FACTFILE:
GCE CHEMISTRY
SHAPES OF MOLECULES AND IONS

Structure

Students should be able to:

1.6.1 demonstrate understanding that the shape of a molecule or ion is determined by the repulsion between the electron pairs surrounding a central atom;

1.6.2 use valence shell electron pair repulsion theory to explain the shapes, and bond angles of molecules and ions with up to six outer pairs of electrons around the central atom to include linear, bent, trigonal planar, tetrahedral, pyramidal, octahedral, square planar, trigonal bipyramid, T-shaped;

1.6.3 explain the departure of the bond angles in NH_3 (107°) and H_2O (104.5°) from the predicted tetrahedral (109.5°), in terms of the increasing repulsion between bonding pair-bonding pair, lone pair-bonding pair and lone pair-lone pair electrons;

1.6.4 demonstrate understanding of the difference between polar bonds and polar molecules and be able to use the shape and dipoles present to predict whether or not a given molecule is polar;

The Shapes of molecules

The shape of a molecule or ion is determined by the repulsion between the electron pairs surrounding a central atom. Lone pair–lone pair repulsion is greater than lone pair–bond pair repulsion, which is greater than bond pair–bond pair repulsion. This is known as the valence shell electron pair repulsion theory (VSEPR). As a result of these differences in size of repulsion, the greatest angles in the shape of the molecule will be between lone pairs of electrons. Bond angles between bonded pairs are often reduced because they are pushed together by lone pair repulsion.

A number of steps are taken in order to predict the shape of a molecule or ion:

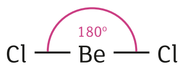
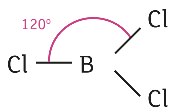
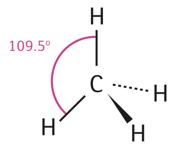
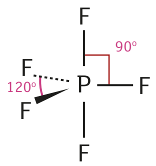
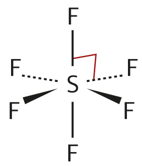
- Write down the number of electrons in the outer shell of the central atom. That will be the same as the Periodic Table group number, except in the case of the noble gases which form compounds, when it will be 8.
- Add one electron for each covalent bond being formed.
- For an ion, adjust the number of electrons based on the charge. For example, if the ion has a 1- charge, add one more electron. For a 1+ charge, deduct an electron.
- You now have the total number of electrons around the central atom — divide this number by two to find the total number of electron pairs.
- Take away the number of bonded atoms to find the number of lone pairs.
- Arrange the electron pairs in order to keep the repulsions between them to a minimum, taking account of the order of repulsion:

  Lone pair-lone pair > lone pair-bonding pair > bonding pair-bonding pair

Molecules with bonding pairs only

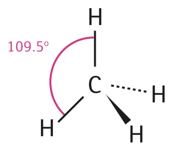
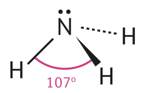
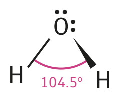
The table below summarises the shapes adopted by molecules with between two and six bonding pairs of electrons around the central atom.

Table needs to be adjusted to create full words in the first column

Bonding pairs	2	3	4	5	6
Example	$BeCl_2$	BCl_3	CH_4	PF_5	SF_6
Name of shape	Linear	Trigonal Planar	Tetrahedral	Trigonal Bipyramidal	Octahedral
Bond angle	180°	120°	109.5°	120°, 90°	90°
Diagram					

Molecules with bonding pairs and lone pairs

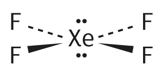
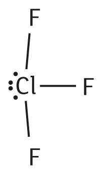
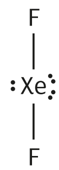
The presence of lone pairs of electrons on the central atom increases repulsion; this results in bonds being forced closer together. For example, methane, CH_4, ammonia, NH_3 and water, H_2O, all have four pairs of electrons around their respective central atoms. However, the four pairs of electrons are different combinations of bonding pairs and lone pairs.

Example	CH_4	NH_3	H_2O
Bonding pairs	4	3	2
Lone pairs	0	1	2
Name of shape	Tetrahedral	Pyramidal	Bent
Bond angle	109.5°	107°	104.5°
Diagram			

As the number of lone pairs of electrons on the central atom increases, the smaller the bond angle due to increased repulsion between the lone pair(s) and the bonding pairs.

