

Shape of molecules

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

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)

Occasionally more complex shapes are seen that are variations of octahedral and trigonal bipyramidal where some of the bonds are replaced with lone pairs. You do not need to learn the names of these but ought to be able to work out these shapes using the method below



Square planar
Bond angle 90°

e.g. XeF_4

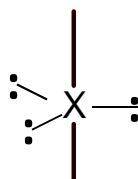


Xe has 8 electrons in its outer shell. 4 F's add 4 more electrons. This makes a total of 12 electrons made up of 4 bond pairs and 2 lone pairs. This means it is a variation of the 6 bond pair shape (octahedral)



Bond angle $\sim 89^\circ$
(Reduced by lone pair)

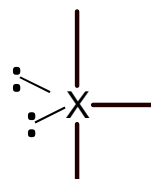
e.g. BrF_5



Bond angle 180°

e.g. I_3^-

Cl has 7 electrons in its outer shell. 3 F's add 3 more electrons. This makes a total of 10 electrons made up of 3 bond pairs and 2 lone pairs. This means it is a variation of the 5 bond pair shape (trigonal bipyramidal)



Bond angle $\sim 89^\circ$
(Reduced by lone pairs)

e.g. ClF_3



I has 7 electrons in its outer shell. 4 F's add 4 more electrons. Remove one electron as positively charged. This makes a total of 10 electrons made up of 4 bond pairs and 1 lone pair. This means it is a variation of the 5 bond pair shape (trigonal bipyramidal)



Bond angles $\sim 119^\circ + 89^\circ$
(Reduced by lone pair)

e.g. SF_4 & IF_4^+



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**

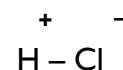
A compound containing elements of very different electronegativity and hence a very **large electronegativity difference** (> 1.7) will be **ionic**

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)** + - ends.

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



Polar and Non Polar molecules

Symmetric molecules

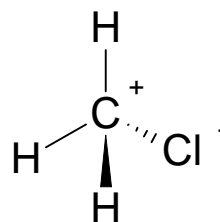
A symmetric molecule (**all bonds identical and no lone pairs**) will **not** be polar *even if individual bonds within the molecular ARE polar*.

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**



CO₂ is a symmetrical molecule and is a non-polar molecule

e.g. CCl₄ will be non-polar whereas CH₃Cl will be polar



Intermolecular Forces

Van der Waals' Forces

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

These are also called **transient, 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 instantaneous 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 Van der Waals

The **more electrons** there are in the molecule the higher the chance that temporary dipoles will form. This makes the **Van der Waals stronger between the molecules** and so boiling points will be greater.

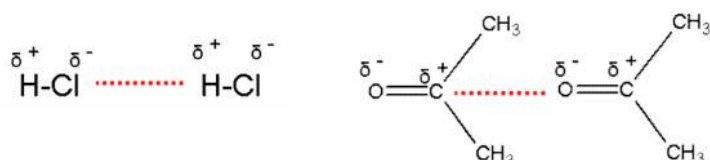
The increasing boiling points of the halogens down the group 7 series can be explained by the increasing number of electrons in the bigger molecules causing an increase in the size of the Van der Waals between the molecules. This is why I_2 is a solid whereas Cl_2 is a gas.

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 Van der Waals between molecules.

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

Permanent dipole-dipole forces

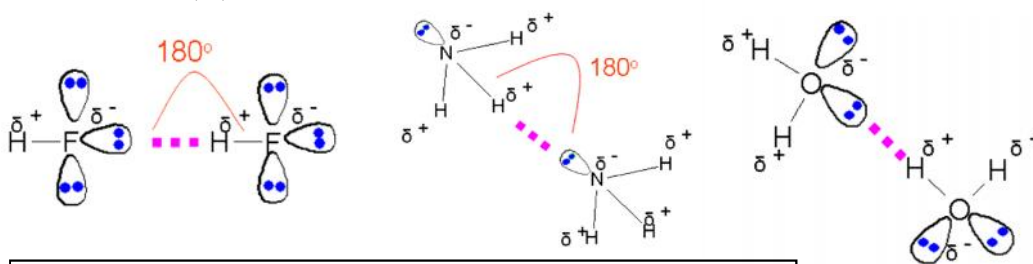
- Permanent dipole-dipole forces occurs between polar molecules
- It is stronger than Van der Waals and so the compounds have higher boiling points
- Polar molecules have a permanent dipole. (commonly compounds with C-Cl, C-F, C-Br H-Cl, C=O bonds)
- Polar molecules are asymmetrical and have a bond where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



