Std-XI Science

Unit IV:

CHEMICAL BONDING
&
MOLECULAR STRUCTURE

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Chemical bond

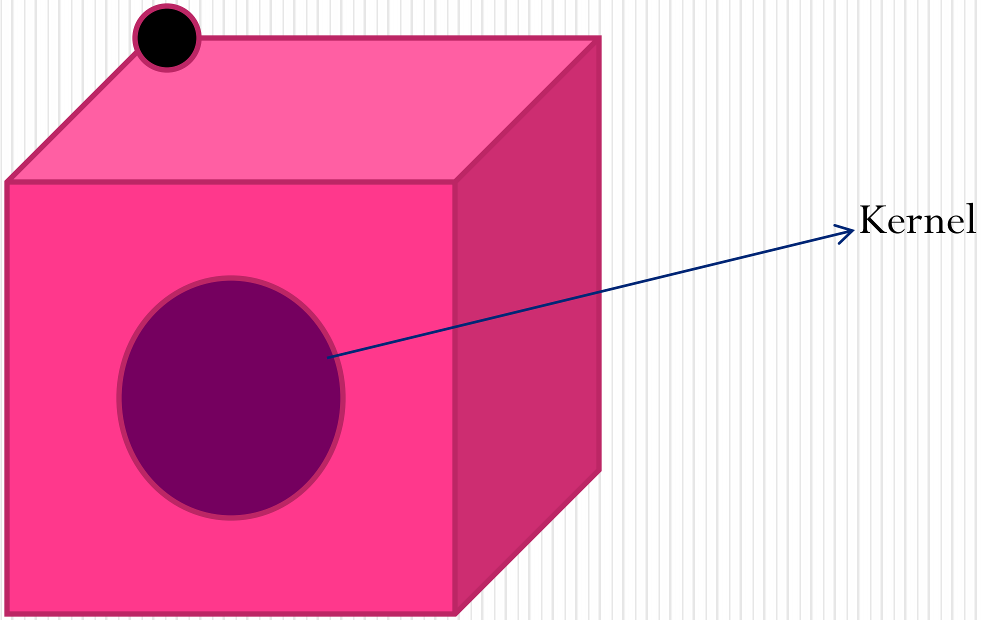
- Matter is made up of one or different type of elements.
- Noble gases elements have independent existence as atoms
- group of atoms is called a molecule
- some force holds these constituent atoms together in the molecules.
- ***The attractive force which holds various constituents (atoms, ions, etc.) together in different chemical species is called a chemical bond.***

- Since the formation of chemical compounds takes place as a result of combination of atoms of various elements in different ways, it raises many questions.
- **Why do atoms combine?**
- **Why are only certain combinations possible?**
- **Why do some atoms combine while certain others do not?**
- **Why do molecules possess definite shapes?**

To answer such questions different theories and concepts have been put forward from time to time.

KÖSSEL-LEWIS APPROACH TO CHEMICAL BONDING

- They were the first to provide some logical explanation of valence which was based on the inertness of noble gases.