Explanation of shape for water:

- electron pairs repel each other
- there are two bonding pairs of electrons and two lone pairs of electrons
- lone pairs of electrons have a greater repulsion
- molecule takes a bent shape to minimise repulsions

Example	XeF_4	ClF_3	XeF_2
Bonding pairs	4	3	2
Lone pairs	2	2	3
Name of shape	Square planar	T-shaped	linear
Bond angle	90°	86°	180°
Diagram			

Examples involving coordinate bonds

When a coordinate bond forms it converts a lone pair of electrons into a bonding pair of electrons.

Ammonium ion, NH_4^+ has a tetrahedral shape, with a bond angle of 109°.

Explanation of shape:

- electron pairs repel each other
- four bonding pairs of electrons repel each other equally
- molecule takes up shape to minimise repulsions

Remember that ammonia (NH_3) is pyramidal (*three* bonding pairs of electrons and one lone pair of electrons), but an ammonium ion is tetrahedral (*four* bonding pairs of electrons).

Molecules with double or triple bonds

A double or a triple bond counts as one bonding pair of electrons when determining shape.

Carbon dioxide, CO_2 has a linear shape with bond angle 180°

Explanation of shape:

- electron pairs repel each other
- two sets of bonding pairs of electrons repel each other equally
- molecule takes a linear shape to minimise repulsions

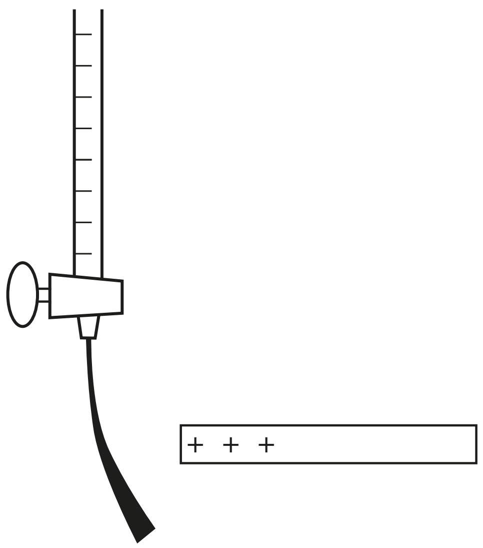
Polar bonds and polar molecules

A polar bond is a covalent bond in which there is unequal sharing of the bonding electrons. This occurs if there is an appreciable difference in electronegativity between the bonding atoms; partial charges, δ^+ and δ^-, appear on the bonding atoms and a dipole is established.

If a molecule contains equally polar bonds arranged *symmetrically*, then the polarities of the bonds cancel each other out and the molecule is non-polar, for example, carbon dioxide, CO_2, is a linear molecule with polar bonds but overall it is non polar.

For example, carbon tetrachloride, CCl_4, contains polar C-Cl bonds. However, as the tetrahedral shape adopted by the molecule is symmetrical, the molecule itself is not considered polar. Water, H_2O, has an unsymmetrical bent shape and so the molecule, which contains polar –OH bonds, is considered polar.

The polarity of molecules can be investigated by bringing a charged rod (positive or negative) to a jet of the flowing liquid; polar molecules will respond to the charged rod, non-polar molecules will not deflect.



Revision Questions

1 In which one of following molecules are the bond angles closest to 107°?

A BF_3
B CH_4
C H_2O
D NH_3

2 Which one of following molecules contains the smallest bond angle?

A $BeCl_2$
B BF_3
C CH_4
D SF_6

3 Phosphorus and nitrogen are in Group V the periodic Table. Nitrogen forms a hydride called ammonia and the hydride of phosphorus is called phosphine, PH_3.

a) (i) Draw a dot and cross diagram to show the bonding in phosphine.

[2]

(ii) Draw and name the shape of a phosphine molecule.

____ [2]

(iii) Explain why a phosphine molecule has the shape you have drawn.

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(iv) Suggest a value for the bond angles in phosphine. Explain your answer.

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.... [2]

4

(i) Draw, name and explain the shape of the SF_6 molecule.

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.... [4]

(ii) Suggest why SF_6 is a non-polar molecule, even through it contains polar bonds.

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