OCR A Chemistry A-level

Module 2.2: Electrons, Bonding and Structure

Detailed Notes

2.2.1 Electron Structure

Energy Levels, Shells, Sub-Shells, Atomic Orbitals, Electron Configuration

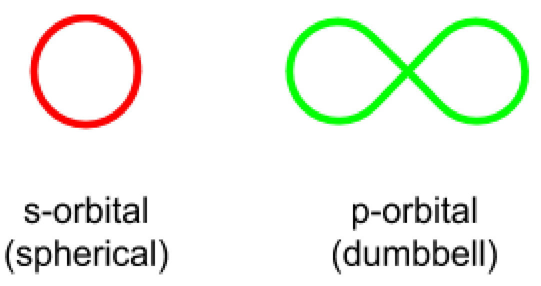
Shells

Electrons orbit the nucleus at different **energy levels**, which are an increasing distance from the nucleus. These are called **shells**. A shell is a **group of atomic orbitals** which have the same value of the principal quantum number, n. They can be split up into separate sub-shells, labelled s, p, d, and f.

The maximum numbers of electrons that can fill the first four shells are: 2, 8, 18, and 32. Given the atomic number of an element, you can deduce its **electron configuration**.

Electron Orbitals

Electrons are held in **clouds of negative charge** called **orbitals**. An atomic orbital is a region around the nucleus that can hold up to two electrons with opposite spins. There are different types of orbital: ***s, p, d,* and *f*.** Each one has a different shape:

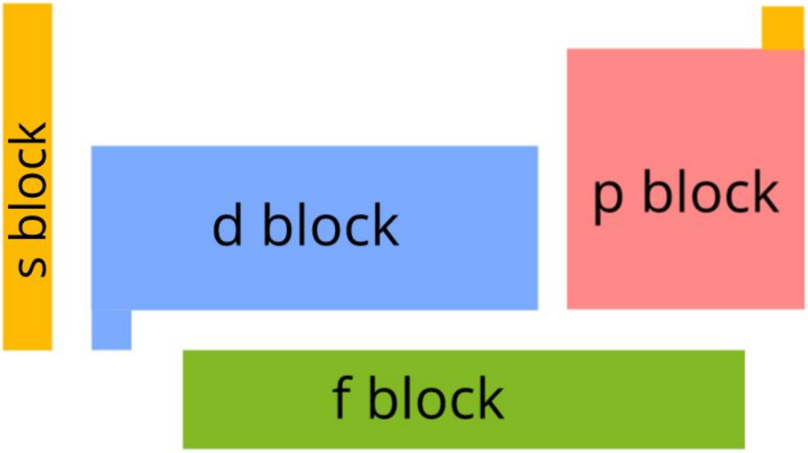


Each subshell has a different number of orbitals and therefore can hold a different number of electrons before the next one is filled:

s-subshell = 2 electrons
p-subshell = 6 electrons
d-subshell = 10 electrons

These orbitals correspond with **blocks** on the Periodic Table. Each element in the block has **outer electrons in that orbital**.

Example: The blocks of the periodic table



The **energy** of the orbitals **increases from s to p to d** meaning the orbitals are **filled in this order**. There is one exception to this rule. The **4s orbital** has a lower energy than the **3d** orbital, and so the 4s orbital is filled first. Each orbital is filled before the next one is used to hold electrons.

Example:

Sodium has 11 electrons. This gives sodium the following configuration:

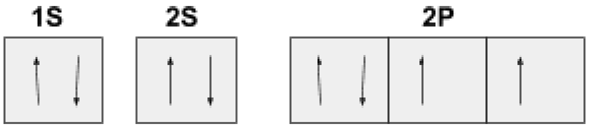
Na = $1s^2 2s^2 2p^6 3s^1$

It has 3 energy levels and 4 orbitals holding the 11 electrons.

Spin

Within an orbital, electrons **pair up with opposite spin** so that the atom is as **stable** as possible. Electrons in the **same orbital must have opposite spins**. Spin is represented by opposite **arrows**.

Example: Electron orbital diagram for oxygen



Overall there are **three rules** for writing out electron configurations:

1. The lowest energy orbital is filled first.
2. For orbitals with the same energy, electrons occupy orbitals singly with the same spin before pairing begins.
3. No single orbital holds more than 2 electrons.