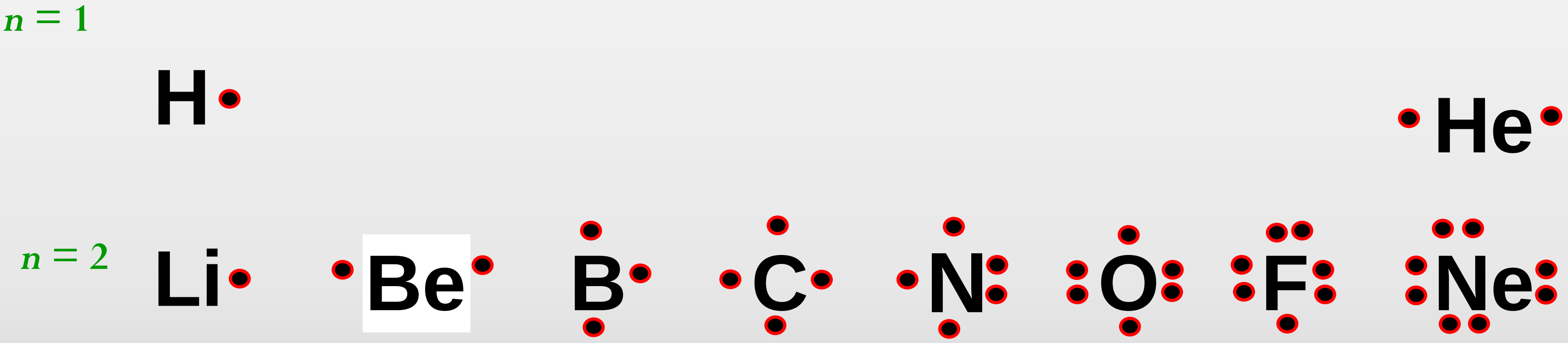
Lewis Symbols:

- G.N. Lewis, an American chemist introduced simple notations to represent valence electrons in an atom.
- These notations are called **Lewis symbols.**

