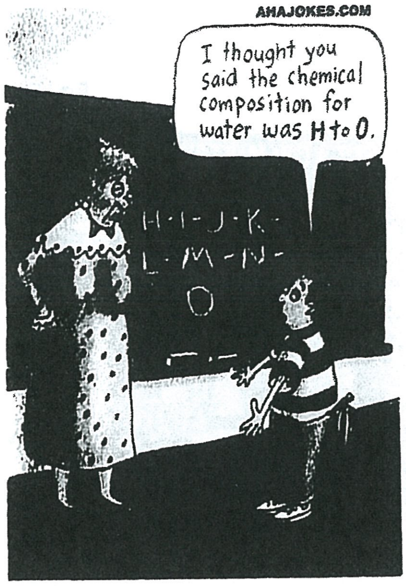


Shapes of Molecules

Using an example, explain what is meant by the term **molecule**.

Carbon dioxide forms molecules which are individual units. The compound is produced when carbon and oxygen atoms are chemically bonded together.

There are **five shapes** of simple molecules that we need to know:

1. **Linear**
2. **Triangular planar**
3. **Tetrahedral**
4. **Pyramidal**
5. **Bent**

These molecular shapes can be explained by the **VSEPR (Valence Shell Electron Pair Repulsion) theory**. According to this theory we assume the following:

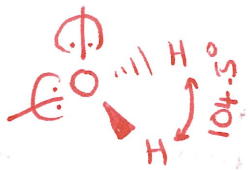
1. All electrons in a molecule are **paired** (either bonded or lone).
2. The pairs of electrons repel each other so that they take up the minimum potential energy positions (ie. as far apart as possible/**largest angle** of separation).

Eg. Water – The bent Molecule

The formula for water is H_20.

There are four pairs of electrons around the central atom. We would expect that, to minimise repulsion, these electrons would be in a tetrahedral arrangement. Experimental evidence shows that this is not the case. The molecule is V shaped or bent with the bond being 104.5°.

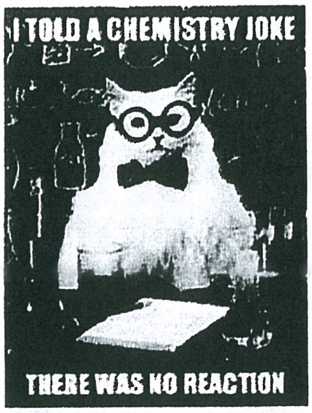
Eg.



The trends seen in other molecules lead us to believe that **lone pairs of electrons required more space than bonding pairs** (ie. as the number of lone pairs increases the bonding pairs are increasingly squeezed together). An explanation for this may be that a bonding pair is shared between two nuclei and the electrons can be close to either nucleus. Therefore, they are confined between the two nuclei. A lone pair is **localised** to only one nucleus, so both electrons are close to that nucleus only.

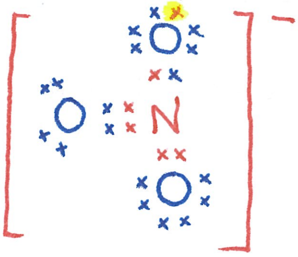
- *CC - use the Valence Shell Electron Pair Repulsion (VSEPR) theory and Lewis structure diagrams to explain and predict and draw the shape of molecules and polyatomic ions (octet only)*

Eg.



The above observations lead us to modify the VSEPR model to include that lone pairs require more room than bonding pairs and tend to compress the angles between the bonding pairs. In substances with multiple bonds the VSEPR model counts multiple bonds as one effective electron pair.

✍ Have a go at determining the shape of the nitrate ion.



Extra electron makes the negative charge.

