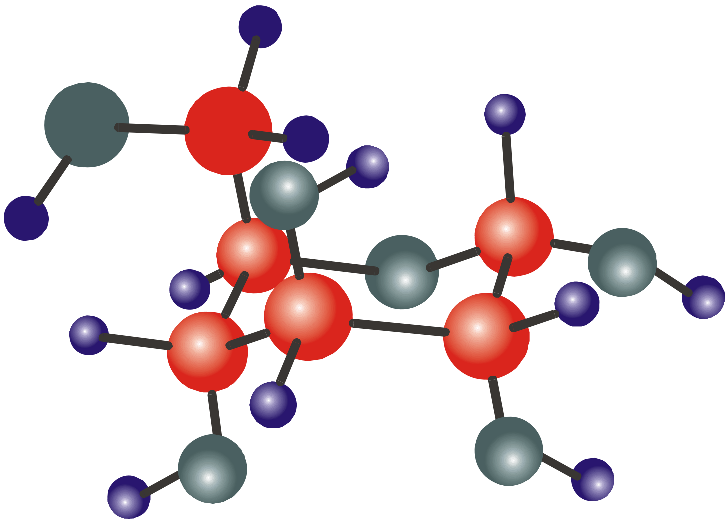
HKDSE Chemistry



Microscopic World II

II. Shape of Simple Molecules

III. Giant Covalent Structures

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Microscopic World II

📖 Shape of simple molecules and polyatomic ions

Since covalent bonds are directional, they have particular spatial arrangement in a molecule, giving molecules a particular shape.

The shape of a molecule can be predicted by the "**Valence Bond Theory**", but there is a simpler method called the "**VSEPR Theory**" or simply "**electron pairs repulsion theory**".

VSEPR stands for **Valence Shell Electron Pairs Repulsion**.

Main points of the **VSEPR theory**

(1) In the **VSEPR Theory**, electron pairs (bond pairs and lone pairs) in the outermost shell of the central atom of a molecule are considered as **electron clouds**. They will **repel each other** and so tend to stay as far apart from each other as possible in order to **minimize the repulsion.**

(2) Thus 2 electron pairs will give a linear arrangement, 3 electrons pairs will give a trigonal planar arrangement, 4 electron pairs will give a tetrahedral arrangement … etc.

(3) The magnitude of repulsion between lone pairs and bond pairs in the central atom are different. In general:

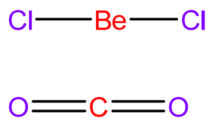
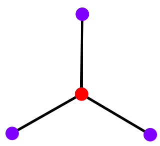
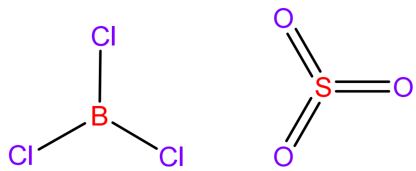
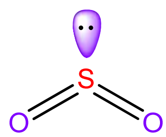
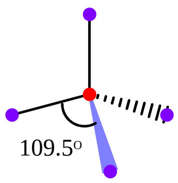
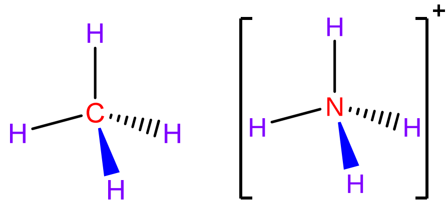
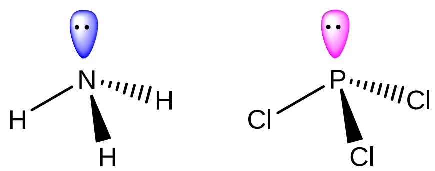
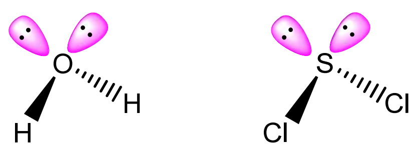
lone pair – lone pair repulsion > **lone pair – bond pair repulsion** > **bond pair – bond pair repulsion**

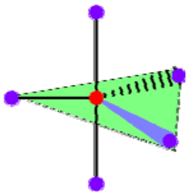
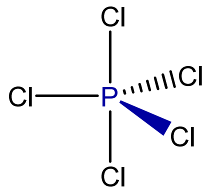
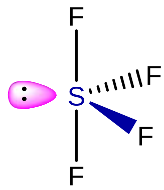
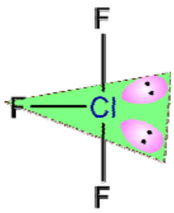
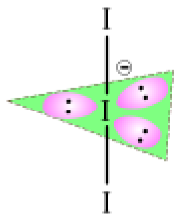
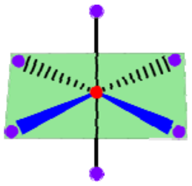
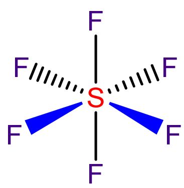
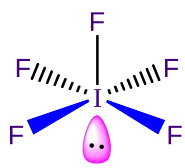
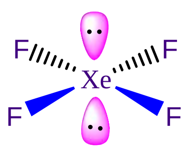
Explanation:
Lone pairs are closer to the nucleus of the central atom than the bond pairs. The reason is: bond pairs are pulled by the two nuclei of the bonded atoms and so are farther away from the nucleus than the lone pairs. So the repulsion between the electron pairs will be in the above order.

