

Demonstrate understanding of bonding, structure, properties and energy changes

Level 2 Credits 5

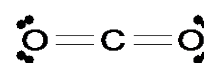
Revision notes for “Lewis structures, shapes & polarities”

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 (CO₂) 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°		3 bond pairs / regions of negative charge – trigonal planar 2 bond pairs & 1 lone pair = angular (approx 120°)
4	Tetrahedral, 109.5°		4 bond pairs = tetrahedral eg NH ₄ ⁺ , CCl ₄ 3 bond pairs & 1 lone pair = trigonal pyramidal eg NH ₃ (approx 107°)* 2 bond pairs & 2 lone pairs = angular or v-shaped eg H ₂ O (approx 105°)**

***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

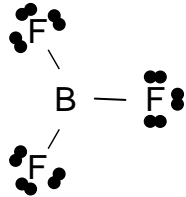
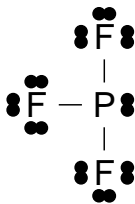
Also the actual shape of the molecule does not include the lone pairs even though they are responsible for determining the shape.

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



Examples

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

BF ₃		trigonal planar	Repulsion of 3 regions of negative charge around - 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....

- Are there polar bonds? (Think F O N/Cl... S...C.. H). If yes draw in the dipole over the bonds.
 $\delta^+ \delta^-$ $\delta^+ \delta^-$
 $\text{H}-\text{O}$ or $\text{H}-\text{O}$
- 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 CO₂ molecule contains (two) polar bonds. O is more electronegative than C. $\delta^+ \delta^-$ $\text{C}-\text{O}$

The CO₂ molecule is linear. It is **symmetrical** so **the centres of +ve and -ve charge coincide** and the **molecule is therefore non polar overall**.

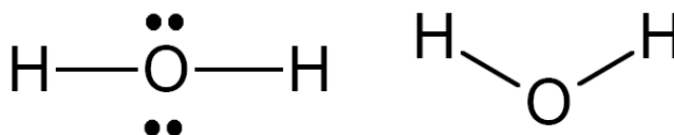
The NH₃ molecule contains (three) polar bonds. N is more electronegative than H. $\delta^- \delta^+$ $\text{N}-\text{H}$

The NH₃ molecule is trigonal pyramidal. It is **asymmetrical** so the **bond dipoles 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 electron repulsions around the central O atom which leads to a tetrahedral shape. This forms a bond angle of 109° .

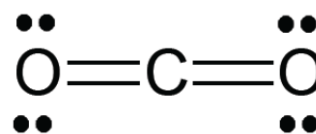


- ◆ There are 3 electron repulsions around the central O atom which leads to a trigonal planar shape. This forms a bond angle of 120°



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 differing electronegativities of C and O. However, as there are only 2 electron repulsions about the central C atom, the polar bonds are symmetrical about the C atom / linear shape, and the effect of these polar bonds / bond dipoles is cancelled, so that the molecule is nonpolar.



- ◆ The S–O bonds of SO_2 are polar due to the differing electronegativities of S and O. There are 3 electron repulsions about the central S atom (trigonal planar), 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 is not cancelled, so that the molecule is polar.