No lone pair spare, 3 bonds

∴ TRIGONAL PLANAR

This theory can be used to predict the shapes of molecules by following a simple procedure:

1. *Decide which is the central atom in a molecule.*
   - *If you are unsure, pick the least electronegative atom as this atom will be better able to share its electrons with the other atoms in the molecule.*
2. *Count up the valence (outer shell) electrons around the central atom.*
3. *When counting pairs, count each multiple bond as a single effective pair.*
4. *Arrange the electron pairs in the way that minimises repulsion. ie. the electron pairs need to be as far apart as possible.*
5. *Lone pairs require more space than bonding pairs.*
6. *Determine the positions of the atoms from the ways the electron pairs are shared.*
7. *Name the structure.*

✍ There are five shapes you need to know. Draw them below:

LINEAR	**TRIANGULAR PLANAR**	**TETRAHEDRAL**	**PYRAMIDAL**	**BENT**
				

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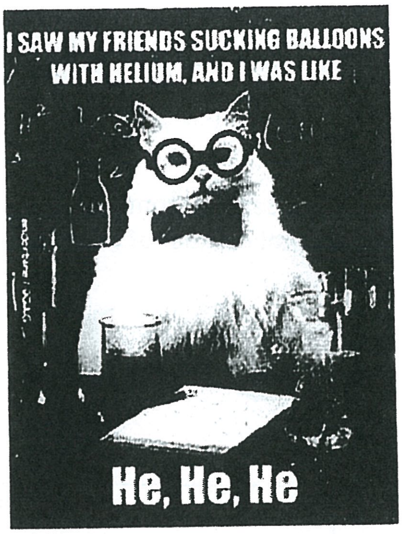
What is meant by the following terms?



Polar bonds:

Non-polar molecules:

A molecule with a 0 net dipole. ie. either the electronegativity of elements oppose one another or are equal in all vector planes (directions).

Polar molecules:

A polar molecule exists when a molecule contains some electronegative elements and the electronegativity is unbalanced due to which elements & the shape of the molecule.

Ideal bond angles:

Molecules are usually arranged in such a way as to provide "enough space" for the bonds. In effect the electrons repel one another evenly.

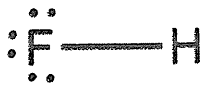
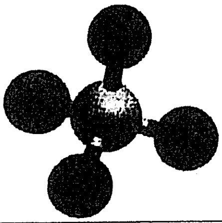
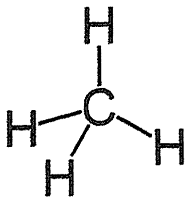
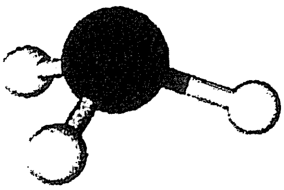
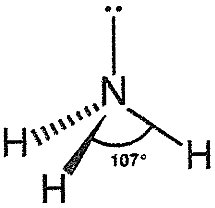
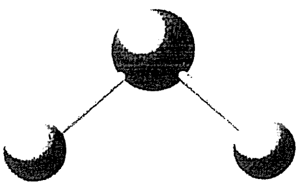
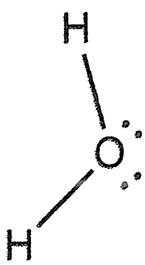
Actual bond angles:

As a result of lone pairs often bond angles are distorted. This is due to "lone pairs" having more repulsion.

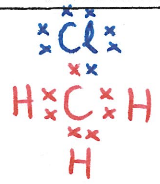
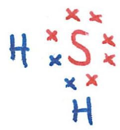
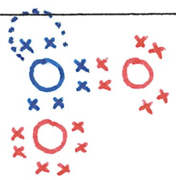
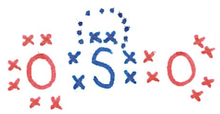
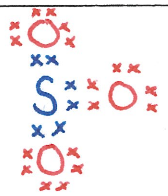
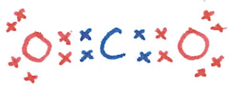
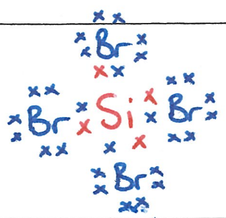
Use the molymods to help you fill out this table.

- *CC - use the Valence Shell Electron Pair Repulsion (VSEPR) theory and Lewis structure diagrams to explain and predict and draw the shape of molecules and polyatomic ions (octet only)*

✋ Use the molymods to help make these molecules now.

