

## Shape of molecules

Name	No bonding pairs	No lone pairs	Diagram	Bond angle	Examples
linear	2	0		180	CO <sub>2</sub> , CS <sub>2</sub> , HCN, BeF <sub>2</sub>
Trigonal planar	3	0		120	BF <sub>3</sub> , AlCl <sub>3</sub> , SO <sub>3</sub> , NO <sub>3</sub> <sup>-</sup> , CO <sub>3</sub> <sup>2-</sup>
Tetrahedral	4	0		109.5	SiCl <sub>4</sub> , SO <sub>4</sub> <sup>2-</sup> , ClO <sub>4</sub> <sup>-</sup> , NH <sub>4</sub> <sup>+</sup>
Trigonal pyramidal	3	1		107	NCl <sub>3</sub> , PF <sub>3</sub> , ClO <sub>3</sub> , H <sub>3</sub> O <sup>+</sup>
Bent	2	2		104.5	OCl <sub>2</sub> , H <sub>2</sub> S, OF <sub>2</sub> , SCl <sub>2</sub>
Trigonal Bipyramidal	5	0		120 and 90	PCl <sub>5</sub>
Octahedral	6	0		90	SF <sub>6</sub>

### How to explain shape

1. State number of bonding pairs and lone pairs of electrons.
2. State that electron pairs repel and try to get as far apart as possible (or to a position of minimum repulsion.)
3. If there are no lone pairs state that the electron pairs repel equally
4. If there are lone pairs of electrons, then state that lone pairs repel more than bonding pairs.
5. State actual shape and bond angle.

Remember lone pairs repel more than bonding pairs and so reduce bond angles (by about 2.5° per lone pair in above examples)

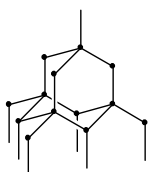
### Effect of multiple bonds on bond strength and length.

Nuclei joined by multiple (i.e. double and triple) bonds have a **greater electron density** between them.

This causes an **greater force of attraction** between the nuclei and the electrons between them, resulting in a **shorter bond length** and **greater bond strength**.

## Carbon Allotropes

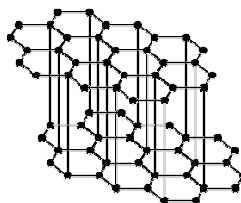
### Macromolecular: diamond



Tetrahedral arrangement of carbon atoms. 4 covalent bonds per atom

Diamond cannot conduct electricity because all 4 electrons per carbon atoms are involved in covalent bonds. They are localised and cannot move

### Macromolecular: Graphite



Planar arrangement of carbon atoms in layers. 3 covalent bonds per atom in each layer. 4<sup>th</sup> outer electron per atom is delocalised. Delocalised electrons between layers.

Graphite can conduct electricity well between layers because one electron per carbon is free and delocalised, so electrons can move easily along layers.

It does not conduct electricity between layers because the energy gap between layers is too large for easy electron transfer.

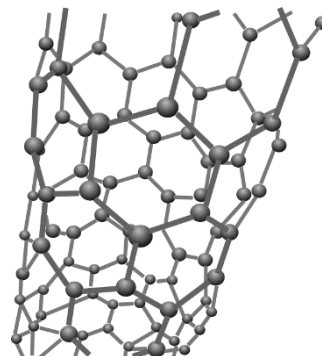
Both these macromolecular structures have very high melting points because of strong covalent forces in the giant structure. It takes a lot of energy to break the **many strong** covalent bonds

### Carbon nanotubes

These have very high tensile strength because of the strong structure of many strong covalent bonds

Nanotubes can conduct electricity well along the tube because one electron per carbon is free and delocalised, so electrons can move easily along the tube.

Nanotubes have potentially many uses. One being the potential to us as vehicles to deliver drugs to cells.



There are delocalized electrons in buckminsterfullerene.

## Electronegativity and intermediate bonding

### Definition

**Electronegativity** is the relative tendency of an **atom in a covalent bond** in a molecule to **attract electrons** in a covalent bond to itself.

F, O, N and Cl are the most electronegative atoms

Electronegativity is measured on the **Pauling scale** (ranges from 0 to 4)

The **most** electronegative element is **fluorine** and it is given a value of 4.0

### Factors affecting electronegativity

Electronegativity increases across a period as the **number of protons increases** and the atomic radius decreases because the **electrons in the same shell** are pulled in more.