2.2.2 Bonding and Structure

Ionic Bonding

Ionic bonding is an **electrostatic attraction** between positive and negative ions.

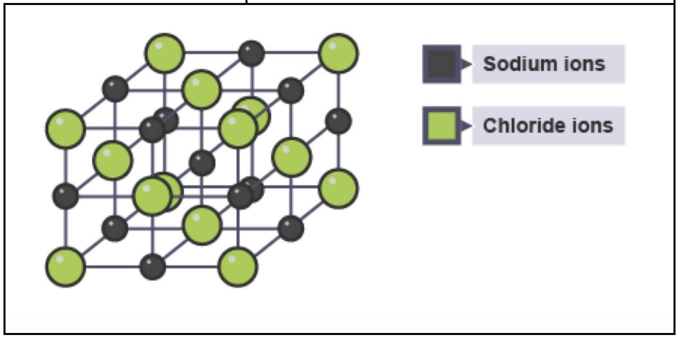
It occurs between a **metal and a nonmetal**. Electrons are **transferred** from the metal to the non-metal so that both elements achieve full outer shells.

When the electrons are transferred, it creates **charged particles** called **ions**. Oppositely charged ions **attract** each other through **electrostatic forces** to form a **giant ionic lattice**.

Example:

Sodium chloride is an ionic compound formed from Na$^+$ and Cl$^-$ ions. Sodium loses an electron and chlorine gains an electron to produce ions with a full outer electron shell. These then form a giant ionic lattice.

Image courtesy of Blogspot IGCSE Chemistry



The **charge** of an ion is related to the strength of the ionic bond that forms. Ions with a **greater charge** will have a **greater attraction** to the other ions resulting in stronger forces of attraction, and therefore **stronger ionic bonding**.

Larger ions that have a **greater ionic radius** will have a **weaker attraction** to the oppositely charged ion because the attractive forces have to act over a **greater distance**.

Cations (+ve) and **anions** (-ve) involved in ionic bonding can be represented using **dot and cross diagrams**. The electrons being transferred from the cation are seen on the outer shell of the anion.

The red dot clearly shows how the electron transfer has produced two ions with full outer electron shells.

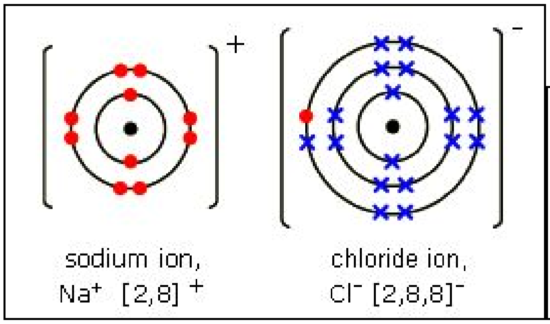


Image courtesy of BBC Bitesize

Physical Properties

Physical properties of a substance include the boiling point, melting point, solubility and conductivity. These properties are different depending on the **type of bonding** and the **crystal structure** of the compound.

Substances with an **ionic crystal structure** have a **high melting and boiling point**. This is because the electrostatic forces holding the ionic lattice together are strong and require a lot of energy to overcome.

When **molten or aqueous** (in solution), ionic substances can **conduct electricity**. In this state, the ions separate and are no longer held in a lattice. Therefore, they are free to move and **carry a flow of charge**.

In the **solid** state, ions are in **fixed positions** with no mobile charge carriers, so the substance can't conduct electricity.

Ionic substances are often **brittle** materials. When the layers of alternating charges are distorted, like charges repel, breaking apart the lattice into fragments.

