Molecular structures (shapes molecules)

This chapter provides the principles used to predict the shapes of molecules of different compounds.

Understanding molecular shapes is very vital because enzyme actions and their inhibitors and activity of many drugs (especially antibiotics) depend exclusively on their molecular structures.

Diatomic molecules, like H_2, Cl_2, O_2, HCl, HF are linear in shape.

However, for poly atomic molecules, i.e., H_2O, CH_4, CO_2, NH_3, etc., the shapes adopted by their molecules depend on: -

1. The total number of electron pairs around the central atom.
2. The number of bonding electrons and lone pairs.

The valence shell electron pair repulsion theory (VSEPR theory)

To predict shapes of poly-atomic molecules, this theory puts into consideration the number of bonding and lone pairs of electrons around the central atoms and the repulsion between the electron pairs.

NB: A lone pair of electrons is found on one atom only; it is under the influence of one nucleus whereas the bonding pair is under the influence of two nuclei. Therefore, the lone pairs of electrons are free compared with the bonding pairs and occupy plenty of space. As lone pairs are closer to the central atom, they cause greater repulsion than the shared (bonding) pairs and the repulsion decreases in this order.

Lone pair - lone pair > lone pair - bond pair > bond pair-bond pair.

Predicting shapes of poly atomic molecules

Using the VSPER theory, we will consider cases in which the central atom is surrounded by a total of two to six electron pairs.

Case 1

Total number of electron pairs around the central atom = 2.
Number of bonding pairs = 2.
Number of lone pairs = 0.

The molecule will be of the form AX_2 and is linear in shape.

X — A — X $\angle XAX = 180^0$

180^0

e.g. $BeCl_2$, BeH_2, CO_2,

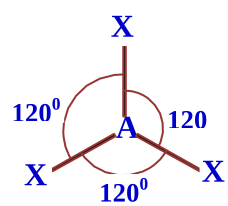
Case 2

Total number of electron pairs around central atom = 3

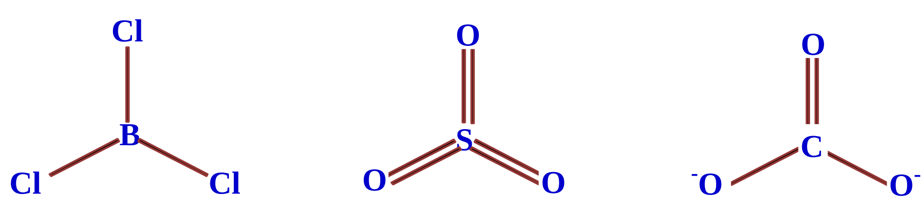
Two possibilities:

a) Total number of electron pairs around the central atom = 3.
Number of bonding pairs = 3.
Number of lone pairs = 0.
The molecule will be of the form AX_3.
Shape: Triangular or trigonal planar, bond angle 120^0.

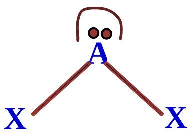
i.e.



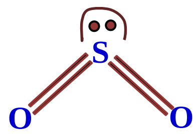
Examples: BCl_3, SO_3, CO_3^{2-}



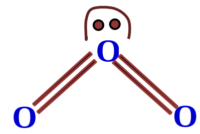
b) Total number of electron pairs around the central atom = 3.
Number of bonding pairs = 2.
Number of lone pairs = 1.
The molecule will be of the form AX_2 but with a lone pair
Shape: Angular /V-shaped.



e.g. SO_2



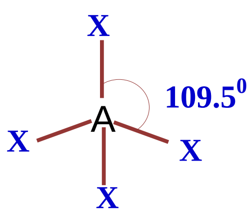
O_3



Case 3

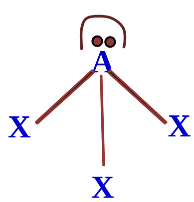
Total number of electron pairs around central atom = 4
Three possibilities:

a) All the four pairs are bonding pairs.
No. of lone pairs = 0
Form of the molecule = AX_4
Shape: Tetrahedral, bonding angle = $109^0.30'$ or 109.5^0



Examples, CH_4, CCl_4, SO_4^{2-}, PO_4^{2-}, MnO_4-, NH_4^+

b) Total number of electron pairs around the central atom = 4.
Number of bonding pairs = 3.
Number of lone pairs = 1.
The molecule will be of the form AX_3 but with a lone pair of electrons.
Shape: Trigonal Pyramidal.

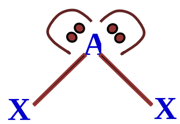


e.g. NH_3, PH_3

The bond angle XÂX, depends on how close to or far from the central atom, the shared pairs of electrons are. The closer they are to the central atom, the stronger the repulsion between them and hence the larger the bond angles, e.g., NH_3 ($\angle$HNH = 107^0), PH_3 ($\angle$HPH = 93^0 20'), AsH_3 ($\angle$HAsH = 91^0 50'), and SbH_3 ($\angle$HSbH = 91^0 50').