It decreases down a group because the **distance** between the nucleus and the outer electrons **increases and the shielding** of inner shell electrons increases

### Intermediate bonding

Ionic and covalent bonding are the extremes of a continuum of bonding type. Differences in electronegativity between elements can determine where a compound lies on this scale

A compound containing elements of similar electronegativity and hence a **small electronegativity difference** will be purely **covalent**

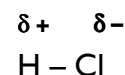
A compound containing elements of very different electronegativity and hence a very **large electronegativity difference** (> 1.7) will be **ionic**

### Formation of a permanent dipole – (polar covalent) bond

A **polar covalent bond** forms when the elements in the bond have **different electronegativities**. (Of around 0.3 to 1.7)

When a bond is a **polar covalent bond** it has an **unequal distribution of electrons** in the bond and produces a **charge separation, (dipole)**  $\delta+$   $\delta-$  ends.

The element with the larger electronegativity in a polar compound will be the  $\delta-$  end



## Polar and Non Polar molecules

### Symmetric molecules

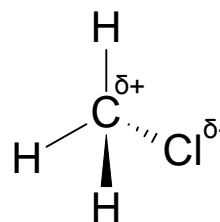
A symmetric molecule (**all bonds identical and no lone pairs**) will **not** be polar **even if individual bonds within the molecular ARE polar**.

The individual dipoles on the bonds '**cancel out**' due to the symmetrical shape of the molecule. There is no **NET** dipole moment: the **molecule is NON POLAR**



CO<sub>2</sub> is a symmetrical molecule and is a non-polar molecule

e.g. CCl<sub>4</sub> will be non-polar whereas CH<sub>3</sub>Cl will be polar

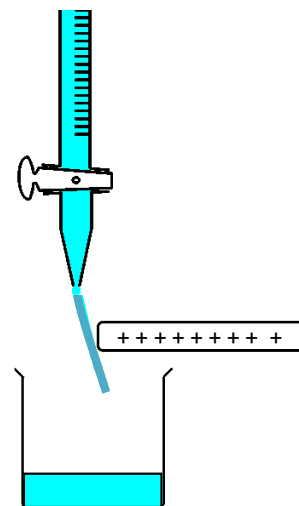


## Experiment effect of charged rod on polar/non-polar liquids

In this experiment, a charged rod (formed by rubbing a plastic rod) is brought close to a jet of liquid flowing from a burette.

If the liquid is polar, the jet of liquid will be attracted to the electrostatic force of the rod. The dipoles in the polar molecules will all align and the negative end  $\delta^-$  will be attracted to the positive rod (or vice versa). The stronger the dipole the more the deflection of the jet.

Non-polar liquids will not be deflected and attracted to the charged rod

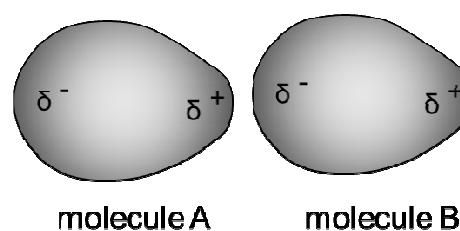


## Intermolecular Forces

### London Forces

London forces occur between **all molecular substances** and noble gases. **They do not occur in ionic substances.**

**London Forces** are also called **instantaneous, induced dipole-dipole interactions**. They occur between all simple covalent molecules and the separate atoms in noble gases. In any molecule the electrons are moving constantly and randomly. As this happens the electron density can fluctuate and parts of the molecule become more or less negative i.e. small temporary or transient dipoles form. These temporary dipoles can cause dipoles to form in neighbouring molecules. These are called induced dipoles. The induced dipole is always the opposite sign to the original one.



### Main factor affecting size of London Forces

The **more electrons** there are in the molecule the higher the chance that temporary dipoles will form. This makes the **London forces stronger between the molecules** and more energy is needed to break them so boiling points will be greater.

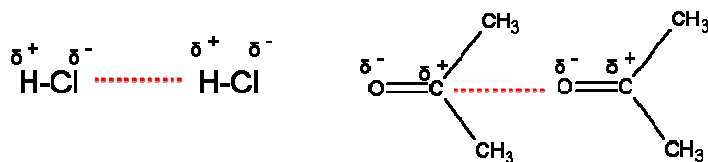
The increasing boiling points of the halogens down the group 7 series can be explained by the increasing number of electrons in the bigger molecules causing an increase in the size of the London forces between the molecules. This is why  $I_2$  is a solid whereas  $Cl_2$  is a gas.