Hydrogen fluoride, HF No central atom Total number of valence electrons = 8  	There is only one bond so there cannot be a bond angle. This shape is **linear**.
Methane, CH_4 Central atom is carbon Total number of valence electrons = 8  	There are four electron pairs around the central carbon and because of their mutual repulsion they take up positions at 109.5° to one another. This shape, with four nuclei arranged symmetrically around a central nucleus and with bond angles of 109.5°, is called **tetrahedral**.
Ammonia, NH_3 Central atom is nitrogen Total number of valence electrons = 8  	There are four electron pairs around the central nitrogen and because of their mutual repulsions these take up positions at about 109.5° to one another. The bond angles in ammonia are actually less than 109.5° because the lone pair has a denser concentration of charge and exerts greater repulsion on the bonding pairs than they do each other. This shape, with three nuclei arranged asymmetrically around the central nucleus and with bond angles of 107.3° is called **pyramidal**.
Water, H_2O Central atom is carbon Total number of valence electrons = 8  	There are four electron pairs around the central oxygen and because of their mutual repulsions these take up positions at about 109.5° to one another. The bond angles in water is actually less than 109.5° because the lone pair has a denser concentration of charge and exerts greater repulsion on the bonding pairs than they do each other. This shape, with two nuclei arranged asymmetrically around the central nucleus and with bond angles of 104.5° is called **bent or v-shaped.**

- *CC - use the Valence Shell Electron Pair Repulsion (VSEPR) theory and Lewis structure diagrams to explain and predict and draw the shape of molecules and polyatomic ions (octet only)*

SUBSTANCE	ELECTRON DOT DIAGRAM	SHAPE	POLARITY
Chloromethane CH_3Cl		Tetrahedral	POLAR.
Hydrogen H_2		Linear	NON-POLAR
DiHydrogen disulfide H_2S		Bent	POLAR
Ozone O_3		Bent (116.8°)	Dipole moment 0.53D. However dissolves very easily in CCl_4. It is polar due to electron density However has non-polar properties.
Sulfur dioxide SO_2		Bent (119°)	Dipole moment 1.62D Due to 'bent' nature POLAR
Sulfur trioxide SO_3		Trigonal Planar	NON-POLAR
Carbon dioxide CO_2		Linear	NON-POLAR
Silicon bromide $SiBr_4$		Tetrahedral	NON-POLAR