Lewis Symbols

Represent the number of valence electrons as dots

Valence number is the same as the Periodic Table Group Number



Groups	1	2	3	4	5	6	7	8

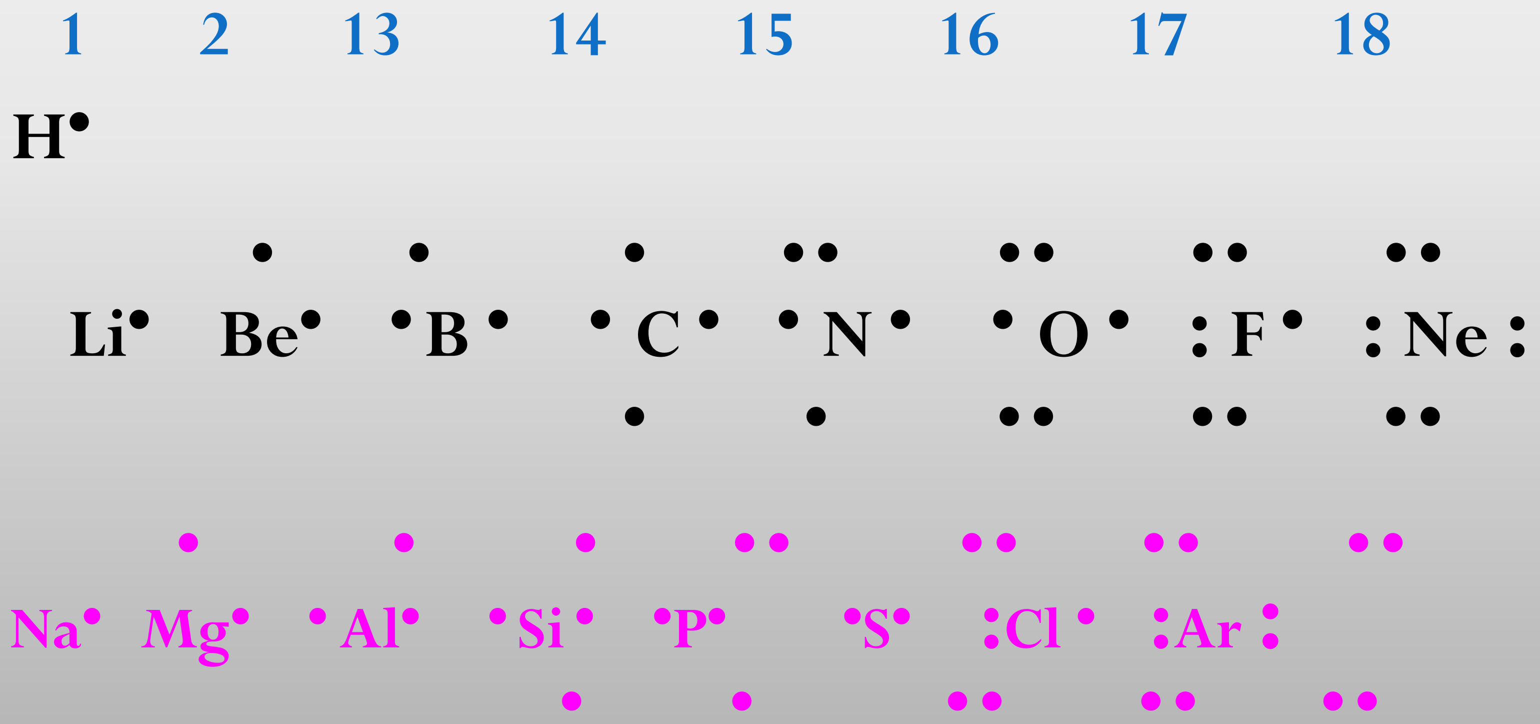
For example,

Na; Is^{2}, 2s^{2}, 2p^{6}, 3s^{1} = [Ne] 3s^{1}

Lewis Structure = Na•

Electron Dot Structures

Symbols of atoms with dots to represent the valence-shell electrons



Significance of Lewis Symbols

- The number of dots around the symbol represents the number of valence electrons.

- This number of valence electrons helps to calculate the common or **group valence of the element.**

- **The** group valence of the elements is generally either equal to the number of dots in Lewis symbols or 8 minus the number of dots or valence electrons.

Kössel’s postulates

- In the periodic table, the highly electronegative halogens and the highly electropositive alkali metals are separated by the noble gases;

- The formation of a negative ion from a halogen atom and a positive ion from an alkali metal atom is associated with the gain and loss of an electron by the respective atoms;

Kössel's postulates

- The negative and positive ions thus formed attain stable noble gas electronic configurations.

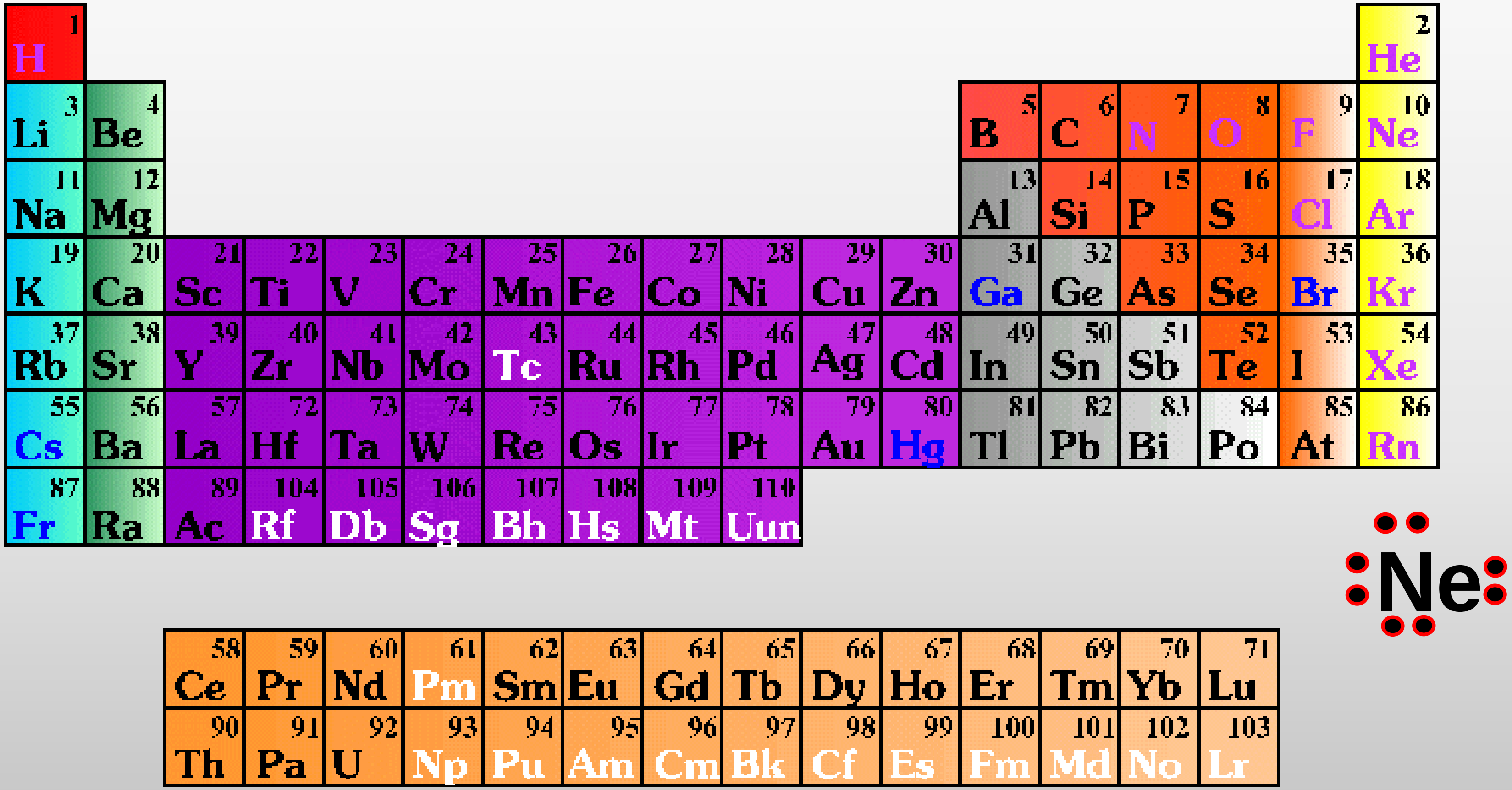
The noble gases (with the exception of helium which has a duplet of electrons) have a particularly stable outer shell configuration of eight (octet) electrons, ns^2np^6.

