Demonstrate understanding of bonding, structure, properties and energy changes

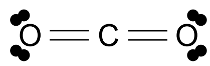
Revision notes for “Lewis structures, shapes & polarities”

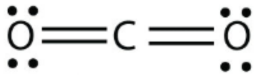
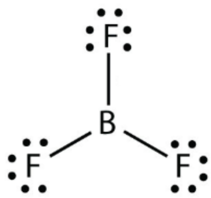
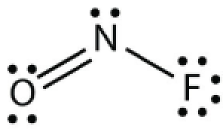
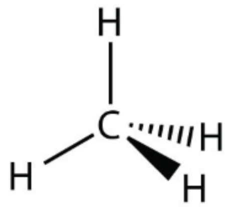
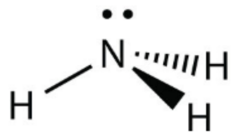
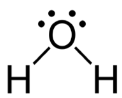
Valence shell electron pair repulsion theory

This is used to predict the shapes of simple molecules and ions by considering the repulsions between pairs of electrons (bonding pairs and non-bonding (lone) pairs). The shape that results is one that keeps repulsive forces to a minimum (i.e. the arrangement that keeps the regions of negative charge as far apart as possible).

Shapes of Molecules with Double or Triple Bonds

Since in a double or triple bond, the electron pairs stay together, we treat them as single regions of negative charge. E.g. in carbon dioxide (CO_2) the oxygen atoms are double bonded to the central carbon atom. The carbon atom has no lone pairs. The two double bonds are two regions of negative charge. The molecule is linear.



Regions of negative charge	Shape around central atom & bond angles	Example	Shapes
2	Linear, 180°		2 bonding regions / regions of negative charge = linear
3	Trigonal planar, 120°		3 bonding regions / regions of negative charge & zero lone pair(s) = trigonal planar
			2 bonding regions / the bond dipoles are NOT arranged symmetrically and do not cancel out & 1 lone pair = bent or V shaped (bond angle approx. 120°)
4	Tetrahedral, 109.5°		4 bonding regions / regions of negative charge & zero lone pair(s) = tetrahedral
			3 bonding regions / regions of negative charge & 1 lone pair = trigonal pyramidal e.g. NH_3 (approx. 107°)*
			2 bonding regions / regions of negative charge & 2 lone pairs = bent or V shaped e.g. H_2O (approx. 105°)**

In some books “regions of negative charge” are referred to as ”regions of electron density” or “electron clouds”. A “lone pair” is also known as a “non-bonding pair”.

***Ammonia: 3 bonding regions** and **1 lone pair** (total = 4 pairs) so the shape is based on a tetrahedron. As the lone pair-bond pair repulsions are greater than bond pair-bond pair repulsions the H-N-H bond angle is reduced from 109.5° to **107°**.

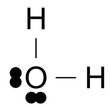
****Water**: **2 bonding regions** and **2 lone pairs** (total = 4 pairs) so the shape is based on a tetrahedron. The lone pair-lone pair repulsion pushes the H-O-H bond angle down further to about **105°**.

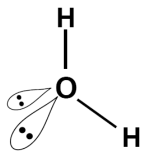
Species with lone pairs. Lone pairs have a greater repulsive force than bonding pairs so their presence affects bond angles. The order of repulsion is:

lone pair – lone pair > lone pair – bonding pair > bonding pair - bonding pair

Note: This is not examined. You will only be asked to suggest bond angles of about 109, 120 and 180 degrees.

When deciding the actual shape of the molecule, don't include the lone pairs in the shape even though they are responsible for determining the shape.

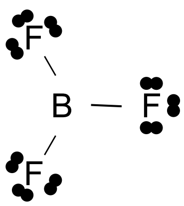
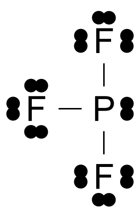




Bond angle is determined by the number of regions of negative charge around the central atom, which are arranged into a position to minimise repulsion by having maximum separation.
There are 4 regions of negative charge around the central O atom which arrange with maximum separation into a tetrahedral arrangement / geometry with a bond angle of approx. 109.5° / 109°.
In H_2O 2 regions are bonding and 2 are non-bonding (lone pairs), and so the shape of the water molecule is V shaped or bent.

Examples – shapes and polarity

$\delta+ \delta-$ $\delta+ \delta-$
The B-F and P-F bonds would be polar.

