SHAPES OF SIMPLE MOLECULES AND IONS

Electron pair repulsion theory

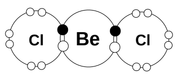
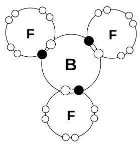
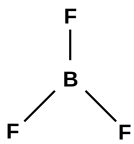
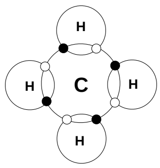
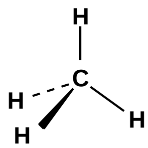
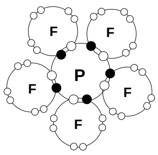
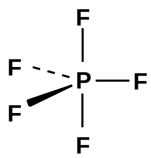
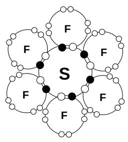
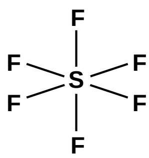
This is used to predict the shapes of simple molecules and ions by considering the repulsions between pairs of electrons (lone pair and bond pair) within the molecule. It states that,

“The shape adopted is the one which keeps repulsive forces to a minimum”

To determine the shape, count up the number of covalent bond pairs and lone pairs around the central atom and work out the shape which keeps the bonds as far apart as possible.

Species without lone pairs

Only bond pair repulsions occur and the basic shapes are regular.

MOLECULE	STRUCTURE		BOND PAIRS	BOND ANGLE(S)	SHAPE
$BeCl_2$			2	180°	Linear
BF_3			3	120°	Trigonal planar
CH_4			4	109.5°	Tetrahedral
PF_5			5	120° 90°	Trigonal bipyramidal
SF_6			6	90°	Octahedral

Species with lone pairs

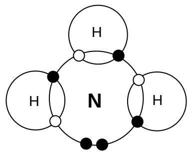
Lone pairs of electrons have a greater repulsive power than bond pairs so their presence will affect the angles of bonds as they push the bond pairs away. The order of repulsive power is ...

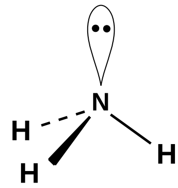
lone pair - lone pair > lone pair - bond pair > bond pair - bond pair

The resulting configuration is based on the number of electron pairs but the actual shape does not include the lone pairs. A water molecule is angular despite the fact that it has 4 electron pairs around oxygen. Two of the pairs are lone pairs and are “invisible”.

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°**.

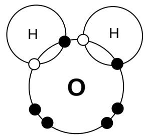
:- shape is **PYRAMIDAL**

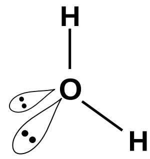




Water **2 bond pairs** and **2 lone pairs** (total = 4 pairs) so the shape is based on a tetrahedron.
The extra lone pair-lone pair repulsion pushes the H-O-H bond angle down further to **104.5°**.

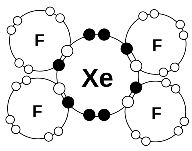
:- shape is **ANGULAR**

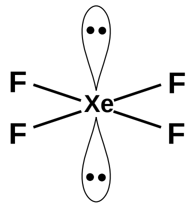




XeF_4 **4 bond pairs** and **2 lone pairs** (total = 6 pairs) so the shape is based on an octahedron.
Lone pairs repel the most so are furthest apart.

:- shape is **SQUARE PLANAR**



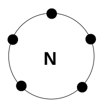
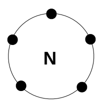
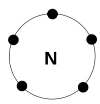
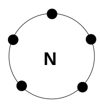
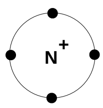
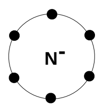
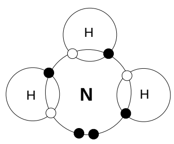
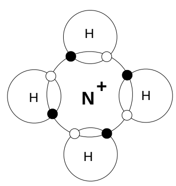
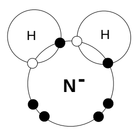


Simple ions

Shapes can be worked out according to the method shown. It allows you to predict the shape but in some cases not the true nature of the bonding.

For ions containing oxygen (e.g. SO_4^{2-}) some bonds are double and some single. In these cases add an electron to an oxygen atom for every -ive charge on the ion. Single bond these oxygens to the central atom and double bond the rest.

e.g. SO_4^{2-}
*Sulphur is the central atom with six electrons in its outer shell. As the ion has a 2- charge, give two of the oxygens an electron each to make them O^- and form a single bond between them and sulphur. The other two oxygens are then double bonded to the sulphur atom. This produces 4 bonds and no lone pairs so the ion is **tetrahedral**..*

	NH_3	NH_4^+	NH_2^-
Draw out the OUTER electronic configuration of the central atom.			
If the species is an ion ... Add one electron for each negative charge or remove one electron for each positive charge			
Pair up the electrons of the central species with those of the atom(s) surrounding it. Count the electron pairs.			
ELECTRON PAIRS	BOND PAIRS 3 LONE PAIRS 1	BOND PAIRS 4 LONE PAIRS 0	BOND PAIRS 2 LONE PAIRS 2
SHAPE	PYRAMIDAL	TETRAHEDRAL	ANGULAR

Q.1 *Determine the shapes of the following molecules and ions.*

a) CCl_4 b) PCl_3 c) AlH_3 d) H_2S e) SO_2 f) SO_3 **
*g) PF_6^- h) PF_4^+ i) AlH_4^- j) BrF_3 k) SO_3^{2-} * l) NO_3^- **

** double bonds are treated as single bonds for repulsion purposes (e.g. CO_2 is linear)*