Example: Diagram showing the brittle property of ionic substances

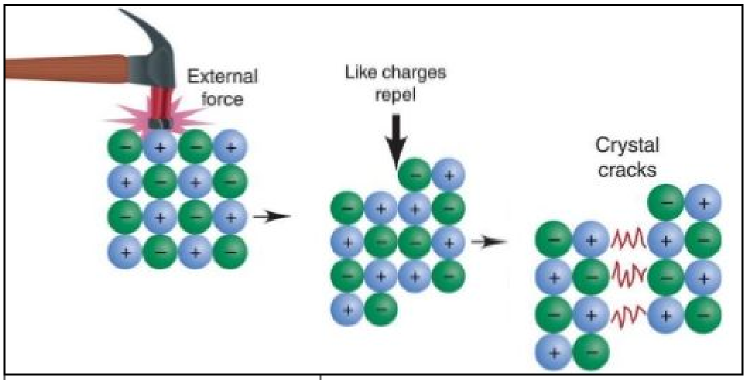


Image courtesy of Saints Chemistry

Covalent Bonding

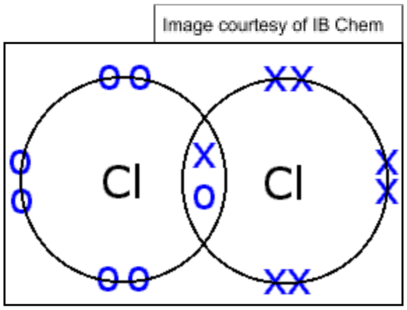
A covalent bond is the strong **electrostatic attraction** between a **shared pair of electrons** and the **nuclei** of the bonded atoms.

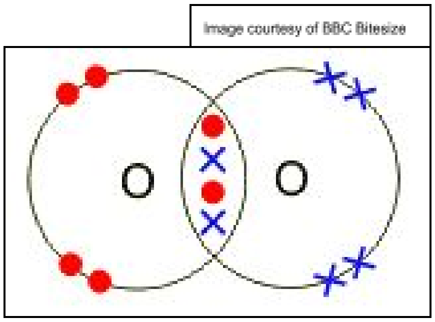
Covalent bonds form between **two nonmetals**. Electrons are **shared** between the two outer shells in order to achieve a **full outer shell**. **Multiple electron pairs** can be shared to produce **multiple covalent bonds**.

The shared electron pairs can be represented using **dot and cross diagrams.**

Double and **triple** bonds can also be shown on dot and cross diagrams with the multiple electron pairs being displayed in the shared segment between the two atoms.

Example: Dot and cross diagrams, chlorine molecule (left) and oxygen molecule (right)





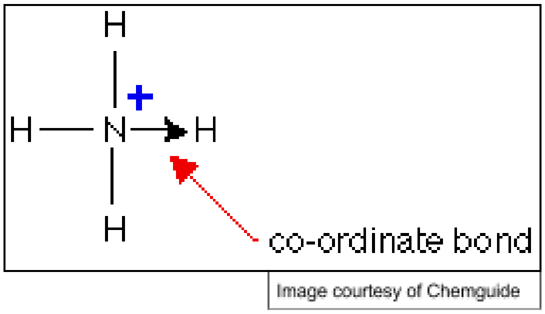
The **length** of a covalent bond is strongly linked to its **strength**. **Shorter bonds** tend to be **stronger** as the atoms are **held closer together** so the forces of attraction are greater, requiring more energy to be overcome. Double and triple bonds are shorter than single covalent bonds, explaining why they are so much stronger. **Average bond enthalpy** is used as a measure of covalent bond strength.

Dative Bonding

Dative or coordinate bonds form when both of the **electrons in the shared pair** are supplied from a **single atom**. It is indicated using an **arrow** from the lone electron pair.

Example:

Ammonia (NH_3) has a lone electron pair that can form a dative bond with a hydrogen ion (H^+) to produce an ammonium ion (NH_4^+).



Once a dative bond has formed, it is treated as a **standard covalent bond** as it **reacts in exactly the same way** and has the same properties regarding length and strength.

The Shapes of Simple Molecules and Ions

The shape of a simple molecule or ion is determined by the number of **electron pairs around the central atom** and the **repulsion** between them. Each electron pair **naturally repels** each other so that the **largest bond angle possible** exists between the covalent bonds.

In **diagrams**, a **solid line** indicates a bond that is in the plane of the paper, a **wedged line** indicates a bond that comes out of the plane of the paper and a **dotted line** indicates a bond that goes into the plane of the paper.

Lone Pair Repulsion

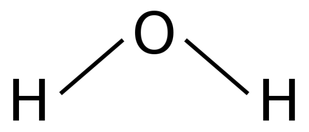
Any lone pairs present around the central atom provide **additional repulsive forces**, which changes the bond angle. For every lone pair present, the bond angle between covalent bonds is **reduced by 2.5°**. This can be seen by looking at methane, ammonia and water in the table below. All molecules have 4 electron pairs, but the bond angle decreases by 2.5° with each lone pair of electrons.