The increasing boiling points of the alkane homologous series can be explained by the increasing number of electrons in the bigger molecules causing an increase in the size of the London forces between molecules.

The **shape** of the molecule can also have an effect on the size of the London forces. Long **straight chain** alkanes have a **larger surface area of contact between molecules** for London forces to form than compared to spherical shaped **branched alkanes** and so have stronger London forces.

## Permanent dipole-dipole bonding

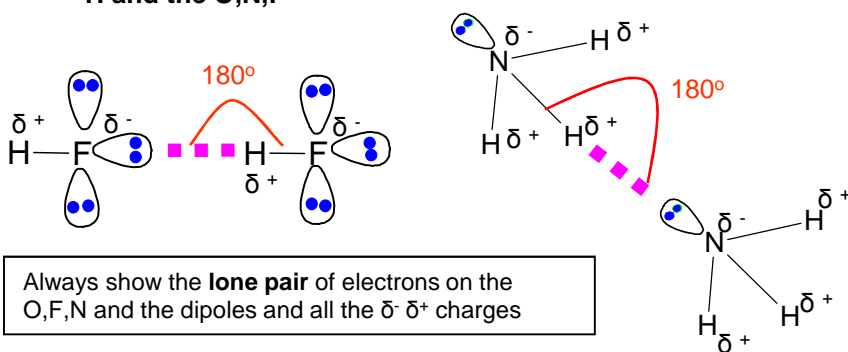
- Permanent dipole-dipole bonding occurs between polar molecules
- It is stronger than van der waals and so the compounds have higher boiling points
- Polar molecules have a permanent dipole. (commonly compounds with C-Cl, C-F, C-Br H-Cl, C=O bonds)
- Polar molecules are asymmetrical and have a bond where there is a significant **difference in electronegativity** between the atoms.



Permanent dipole bonding occurs in addition to London forces

## Hydrogen bonding

It occurs in compounds that have a **hydrogen atom attached to one of the three most electronegative atoms of nitrogen, oxygen and fluorine**, which must have an available lone pair of electrons. e.g. a **-O-H -N-H F-H** bond. There is a **large electronegativity difference** between the **H and the O,N,F**



Always show the **lone pair** of electrons on the O,F,N and the dipoles and all the  $\delta^- \delta^+$  charges

Hydrogen bonding occurs in addition to London forces

The hydrogen bond should have an bond angle of  $180^\circ$  with one of the bonds in one of the molecules

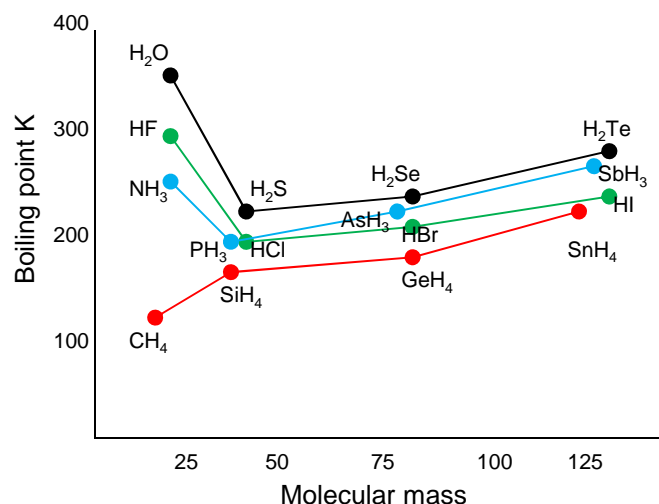
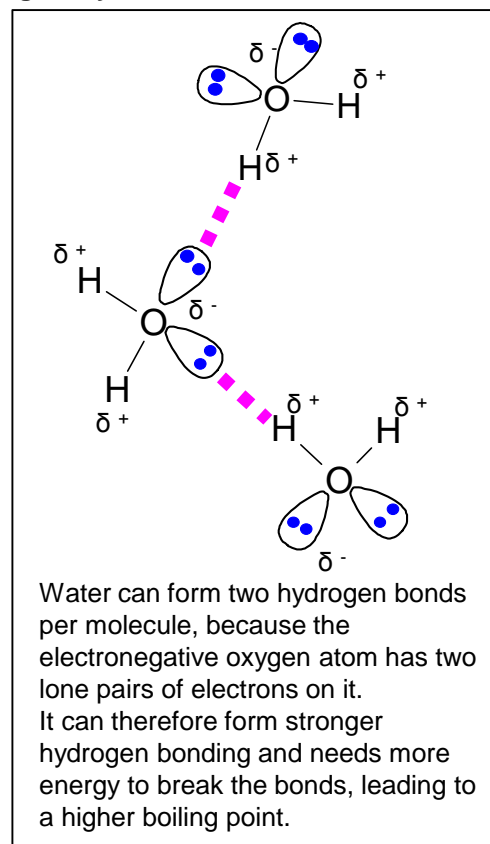
The bond angle is  $180^\circ$  around the H atom because there are two pairs of electrons around the H atom involved in the hydrogen bond. These pairs of electrons repel to a position of minimum repulsion, as far apart as possible.