Once the spatial arrangement of the electron pairs is worked out by the VSEPR theory, **the shape of the molecule is obtained by joining the positions of the atoms in the molecule**.

Remember: Only the positions of the atoms are considered when talking about molecular shape. So, the shape of the molecule **may not be the same** as the spatial arrangement of the electron pairs.

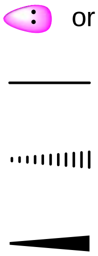
The following table summarizes the spatial arrangements of different number of electron clouds and the shapes of some corresponding molecules.

No. of e^- pairs	Spatial arrangement of e^- pairs	Examples of molecules	No. of lone pairs	Shape of molecule
2	linear 	$BeCl_2$, CO_2	0	Linear 
3	trigonal planar 	BCl_3, SO_3	0	trigonal planar 
		SO_2	1	V-shaped 
4	tetrahedral 	CH_4, NH_4^+	0	tetrahedral 
		NH_3, PCl_3	1	trigonal pyramidal 
		H_2O, H_2S, SCl_2, Cl_2O	2	V-shaped 

5	trigonal bipyramidal 	PCl_5	0	trigonal bipyramidal 
		SF_4	1	distorted tetrahedral 
		ClF_3	2	T-shaped 
		I_3^-	3	linear 
6	octahedral 	SF_6	0	octahedral 
		IF_5	1	(distorted) square pyramidal 
		XeF_4	2	square planar 

Note the following points:

- The following symbols are used when drawing the shape of a molecule:



or : lone pair of electrons

bond on the plane of the paper

bond pointing back into the paper

bond pair pointing out of the paper

- A **multiple bond** or **an unpaired electron** are regarded as a single electron cloud when considering repulsion. The following two examples, **HCN** and **NO_2**, illustrate this point.

Q. Draw the electron diagram of the above two molecules.

HCN	**NO_2**

Thus in $H-C\equiv N$, two electron clouds are repelling each other, giving the molecule a linear shape.

In NO_2, ____________ electron clouds are repelling each other, giving the molecule a _____________ shape.

- For **5 electron pairs**, their arrangement is trigonal bipyramdial. If there are lone pairs, **the lone pairs occupy the equatorial position, not the axial position**.

Why? ____

Thus the shape of SF_4 is **distorted tetrahedral**; ClF_3 is **T-shaped** and I_3^- is **linear shaped**.

- For **6 electron pairs**, their arrangement is octahedral. If there are lone pairs, **the lone pairs occupy the axial position, not the equatorial position**.

  Why? ____

  Thus the shape of IF_5 is **square pyramidal** and that of XeF_4 is **square planar**.

Exercise

For each of the following molecules,

(i) drawn its electron diagram, showing the outermost shell electrons only,

(ii) Predict and draw the shape of the molecule.

	Molecule	Electron diagram	Shape of molecule
(1)	N_2O		
(2)	ICl_2^-		
(3)	SF_2		

	Molecule	Electron diagram	Shape of molecule
(4)	CO_3^{2-}		
(5)	SO_4^{2-}		
(6)	BeH_2		
(7)	$SOCl_2$		
(8)	HOCl		

(9)	O_3		
(10)	NO_3^-		
(11)	NO_2^-		
(12)	IO_3^-		
(13)	IF_4^-		

🕮 Giant Covalent Structures

Whereas simple molecular substances (such as oxygen, water, sugars etc.) are made up of discrete molecules, giant covalent structures like diamond and graphite are not. They consist of a **giant 3-dimentsional network of atoms** that make up the crystal.

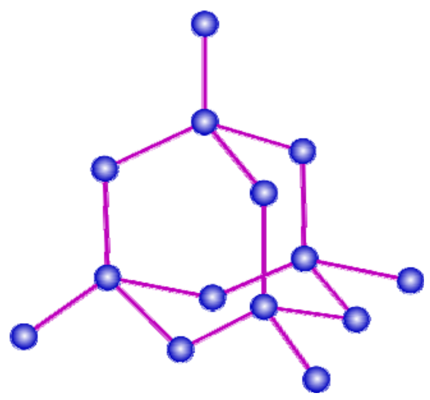
1. Diamond

(a) Bonding and structure of diamond

Electronic configuration of C: 2,4

To attain a stable octet electronic configuration, each carbon atom shares electrons with four other carbon atoms, forming four single covalent bonds that arrange tetrahedrally with each other.

Thus in diamond, **each carbon atom is bonded tetrahedrally to four other carbon atoms**. Such arrangement is repeated in 3 dimensions, forming a giant covalent network of atoms called '**giant covalent structure**'. The following figure shows the structure of diamond.



Note the tetrahedral arrangement of the carbon atoms. In the diagram, not all bonds of carbon are drawn because the figure shows only part of the whole giant covalent structure.

Structure of diamond

How to draw the structure of diamond

Don't try to draw too much of the structure otherwise you may lose marks if you are wrong with the details! The above figure is good enough for exam purpose.

Learn to draw the diagram given above by following the steps below:

未完，待續