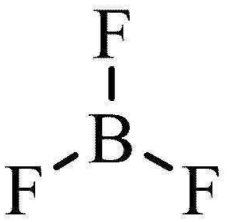
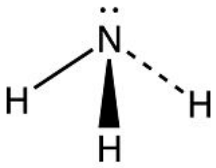
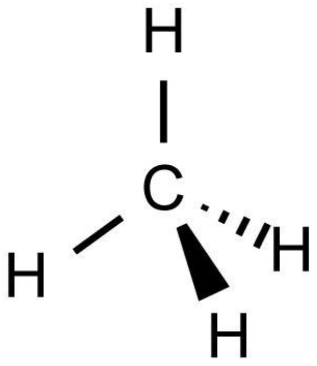
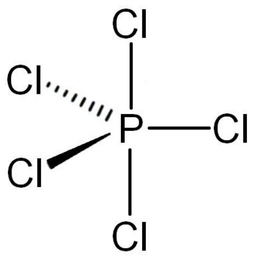
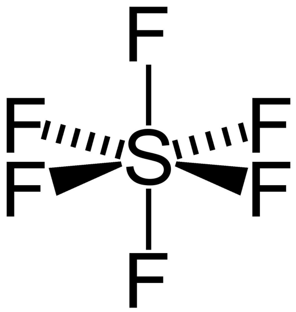
Molecule Shapes

The shape of a molecule can be determined by considering the **type and quantity of electron pairs**:

1. Find the number of electron pairs.
2. Determine how many of the pairs are bonding pairs and how many are lone pairs.
3. Bonding pairs indicate the basic shape and lone pairs indicate any additional repulsion.

This table shows some common molecule shapes:

Name	**Bonding e^- Pairs**	**Lone e^- Pairs**	**Bond Angle (°)**	**Example**
Linear	2	0	180	Cl - Be - Cl
Bent	2	2	104.5	

Trigonal Planar	3	0	120	
Triangular Pyramid	3	1	107	
Tetrahedral	4	0	109.5	
Trigonal Bipyramid	5	0	180 and 120	
Octahedral	6	0	90	

Images courtesy of World of Chemicals, Socratic, Quora, and Alchetron

Electronegativity and Bond Polarity

The negative charge around a covalent bond is **not evenly distributed** around the orbitals of the bonded atoms.

Electronegativity

Every atom has electronegativity, which is defined as:

The ability of an atom to attract the bonding electrons in a covalent bond towards itself.

This 'power' is different for every atom depending on its **size and nuclear charge**.

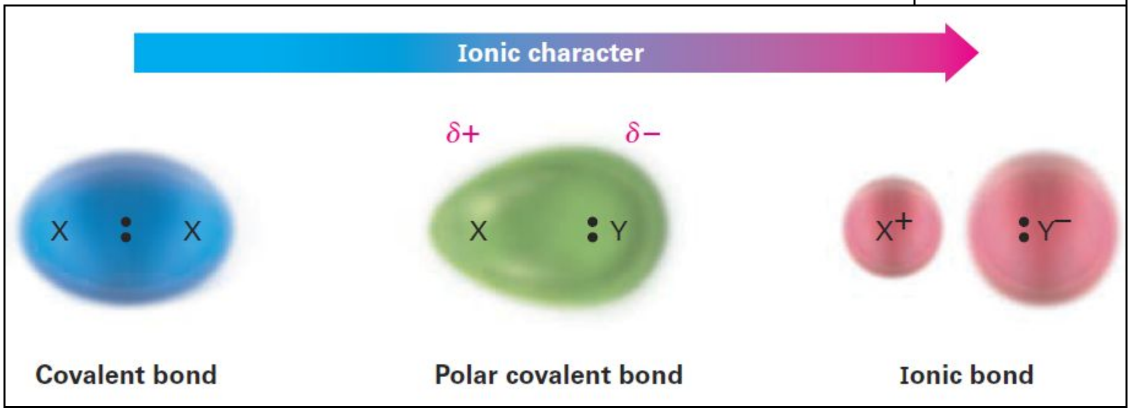
- Electronegativity **increases along a period** as atomic radius decreases and charge density increases.
- Electronegativity **decreases down a group** as shielding increases and atomic radius increases so charge density decreases.

Pauling electronegativity values can be used to compare the electronegativity of atoms. A **higher value** on the pauling scale indicates a **greater electronegativity**. Fluorine is the most electronegative atom and has a value of 4.0.