Permanent dipole-dipole forces occurs in addition to Van der Waals 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**



Hydrogen bonding occurs in addition to van der waals forces

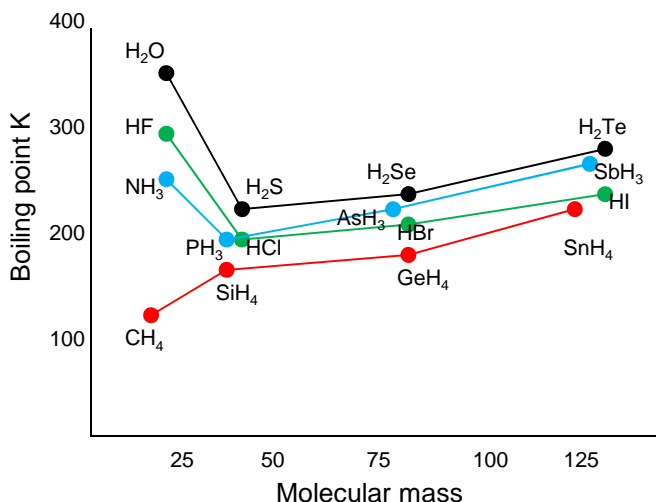
Always show the **lone pair** of electrons on the O,F,N and the dipoles and all the δ^- δ^+ charges

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

The **anomalously high** boiling points of H_2O , NH_3 and HF are caused by the hydrogen bonding between the molecules

The general increase in boiling point from H_2S to H_2Te is caused by increasing Van der Waals forces between molecules due to an increasing number of electrons.

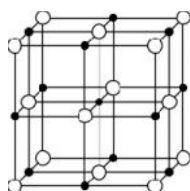
Alcohols, carboxylic acids, proteins, amides all can form hydrogen bonds



Four types of crystal structure: ionic, metallic, molecular and giant covalent (macromolecular).

You should be able to draw the following diagrams or describe the structure in words to show the four different types of crystal. You should also be able to explain the properties of these solids. The tables earlier in the revision guide explain these properties.

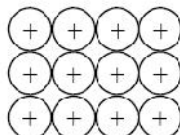
Ionic: sodium chloride



Giant ionic lattice showing alternate Na^+ and Cl^- ions

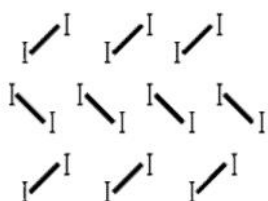
Metallic: magnesium or sodium

Use this diagram for any metal



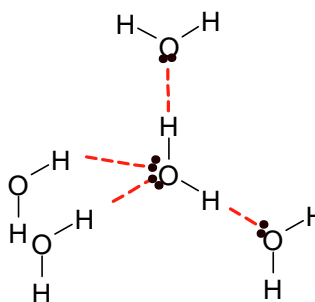
Giant metallic lattice showing close packing magnesium **ions**

Molecular: iodine



Regular arrangement of I_2 molecules held together by weak van der Waals forces

Molecular: Ice

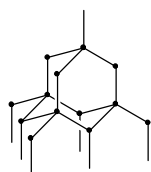


This is a difficult diagram to draw.

The main point to show is a central water molecule with two ordinary covalent bonds and two hydrogen bonds in a tetrahedral arrangement

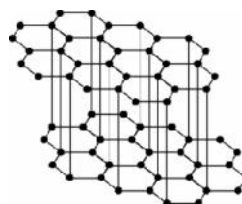
The molecules are held further apart than in liquid water and this explains the lower density of ice

Macromolecular: diamond



Tetrahedral arrangement of carbon atoms. 4 covalent bonds per atom

Macromolecular: Graphite



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

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.