SHAPES OF SIMPLE MOLECULES AND IONS

Electron pair repulsion theory

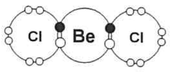
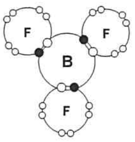
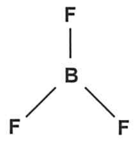
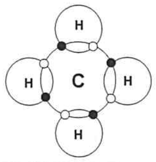
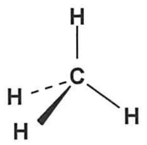
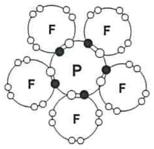
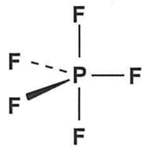
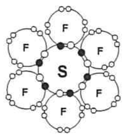
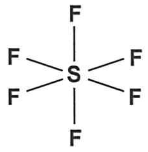
This is used to predict the shapes of simple molecules and ions by considering the repulsions between pairs of electrons (lone pair and bond pair) within the molecule. It states that,

> *"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
$BeCl_2$		Cl—Be—Cl	**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

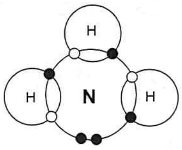
Lone pairs of electrons have a greater repulsive power than bond pairs so their presence will affect the angles of bonds as they push the bond pairs away. The order of repulsive power is ...

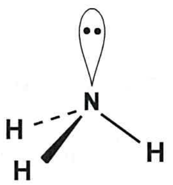
lone pair - lone pair > lone pair - bond pair > bond pair - bond pair

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°**.

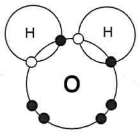
:- shape is **PYRAMIDAL**

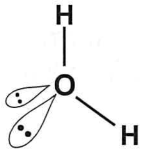




Water **2 bond pairs** and **2 lone pairs** (total = 4 pairs) so the shape is based on a tetrahedron.
The extra lone pair-lone pair repulsion pushes the H-O-H bond angle down further to **104.5°**.

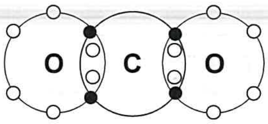
:- shape is **ANGULAR**





Carbon dioxide **2 double bond pairs** and **no lone pairs**
For repulsive purposes, double bonds act like single bonds. The shape will be based on two bond pairs repelling each other.
The bond angle is **180°**.

:- shape is **LINEAR**



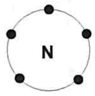
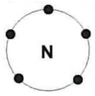
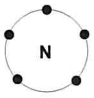
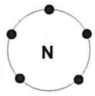
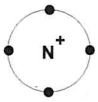
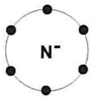
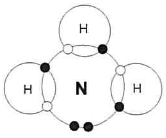
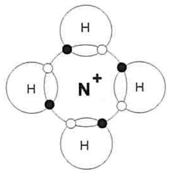
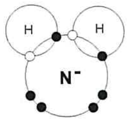
$O=C=O$

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 has 6electrons in its outer shell. As the ion has a 2- charge, give two of the O's an electron each to make them O^- and form a single bond between them and S. The other two O's are then double bonded to the sulphur. 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) PCl_3 b) AlH_3 c) H_2S d) SO_2 e) SO_3 * f) PF_6^- g) AlH_4^-*

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

Worksheet 3.1

Intermolecular bonding

NAME: **CLASS:**

INTRODUCTION

This worksheet focuses on the importance of the polarity of molecules to intermolecular bonding, and the relationship between intermolecular bonding and the boiling points of molecular compounds.

No.	Question	Answer
1	Define the terms: **a** electronegativity **b** permanent dipole **c** polar molecule.	
2	Use the electronegativity values in Table 1.7 to label the atoms in each of the following as δ+ or δ–. **a** HBr **b** PF_3 **c** CO_2 **d** H_2S	
3	Complete the following table.	

Molecule	OCl_2	CCl_4	CH_3Cl	NI_3
Line structure				
Name of shape				
Symmetrical: yes or no?				
Polar or non-polar?				

