AS90780

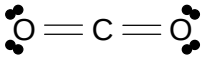
Describe properties of particles and thermochemical principles

Revision notes for "Lewis structures, shapes & polarities"

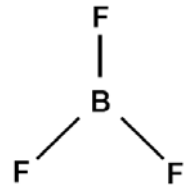
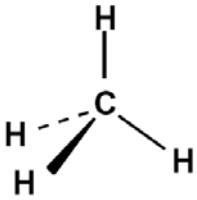
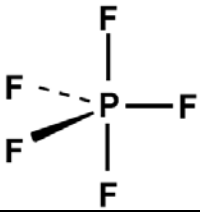
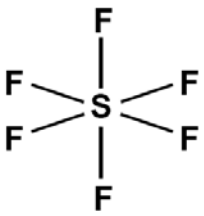
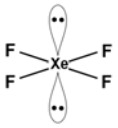
Valence shell electron pair repulsion theory

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 (ie 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. Eg, 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^o	Cl — Be — Cl	linear
3	Trigonal planar, 120^o		2 bond pairs & 1 lone pair = angular (approx 120^o)
4	Tetrahedral, 109.5^o		4 bond pairs = tetrahedral eg NH_4^+, CCl_4 3 bond pairs & 1 lone pair = trigonal pyramidal eg NH_3 (approx 107^o)* 2 bond pairs & 2 lone pairs = angular or v-shaped eg H_2O (approx 105^o)**
5	Trigonal bipyramidal, 120^o & 90^o		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^o		5 bond pairs & 1 lone pair = square pyramidal 4 bond pairs & 2 lone pairs = square planar Eg XeF_4 

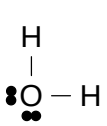
*Ammonia: 3 bond pairs and 1 lone pair (total = 4 pairs) so the shape is based on a tetrahedron. As the lone pair-bond pair repulsions are greater than bond pair-bond pair repulsions the H-N-H bond angle is reduced from 109.5° to 107°. **Water: 2 bond pairs and 2 lone pairs (total = 4 pairs) so the shape is based on a tetrahedron. The lone pair-lone pair repulsion pushes the H-O-H bond angle down further to about 105°.

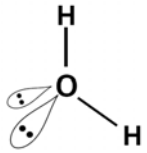
Species with lone pairs. Lone pairs have a greater repulsive force than bonding pairs so their presence affects bond angles. The order of repulsion is:

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

Also the actual shape of the molecule does not include the lone pairs even though they are responsible for determining the shape.

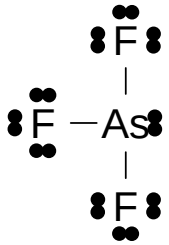
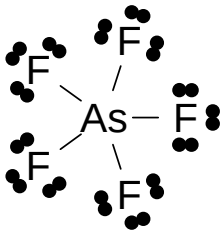
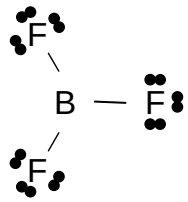
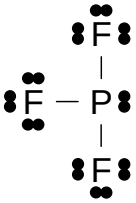
Eg water has 4 electron pairs around the O atom but the shape overall is angular or V-shaped.





Examples

F is different in electronegativity to As: so the As-F bond is polar. $\overset{\delta+}{As} - \overset{\delta-}{F}$ The B-F and P-F bonds would also be polar.

AsF_3		trigonal pyramid	Repulsion of four regions of negative charge around As - three bonding, one non bonding	AsF_3 is polar. The trigonal pyramid molecule asymmetrical. Dipoles of AsF bonds don't cancel out OR Centres of +ve and –ve charge do not coincide OR there is an asymetric/uneven distribution of charge about central atom.
AsF_5		trigonal bipyramid	Repulsion of 5 regions of negative charge around As - all are bonding	AsF_5 is non-polar. The trigonal bipyramid molecule is symmetrical. Polarities of AsF bonds cancel OR centres of +ve and –ve charge coincide
BF_3		trigonal planar	Repulsion of 3 regions of negative charge around - all are bonding B is electron deficient	BF_3 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_3		trigonal pyramid	Repulsion of four regions of negative charge around P - three 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… H). If yes draw in the dipole over the bonds.
   $\overset{\delta+\ \delta-}{H-O}$ or $\overset{\longrightarrow}{H-O}$
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 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

Eg

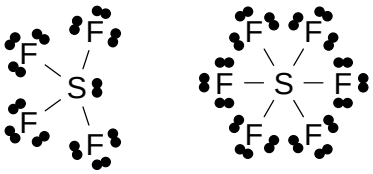
The CO_2 molecule contains (two) polar bonds. O is more electronegative than C. $\overset{\delta+\ \delta-}{C-O}$

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. $\overset{\delta-\ \delta+}{N-H}$

The NH_3 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_4 and SF_6.

- Work out shape of each from their Lewis diagrams.
- SF_4 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's 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_6 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.