BF_3		trigonal planar	Repulsion of 3 regions of negative charge around B atom. All are bonding B is electron deficient	BF_3 is non-polar. The trigonal planar molecule is symmetrical about the central B atom, so the bond dipoles cancel / there is a symmetrical distribution of charge about the central atom.
PF_3		trigonal pyramid	Repulsion of four regions of negative charge around P atom: Three are bonding, one non-bonding	PF_3 is polar. The trigonal pyramid molecule is asymmetrical about the central P atom, so the P–F bond dipoles <u>add</u> to give a <u>net dipole</u> / there is an asymmetric distribution of charge about the central atom.

Explaining why a molecule is polar or not. Think….

1. Are there polar bonds? (Think F O N/Cl… S…C.. H). If yes, draw in the dipole over the bonds.

   $\overset{\delta+}{\text{H}} - \overset{\delta-}{\text{O}}$ or $\overset{+\!\!\!\longrightarrow}{\text{H - O}}$

   You MUST explain <u>how</u> bonds are polar. This is because of the difference in electronegativity between the different atoms e.g. H and O.

2. Consider the shape of the overall molecule; write one of the following statements: Choose ONE of the middle four options (!) but don't mix and match "dipoles" and "centres" and "charge distribution" randomly. Learn a pair of statements you will be able to remember and use.

Molecule is symmetrical	SO	bond dipoles cancel out there is no net dipole the centres of +ve and –ve charge coincide the bond dipoles are arranged symmetrically and cancel out	AND	molecule is therefore NON POLAR OVERALL
Molecule is asymmetrical (not symmetrical)	SO	the bond dipoles do not cancel out the dipoles add to give a net dipole centres of +ve and –ve charge do not coincide the bond dipoles are NOT arranged symmetrically and do not cancel out	AND	molecule is therefore POLAR OVERALL

E.g. The CO_2 molecule contains (two) polar bonds. O is more electronegative than C. $\overset{\delta+}{\text{C}} - \overset{\delta-}{\text{O}}$

The CO_2 molecule is linear. It is **symmetrical** so **the centres of +ve and –ve charge coincide** and the **molecule is therefore non polar overall**.

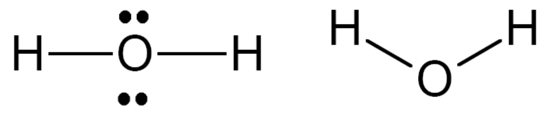
The NH_3 molecule contains (three) polar bonds. N is more electronegative than H. $\overset{\delta-}{\text{N}} - \overset{\delta+}{\text{H}}$

The NH_3 molecule is trigonal pyramidal. It is **asymmetrical** so the **bond dipoles are NOT arranged symmetrically and do not cancel out** and the **molecule is therefore polar overall**.

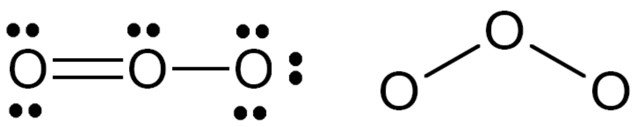
SAMPLE QUESTIONS & ANSWERS

Molecules of water (H_2O) and ozone (O_3) each contain 3 atoms and both the molecules are bent. However, the bond angle in H_2O is significantly smaller than the bond angle in O_3. Using Lewis structures, discuss the reasons for the difference in bond angles of these two molecules.

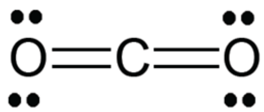
There are 4 regions of electron density around the central O atom which leads to a tetrahedral arrangement. 2 regions are bonding and 2 are non-bonding leading to a V-shaped molecule with a bond angle of approx. 109^o.



There are 3 regions of electron density around the central O tom which leads to a trigonal planar arrangement. 2 regions are bonding and 1 is non-bonding leading to a V-shaped molecule with a bond angle of approx. 120^o



Discuss the reasons for the difference in the polarity of CO_2 and SO_2.



Work out shape of each from their Lewis diagrams.

The C−O bonds of CO_2 are polar due to the different electronegativities of C and O.

However, as there are only 2 regions of electron density about the central C atom, the polar bonds are symmetrically arranged about the C atom / the molecule is a linear shape, and the effect of these polar bonds / bond dipoles cancels out, so that the molecule is nonpolar overall.

The S−O bonds of SO_2 are polar due to the different electronegativities of S and O. There are 3 regions of electron density about the central S atom (which repel into a trigonal planar arrangement). However, the lone pair of electrons on the S atom causes the S−O bonds to occupy a bent or V shape around the central S. Therefore, the effect of these polar bonds / bond dipoles do not cancel out, so that the molecule is polar overall.