- The negative and positive ions are stabilized by electrostatic attraction.

Octet Rule

- Kössel and Lewis in 1916 developed an important theory of chemical combination between atoms known as **electronic theory** of **chemical bonding.**
- **According to this,** atoms can combine either by transfer of valence electrons from one atom to another *(gaining or losing)* or by sharing of valence electrons in order to have an octet in their valence shells.
- This is known as **octet rule.**

Elements want to achieve the stable electron configuration of the nearest noble gas



	1 H																	2 He
n = 2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
n = 3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
	87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Uun								
				58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
				90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

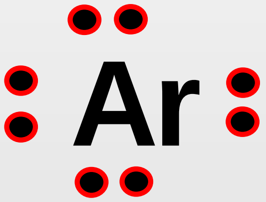
Atoms tend to gain, lose or share electrons until they are surrounded by 8 electrons

Octet Rule

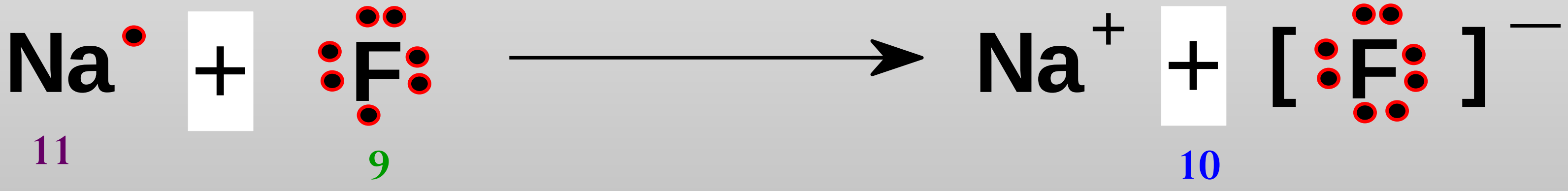
Nobel Gas Has a Stable Electron Configuration