Alcohols, carboxylic acids, proteins, amides all can form hydrogen bonds

Hydrogen bonding is stronger than the other two types of intermolecular bonding.

The **anomalously high** boiling points of  $\text{H}_2\text{O}$ ,  $\text{NH}_3$  and  $\text{HF}$  are caused by the hydrogen bonding between these molecules in addition to their London forces. The additional forces require more energy to break and so have higher boiling points

The general increase in boiling point from  $\text{H}_2\text{S}$  to  $\text{H}_2\text{Te}$  or from  $\text{HCl}$  to  $\text{HI}$  is caused by increasing London forces between molecules due to an increasing number of electrons.



## Solvents and Solubility

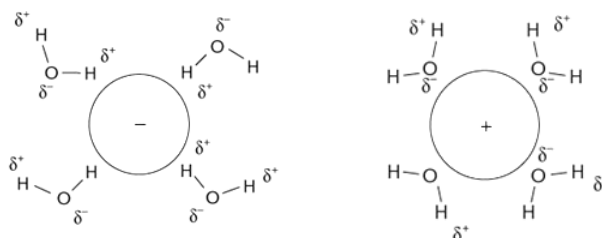
Solubility of a solute in a solvent is a complicated balance of energy required to break bonds in the solute and solvent against energy given out making new bonds between the solute and solvent.

### Ionic substances dissolving in water

When an ionic lattice dissolves in water it involves breaking up the bonds in the lattice and forming new bonds between the metal ions and water molecules.

The **negative** ions are attracted to the  $\delta^+$  **hydrogens** on the **polar water** molecules and the positive ions are attracted to the  $\delta^-$  oxygen on the polar water molecules.

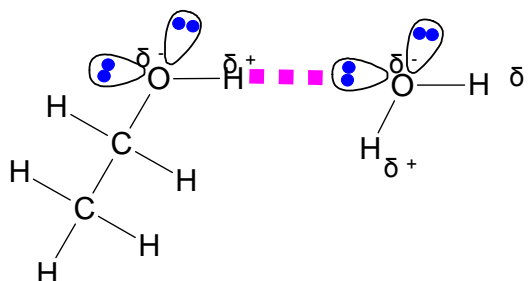
hydration of the ions



The higher the **charge density** the greater the hydration enthalpy (e.g. **smaller ions** or **ions with larger charges**) as the ions attract the water molecules more strongly.

### Solubility of simple alcohols

The smaller alcohols are soluble in water because they can form hydrogen bonds with water. The longer the hydrocarbon chain the less soluble the alcohol.



### Insolubility of compounds in water

Compounds that cannot form hydrogen bonds with water molecules, e.g. polar molecules such as halogenoalkanes or non polar substances like hexane will be insoluble in water.

### Solubility in non-aqueous solvents

Compounds which have similar intermolecular forces to those in the solvent will generally dissolve

**Non-polar solutes will dissolve in non-polar solvents.** e.g. Iodine which has only London forces between its molecules will dissolve in a non polar solvent such as hexane which also only has London forces.

Propanone is a useful solvent because it has both polar and non polar characteristics. It can form London forces with some non polar substances such as octane with its  $\text{CH}_3$  groups. Its polar  $\text{C}=\text{O}$  bond can also hydrogen bond with water.

