style-type: none"> • Solid at room temperature • High MPt/BPt • Poor conductor of electricity • Insoluble in water and non-polar solvents

Table 5. Specific examples of molecular structures

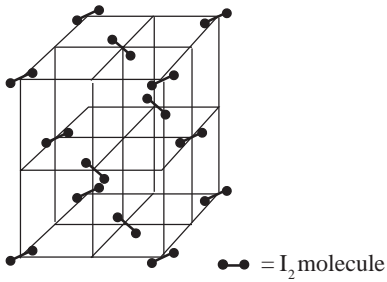
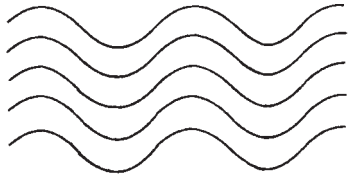
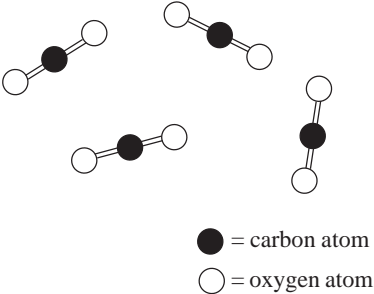
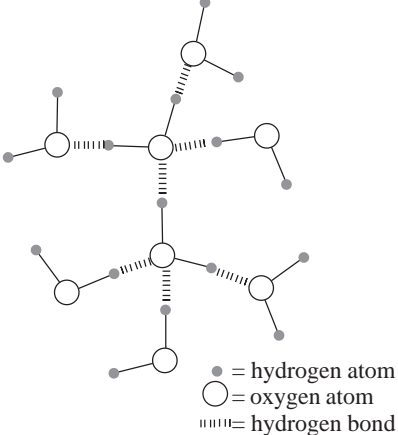
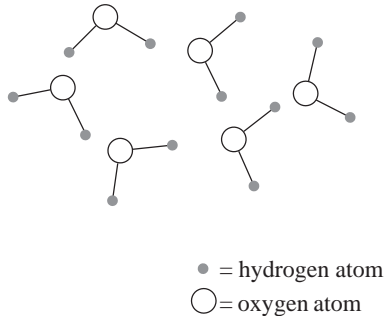
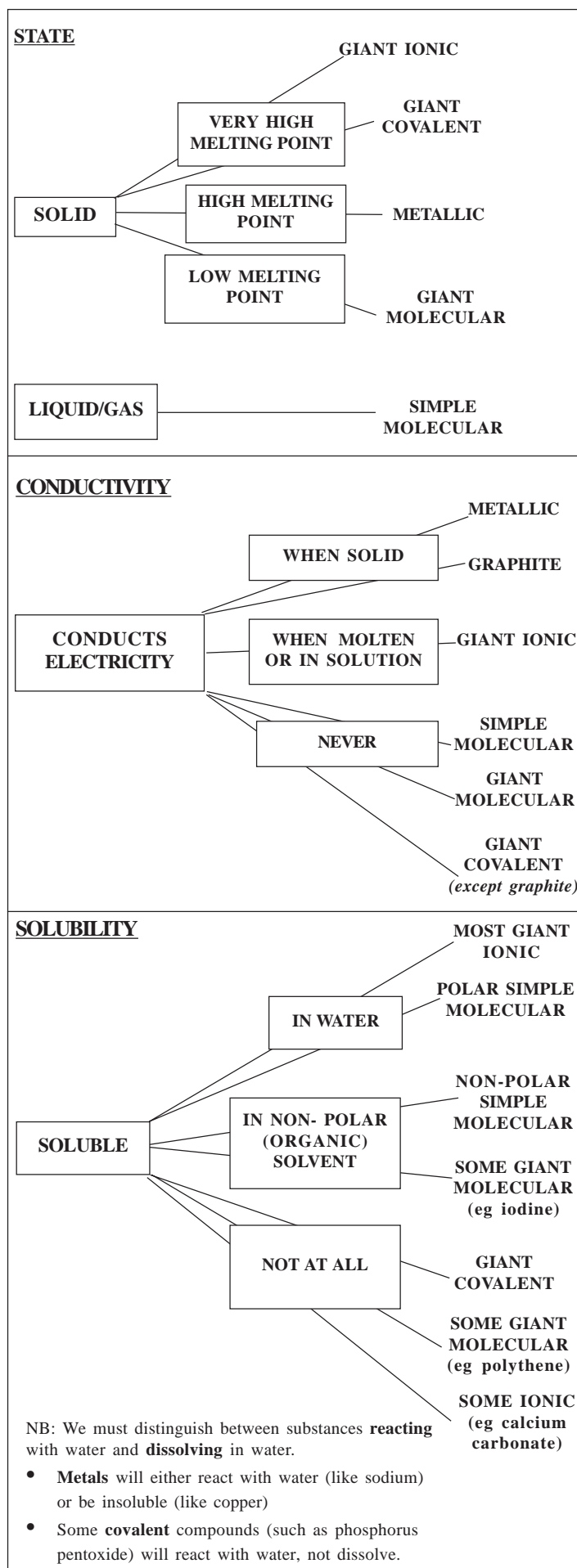
Name/Formula	Structure	Description	Physical Properties
Iodine $I_2(s)$		Giant molecular structure. Weak van der Waals forces hold the I_2 molecules in a 3-dimensional structure.	<ul style="list-style-type: none"> • Solid at room temperature • Low MPt/BPt • Soft • Does not conduct electricity • Virtually insoluble in water, very soluble in non-polar solvents
Polythene (C_2H_4) _n		Giant molecular structures, where long chains of carbon atoms lie alongside each other, attracted together by van der Waals forces.	<ul style="list-style-type: none"> • Solid at room temperature • Low MPt i.e. softens easily when heated • Does not conduct electricity • Will stretch • Insoluble in water
Carbon dioxide $CO_2(g)$		Simple molecular structure, strong covalent bonding within molecule, but only weak van der Waals forces between the molecules. A small light molecule. (RMM = 44)	<ul style="list-style-type: none"> • Gas at room temperature • Low MPt/BPt
Ice $H_2O(s)$		Giant structure of water molecules held together by strong hydrogen bonding. This 3-dimensional network of covalent bonds and hydrogen bonds keeps the H_2O molecules further apart than in liquid water (this is why its density is less than water, so it will float on water).	<ul style="list-style-type: none"> • Solid at, or below, $0^\circ C$ • Less dense than water
Water $H_2O(l)$		Polar molecules held together by hydrogen-bonding. Because the molecules are moving about the hydrogen-bonds are frequently broken and reformed but still cause the molecules to be attracted to one another.	<ul style="list-style-type: none"> • Liquid between 0°-$100^\circ C$