Ne; $1s^2, 2s^2, 2p^6$

Ar; $[Ne]\ 3s^2, 3p^6$

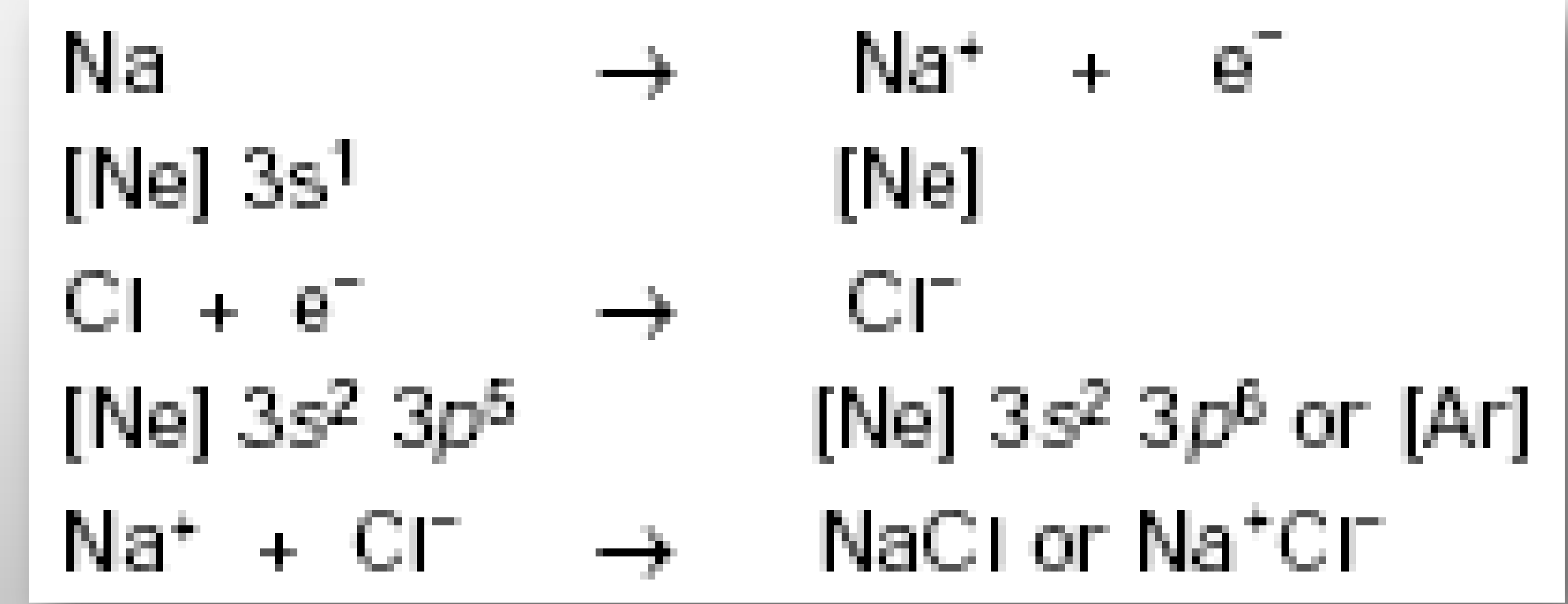


Example



Electronic *configuration* of Neon achieved in both cases

For example, the formation of NaCl from sodium and chlorine, according to the above scheme, can be explained as:



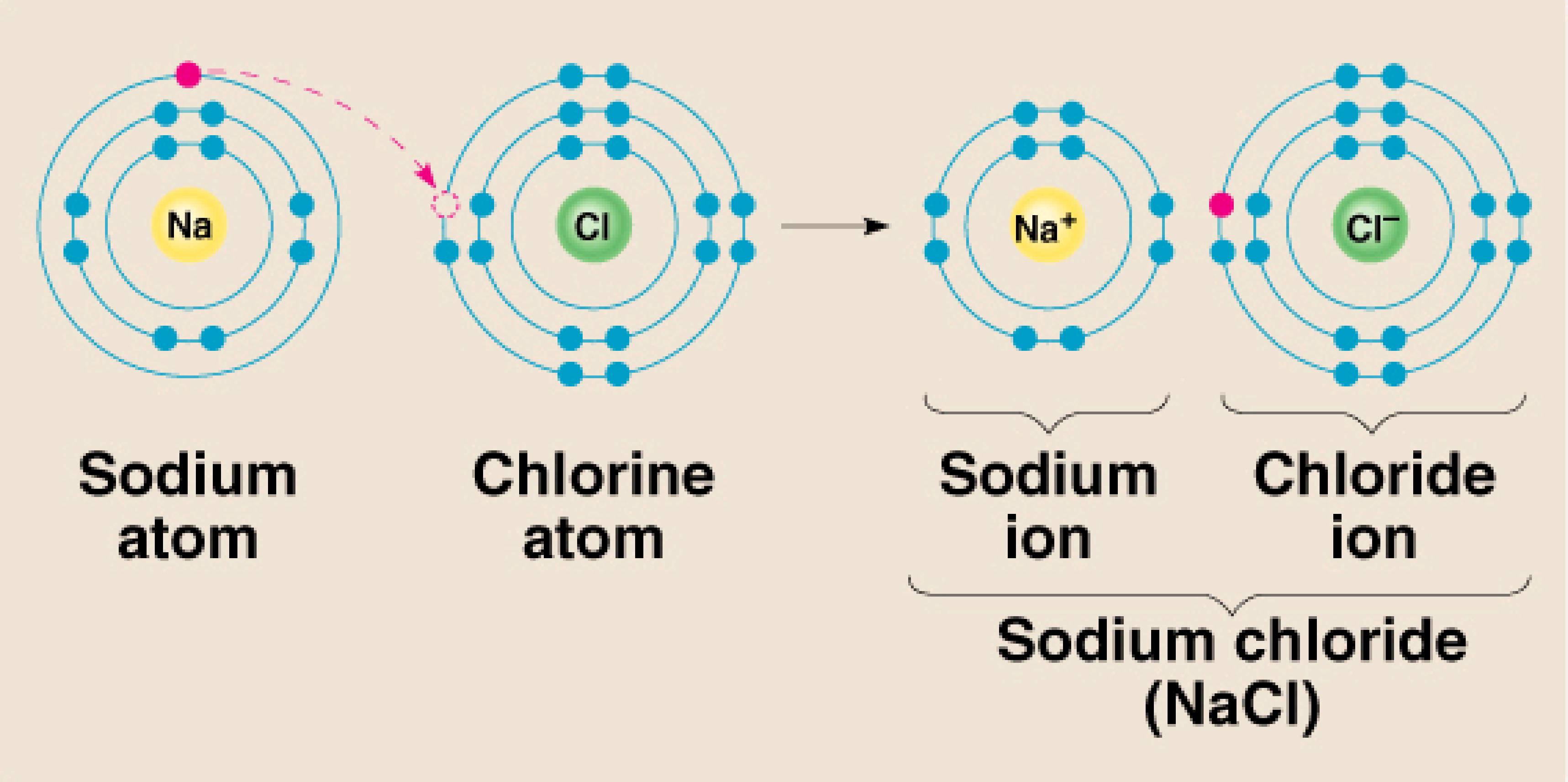
$$\mathrm{Na} \rightarrow \mathrm{Na}^{+} + e^{-}$$