The decrease in the bond angle in passing from NH_3 to SbH_3 is due to the decrease in electronegativity of the central atom. The electronegativity of the central atoms decreases in the order: N $\rangle$ P $\rangle$ As $\rangle$ Sb.

c) Total number of electron pairs around the central atom = 4.
Number of bonding pairs = 4.
Number of lone pairs = 2.
The molecule will be of the form AX_2 but with two lone pairs.
Shape: Angular

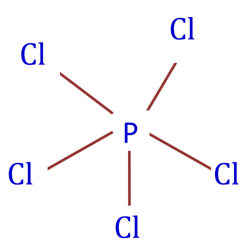


e.g. H_2O, H_2S, H_2Se, H_2Te

Case 4

Total number of electron pairs around central atom = 4

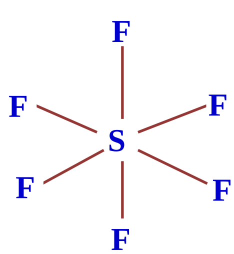
(a)	Total number of electron pairs	= 5
	Number of lone pairs	= 0
	Number of bond pairs	= 5
	Formula	AX_5 e.g. PCl_5
	Shape:	Trigonal bipyramidal



se 5

Total number of electron pairs around central atom = 6

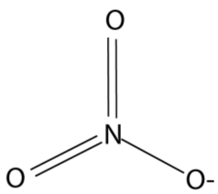
(a)	Total number of electron pairs	= 6
	Number of lone pairs	= 0
	Number of bond pairs	= 6
	Formula	AX_6 e.g. SiF_6, $[Al(H_2O)_6]^{3+}$
	Shape:	octahedral



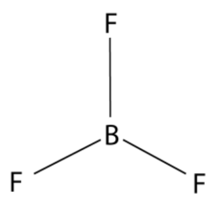
NB: Structures of molecules that do not involve lone pairs on the central atom are highly symmetrical, i.e., linear, triangular, and tetrahedral. This is because such structures involve only one kind of repulsion (bond pair - bond pair) and in such structures there is a constant bond angle, i.e., linear - 180^0, triangular = 120^0 and tetrahedral 109.5^0, triangular bipyramidal, octahedral, etc.

Common shapes in examination

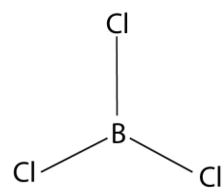
Triangular planar molecule have uniform repulsion among bond pairs; bond angle is 120^0.



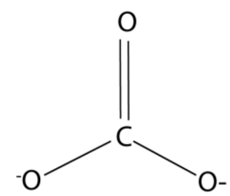
NO_3^-



BF_3

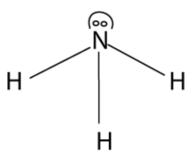


BCl_3

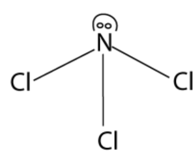


CO_3^{2-}

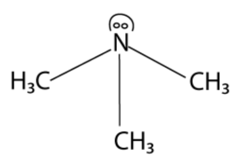
Triangular pyramidal shape: there is strong repulsion between pair and bond pair



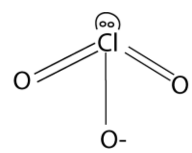
NH_3



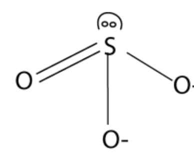
NCl_3



$N(CH_3)_3$

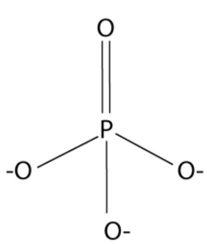


ClO_3^-

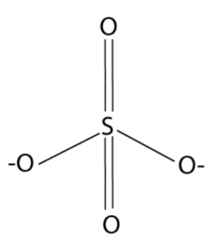


SO_3^{2-}

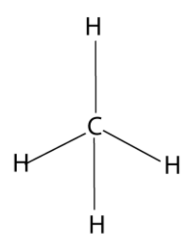
Tetrahedral shape: uniform repulsion among bonding pairs; bond angle 109.5^0



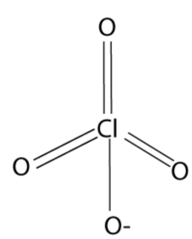
PO_4^{3-}



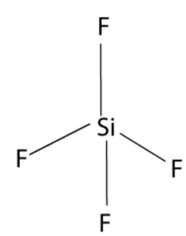
SO_4^{2-}



CH_4

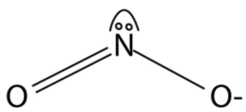


ClO_4^-

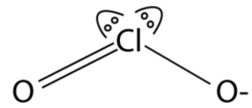


SiF_4

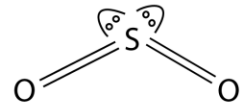
Angular:



NO_2^-



ClO_2^-



SO_2

H_2O

Trial 2

(a) Sketch the shapes of the following molecules. (3marks)

(i) NH_3 (ii) BF_3 (iii) H_2S

(b) Briefly explain why each molecule adapts the shapes in (a) above. (6marks)

(c) Sketch the following molecules, SO_2Cl_2, PO_4^{3-}, ClO_4^-, MnO_4^-, ClF_3, ClO_3^-, ClO_2^-,NO_2^-,NO_3^-, SiF_4, $(CH_3)_3N$, CO_3^{2-}, NCl_3, PCl_5