4	Choose a molecule from the list below to match its description. You may use each molecule from the list only once. • Ammonia (NH_3) • Tetrachloromethane (CCl_4) • Hydrogen bromide (HBr) • Oxygen gas (O_2) • Sulfur dioxide (SO_2) **a** Contains polar bonds, but is non-polar overall **b** Exhibits hydrogen bonds between molecules **c** Has V-shaped molecules **d** Has a permanent dipole	
5	The group 17 elements fluorine (F_2) and iodine (I_2) have very different boiling points of –188°C and 183°C respectively. Explain the significant difference in these boiling points.	
6	The alkane group of hydrocarbons are non-polar molecules. Explain why, at room temperature, methane (CH_4) is a gas while octane (C_8H_{18}) is a liquid.	
7	Hydrogen fluoride (HF) and hydrogen chloride (HCl) are both group 17 hydrides. While HF has a boiling point of 19°C, HCl boils at the considerably lower temperature of –85°C. In terms of the intermolecular bonding present, explain the significant difference in boiling points between these two substances.	
8	The boiling points of HCl, HBr and HI are, in order, –85°C, –67°C and –35°C. **a** Name the two types of intermolecular bonding between these HX molecules. **b** Based on the trend in their boiling points, which type of bonding appears to be the more significant for these molecules?	

Worksheet 3.1: Solutions
Intermolecular bonding

<table>
<tr><th>No.</th><th>Question</th><th>Answer</th></tr>
<tr><td>1</td><td colspan="2">a Electronegativity is a numerical measure of the electron-attracting power of an atom when bonded to another atom.
b A permanent dipole has positive and negative ends separated by a distance. A permanent dipolar bond results from an uneven sharing of electrons between two atoms.
c Polar molecules have an uneven overall distribution of electrons in their bonds (an unsymmetrical molecule with polar bonds).</td></tr>
<tr><td>2</td><td colspan="2">a Hydrogen atom is $\delta+$, bromine atom is $\delta-$.
b Phosphorus atom is $\delta+$, fluorine atoms are $\delta-$.
c Carbon atom is $\delta+$, oxygen atoms are $\delta-$.
d Hydrogen atoms are $\delta+$, sulfur atom is $\delta-$.</td></tr>
<tr><td>3</td><td colspan="2">
<table>
<tr><th>Molecule</th><th>OCl_2</th><th>CCl_4</th><th>CH_3Cl</th><th>NI_3</th></tr>
<tr><td>Line structure</td><td>Similar to SBr_2, page 60</td><td>Similar to SiF_4, page 60</td><td>See Figure 3.14</td><td>Similar to NF_3, page 69</td></tr>
<tr><td>Name of shape</td><td>V-shaped</td><td>Tetrahedral</td><td>Tetrahedral</td><td>Pyramidal</td></tr>
<tr><td>Symmetrical: yes or no?</td><td>No</td><td>Yes</td><td>No</td><td>No</td></tr>
<tr><td>Polar or non-polar?</td><td>Polar</td><td>Non-polar</td><td>Polar</td><td>Polar</td></tr>
</table>
</td></tr>
<tr><td>4</td><td colspan="2">a Tetrachloromethane
b Ammonia
c Sulfur dioxide
d Hydrogen bromide</td></tr>
<tr><td>5</td><td colspan="2">Both of these molecules are non-polar and so exhibit only dispersion forces between molecules. Iodine is a much larger atom and has far more electrons; therefore it has much stronger dispersion forces than F_2 and so has a higher melting point.</td></tr>
<tr><td>6</td><td colspan="2">Both of these hydrocarbon molecules are non-polar and so exhibit only dispersion forces between molecules. Octane is a much larger molecule and has far more electrons than methane; therefore it has much stronger dispersion forces and so has a higher boiling point.</td></tr>
<tr><td>7</td><td colspan="2">HF has a much higher boiling point than HCl because HF exhibits hydrogen bonds between its molecules, rather than the weaker dipole–dipole interactions in HCl. The stronger the intermolecular attractive forces, the higher the boiling point of the substance.</td></tr>
</table>

Intermolecular bonding

8	**a**	Dipole–dipole bonds and dispersion forces
	b	Moving down the group (from Cl to I), electronegativity decreases. The dipole moments will therefore decrease, and so the dipole–dipole bond strength will decrease. This would lead to a decrease in the boiling points. Dispersion forces increase down the group, due to an increasing number of electrons. This would lead to an increase in boiling points. Since boiling points increase, dispersion forces appear to be the more important influence in this case.