Fig 2. Physical properties and structure



Exam hint:- Questions on this topic may require:

- deduction of the properties of a compound from the elements in it
- diagrams of the structure of named compounds (see Tables 4 and 5)
- deduction of the structure of a compound from its properties, and possibly identification of the compound (from a list) (see Fig 2)

Questions

- PbCl_4 is a liquid at room temperature which does not conduct electricity, and is insoluble in water. PbCl_2 is a solid at room temperature which dissolves in water to form a solution which conducts electricity. What can be deduced from these physical properties about the structure and bonding of PbCl_4 and PbCl_2 ?
- Why is H_2O a liquid at room temperature, and not a gas?
- Carbon and silicon are both in group 4 of the periodic table. SiO_2 is a solid with a high melting point, whereas CO_2 is a gas. Explain this.
- Graphite conducts electricity only in one plane, whereas metals conduct in all planes. Why is this?
- Put the following compounds and elements into their correct positions in the table.
KBr, Hg, SO_2 , Ne, SiCl_4 , Rb_2O , PVC.

STRUCTURE	ELEMENT/COMPOUND
Giant ionic lattice	
Metallic	
Simple molecular	
Simple atomic	
Giant molecular	

Answers

- PbCl_4 -covalent, simple molecular. PbCl_2 -ionic, giant ionic lattice.
- Presence of H-bonding causes polar molecules to be attracted to one another, so more energy is required to separate the molecules.
- SiO_2 - giant covalent structure, with many Si and O atoms inter-linked. CO_2 -simple molecular structure. Only weak inter-molecular forces.
- Graphite is made of layers of C atoms arranged in hexagonal rings, along which electrons can flow. Electrons cannot move in between layers – hence conduction in 1 plane.
The de-localised electrons in metals can move in any direction because the structure is symmetrical.
- | | |
|---------------------|---------------------------------|
| Giant ionic lattice | KBr, Rb_2O |
| Metallic | Hg |
| Simple molecular | SO_2 , SiCl_4 |
| Simple atomic | Ne |
| Giant molecular | PVC |

Acknowledgements: This Factsheet was researched and written by Kieron Heath. Curriculum Press, Unit 305B, The Big Peg, 120 Vyse Street, Birmingham, B18 6NF. ChemistryFactsheets may be copied free of charge by teaching staff or students, provided that their school is a registered subscriber. No part of these Factsheets may be reproduced, stored in a retrieval system, or transmitted, in any other form or by any other means, without the prior permission of the publisher. ISSN 1351-5136