

### AS 91390

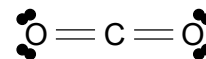
Demonstrate understanding of thermochemical principles and the properties of particles and substances

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 / electron density / electron cloud. E.g. in carbon dioxide (CO<sub>2</sub>) 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°	Cl—Be—Cl	linear
3	Trigonal planar, 120°		2 bond pairs & 1 lone pair = angular (approx 120°)
4	Tetrahedral, 109.5°		4 bond pairs = tetrahedral e.g. NH <sub>4</sub> <sup>+</sup> , CCl <sub>4</sub> 3 bond pairs & 1 lone pair = trigonal pyramidal e.g. NH <sub>3</sub> (approx. 107°)* 2 bond pairs & 2 lone pairs = angular or v-shaped or bent e.g. H <sub>2</sub> O (approx. 105°)**
5	Trigonal bipyramidal, 120° & 90°		4 bond pairs & 1 lone pair = see-saw or unsymmetrical tetrahedron 3 bond pairs & 2 lone pairs = t-shape 2 bond pairs & 3 lone pairs = linear
6	Octahedral, 90°		5 bond pairs & 1 lone pair = square pyramidal 4 bond pairs & 2 lone pairs = square planar E.g. XeF <sub>4</sub>

\*Ammonia: 3 bond pairs 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 bond pairs 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°. However this is not assessed @ L3 and 109° or 109.5° is accepted,

**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:



The actual shape of the molecule does not include the lone pairs even though they are responsible for determining the shape. E.g. don't see water has a tetrahedral shape.

E.g. water has 4 regions of electron density around the O atom but the shape overall is angular or V-shaped or bent.



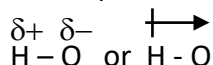
**Examples**

F is different in electronegativity to As: so the As-F bond is polar.  $\delta^+ \delta^-$  As – F  $\delta^+ \delta^-$  The B-F and P-F bonds would also be polar. (F is more electronegative than As, B and P).

AsF <sub>3</sub>		trigonal pyramid / pyramidal	Repulsion of four regions of electron density around As - three bonding, one non-bonding	AsF <sub>3</sub> is polar. The trigonal pyramid molecule asymmetrical. Dipoles of AsF bonds don't cancel out <b>OR</b> Centres of +ve and -ve charge do not coincide <b>OR</b> there is an asymmetric/uneven distribution of charge about central atom.
AsF <sub>5</sub>		trigonal bipyramid / bipyramidal	Repulsion of 5 regions of negative charge around As - all are bonding	AsF <sub>5</sub> is non-polar. The trigonal bipyramid molecule is symmetrical. Polarities of AsF bonds cancel <b>OR</b> centres of +ve and -ve charge coincide
BF <sub>3</sub>		trigonal planar	Repulsion of 3 regions of negative charge around - all are bonding B is electron deficient	BF <sub>3</sub> is non-polar. The trigonal pyramid molecule is symmetrical about the central B atom, so bond dipoles cancel / there is a symmetrical distribution of charge about the central atom.
PF <sub>3</sub>		trigonal pyramid / pyramidal	Repulsion of four regions of negative charge around P - three bonding, one non-bonding	PF <sub>3</sub> 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... H). If yes draw in the dipole over the bonds.



If you don't know which element is the more electronegative but they are different just say that because the elements are different they will have different electronegativities and so the bond will be polar as the bonding electrons will not be equally shared.

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	the bond dipoles cancel out there is no net dipole the centres of +ve and -ve charge coincide there is an even distribution of charge about central atom	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 there is an asymmetric or uneven distribution of charge about central atom	AND	molecule is therefore POLAR OVERALL

E.g.

The CO<sub>2</sub> molecule contains (two) polar bonds. O is more electronegative than C.  $\delta^+ \quad \delta^-$  C - O

The CO<sub>2</sub> 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<sub>3</sub> molecule contains (three) polar bonds. N is more electronegative than H.  $\delta^- \quad \delta^+$  N - H

The NH<sub>3</sub> molecule is trigonal pyramidal. It is **asymmetrical** so the **bond dipoles do not cancel out** and the **molecule is therefore polar overall**.

### SAMPLE ANSWER

Discuss the reasons for the difference in the polarity of SF<sub>4</sub> and SF<sub>6</sub>.

- ◆ Work out shape of each from their Lewis diagrams.
- ◆ SF<sub>4</sub> has 5 regions of negative charge around the S so will be based around a trigonal bipyramid but one region is non-bonding so it has a distorted tetrahedral / see-saw shape. The S-F bonds are polar (S is  $\delta^+$  and F is  $\delta^-$ ) because F is more electronegative than S. Because the molecule is asymmetrical there is an uneven distribution of charge about central atom and the molecule is therefore polar overall.
- ◆ SF<sub>6</sub> has 6 regions of negative charge so will be octahedral shape. Although the S-F bonds are polar, the molecule is symmetrical so the bond dipoles cancel out and the molecule is non polar overall.