The pauling values can be used to calculate **electronegativity differences** in a covalent bond. The greater the electronegativity difference, the greater the bond polarity. This leads to a greater degree of **ionic character**. Ionic and covalent bonding are the extremes in a continuous scale of bonding as shown below.

Example:

Image courtesy of almerja.com

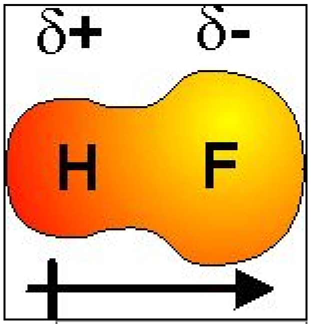


This bond polarity can be **permanent** or **induced**, depending on the molecule and how it interacts with things around it.

Permanent Dipole

If the two atoms that are bonded have different electronegativities, a **polar bond** forms. The more electronegative atom **draws more of the negative charge towards itself** and away from other atom, producing a **∂-** region and a **∂+** region. This is a **permanent dipole**.

Example:



Images courtesy of Socratic

Hydrogen fluoride is a polar molecule as fluorine is a lot more electronegative than hydrogen. This means electrons are drawn towards the fluorine atom.

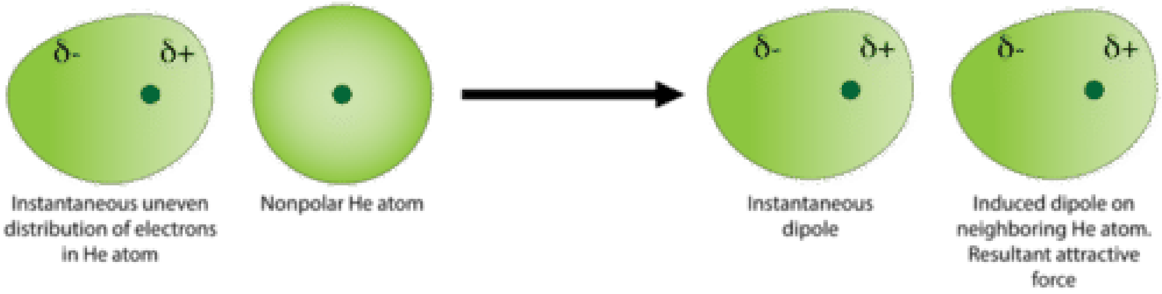
A **polar molecule** requires **polar bonds** with dipoles that do not cancel due to their direction. CO_2 contains two polar bonds since oxygen is more electronegative than carbon. However, these dipoles cancel due to the linear shape. Hence, CO_2 is **non-polar**.

Polar molecules with a permanent dipole can align to form a **lattice of molecules** similar to an ionic lattice.

Induced Dipole

An induced dipole can form when the electron orbitals around a molecule are **influenced by the distributions of electrons on another particle**.

Example:



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Intermolecular Forces

There are **three main types of intermolecular force**. Each one differs in strength and in what they act between.

Van der Waals Forces

Van der Waals forces are the **weakest** type of intermolecular force. They act as an **induced dipole** between molecules.

The strength of van der Waals forces varies depending on the Mr of the molecule and its shape. The **larger the Mr** of the molecule, the **stronger the intermolecular forces**. Straight chain molecules experience stronger van der Waals forces than branched chain molecules as they can **pack closer together**. This **reduces the distance** over which the force acts, making it stronger.

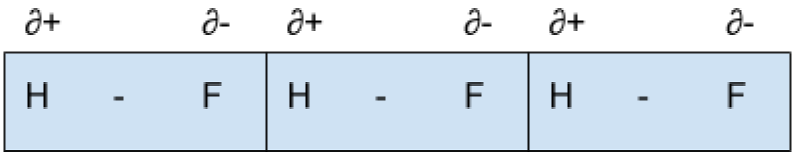
Van der Waals forces act between organic **alkane chains** and are affected by the **chain length** and the presence of **branching**. As the chain length of the alkane increases, so does the **Mr** of the molecule. This results in **stronger** intermolecular forces between the chains and the compound has a **higher boiling point** as a result.

Branching of alkane chains weakens van der Waal forces between the chains as they are less able to **pack tightly** together. Therefore, the distance over which the intermolecular forces act is increased and the **attractive forces** are **weakened**. This means branched chain alkanes have **lower boiling points** than straight chain alkanes.