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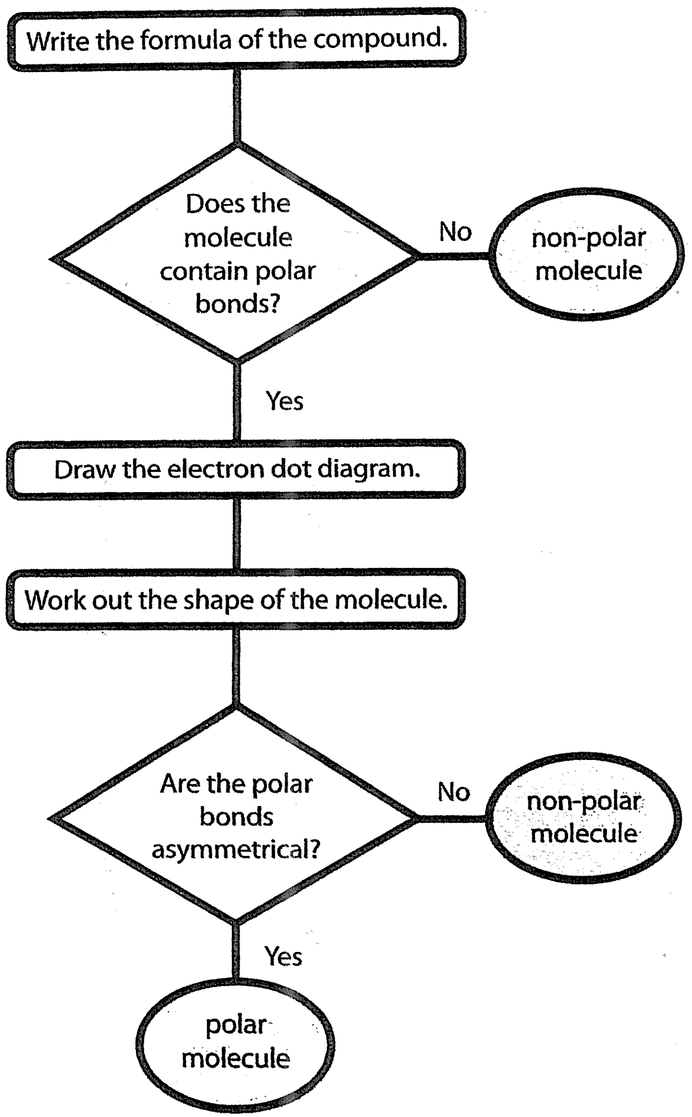
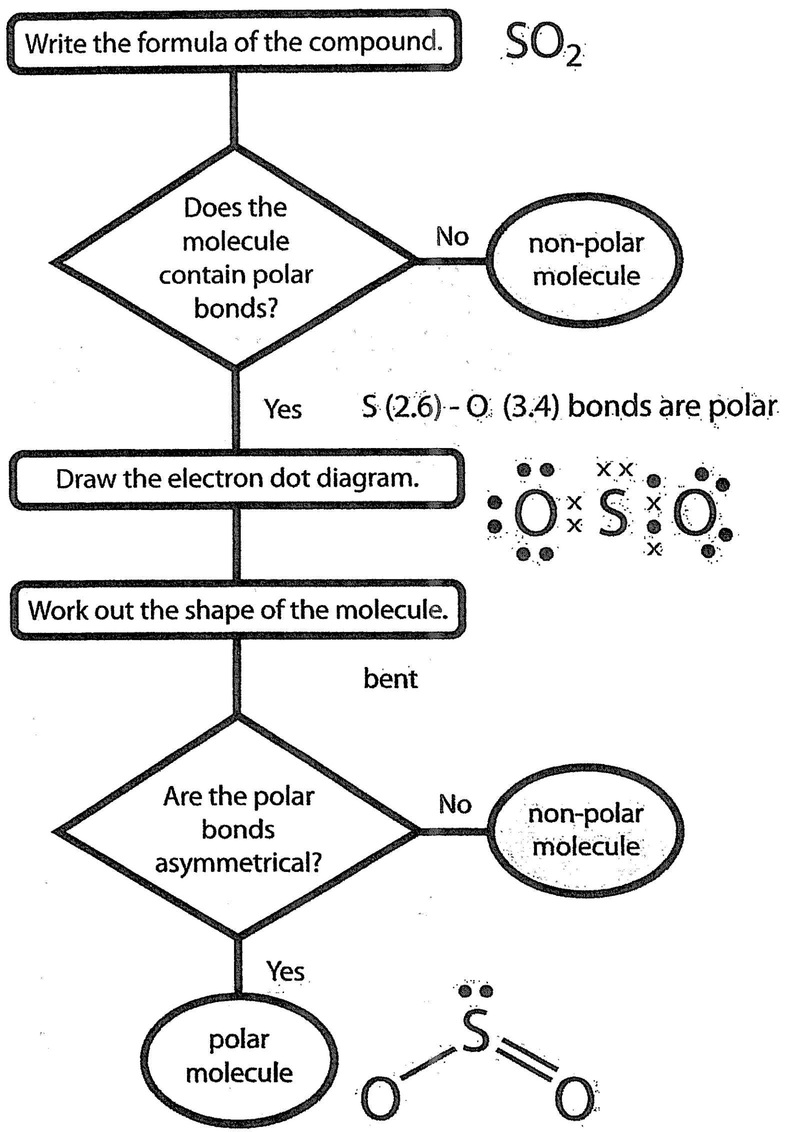
Predicting the polarity of molecules

Use the flow chart to decide whether a molecule is polar or not. An example is given on the next page.



Example: Sulfur dioxide



Therefore sulfur dioxide is a polar molecule.