Permanent Dipole

Permanent dipoles are a type of intermolecular force which acts between molecules with a **polar bond**. The **∂+** and **∂-** regions on adjacent molecules attract each other and hold the molecules together in a **lattice-like structure**. These interactions are stronger than induced dipole-dipole interactions, so more energy is needed to overcome them, so melting and boiling points will be higher.

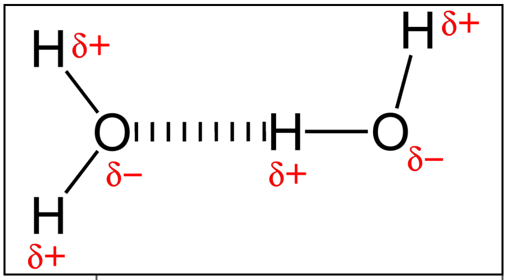
Example:



Hydrogen Bonding

Hydrogen bonds are the **strongest** type of intermolecular forces. Hydrogen bonds only act between hydrogen and the three most electronegative atoms: **nitrogen, oxygen and fluorine**. The **lone pair** of electrons on these electronegative atoms forms a bond with the **∂+** hydrogen atom from another molecule. As seen in the diagram below, the hydrogen bond is often shown by a **dotted line**.

Example:



Images courtesy of The Curious Wavefunction

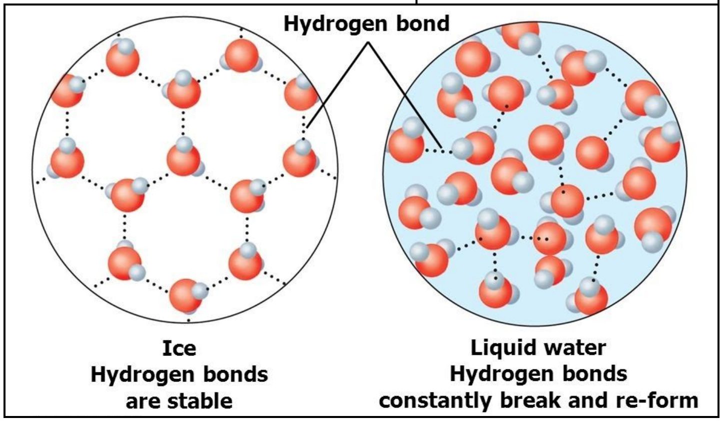
Molecules held together with hydrogen bonds have **much higher melting and boiling points** compared to similar sized molecules without hydrogen bonding. This shows how the type of intermolecular force heavily influences the **physical properties** of a substance.

Water has a simple molecular structure but has **unusually high melting and boiling points** for the size of the molecule due to the presence of hydrogen bonds.

The hydrogen bonds in water also result in **ice** having a much **lower density** than liquid water, as they hold the molecules in a **rigid structure** with a lot of **air gaps**.

Example: Diagram indicating how the hydrogen bonds affect the density of ice

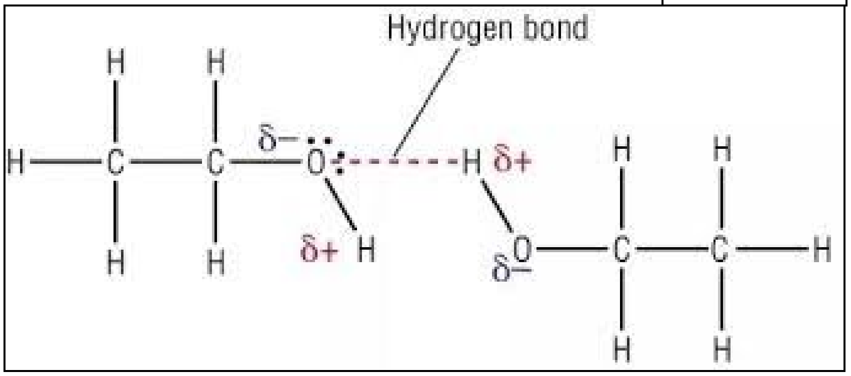
Image courtesy of Chemistry Stack Exchange



Hydrogen bonding is also responsible for the fact that **alcohols** have **much higher boiling points** than alkanes with a similar Mr value. This is because the lone electron pair on the oxygen atom is able to form **hydrogen bonds** with a hydrogen bonded to an oxygen on a neighbouring alcohol molecule.

Example: Hydrogen bonds between ethanol molecules

Image courtesy of Quora



This same property makes alcohols and water **good solvents** for compounds that are able to form hydrogen bonds in solution. However, alcohols and water can be poor for the dissolving of some **polar molecules** such as halogenoalkanes which cannot form hydrogen bonds.

Hydrogen bonds are also present in **DNA**. The **AT base pair** is held together by two hydrogen bonds and the **GC base pair** is held together by three hydrogen bonds.

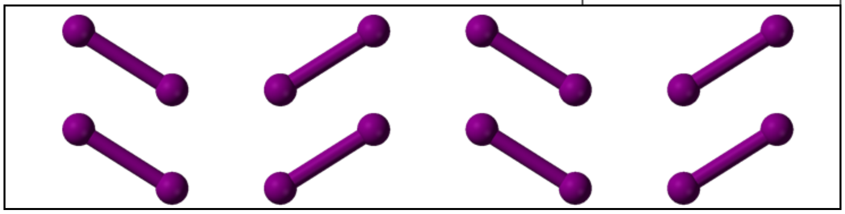
Covalent Structures

Simple Molecular

Substances with a simple molecular structure consist of **covalently bonded molecules** held together with weak **van der Waals** forces. These are a type of intermolecular force that act between the molecules and hold their structure.

Example:

Image courtesy of Wikimedia



Van der Waals forces are **very weak** and not much energy is required to overcome them, meaning simple molecular substances have **low melting and boiling points**. Simple molecular substances are **very poor conductors** as their structure contains no charged particles.

Macromolecular - Diamond

Substances that have a macromolecular structure are **covalently bonded** into a **giant lattice** structure. Each atom has **multiple covalent bonds** which are very strong, giving the substance a **very high melting point**.

The strength of the covalent lattice makes **macromolecular** substances **rigid**. **Diamond** is a macromolecular structure made up of carbon atoms each bonded to four further carbon atoms. This makes diamond one of the **hardest**, strongest materials known.

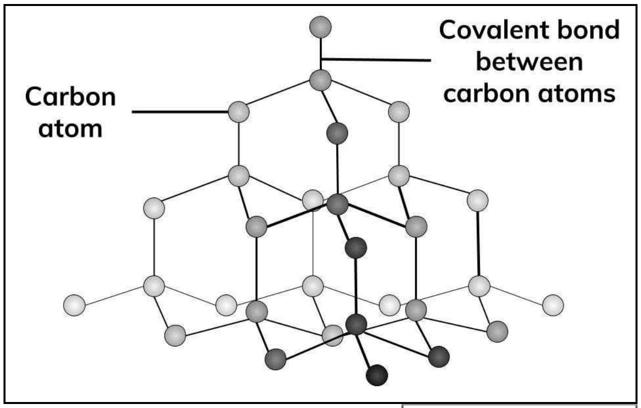
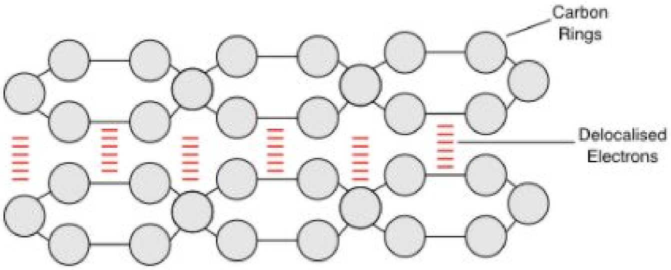


Image courtesy of Seneca

Macromolecular - Graphite

Graphite is a macromolecular structure made up of carbon atoms. However, in graphite, each carbon atom is bonded to three others in **flat sheets**. The electrons not used in bonding are released as **free electrons** which move between layers, meaning it can **conduct electricity**. There are **strong covalent bonds** between carbon atoms within a layer and **weak van der Waals** forces between such layers. These weak intermolecular forces allow layers to slide over each other easily. This property makes graphite a good lubricant.

Example:



Graphene

Graphene is a relatively recent material consisting of single, **2D sheets of graphite** that are just **one atom thick**.

These sheets are formed of **hexagonal carbon rings** that create a very strong, rigid material that is extremely **lightweight**. Delocalised electrons move through each layer allowing graphene to **conduct** electricity.