$$[\mathrm{Ne}]\ 3s^{1} \qquad [\mathrm{Ne}]$$

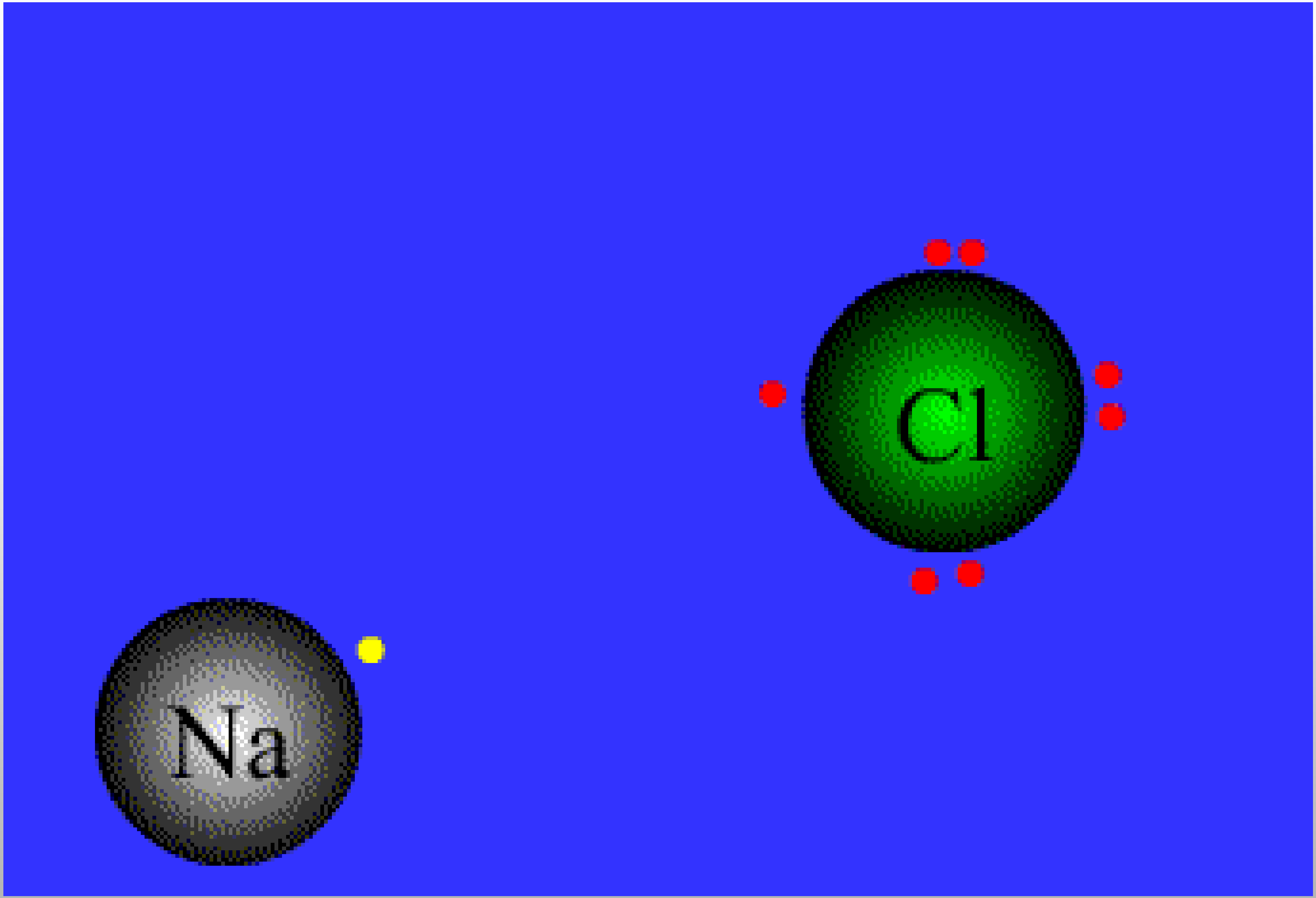
$$\mathrm{Cl} + e^{-} \rightarrow \mathrm{Cl}^{-}$$

$$[\mathrm{Ne}]\ 3s^{2}\ 3p^{5} \qquad [\mathrm{Ne}]\ 3s^{2}\ 3p^{6} \text{ or } [\mathrm{Ar}]$$

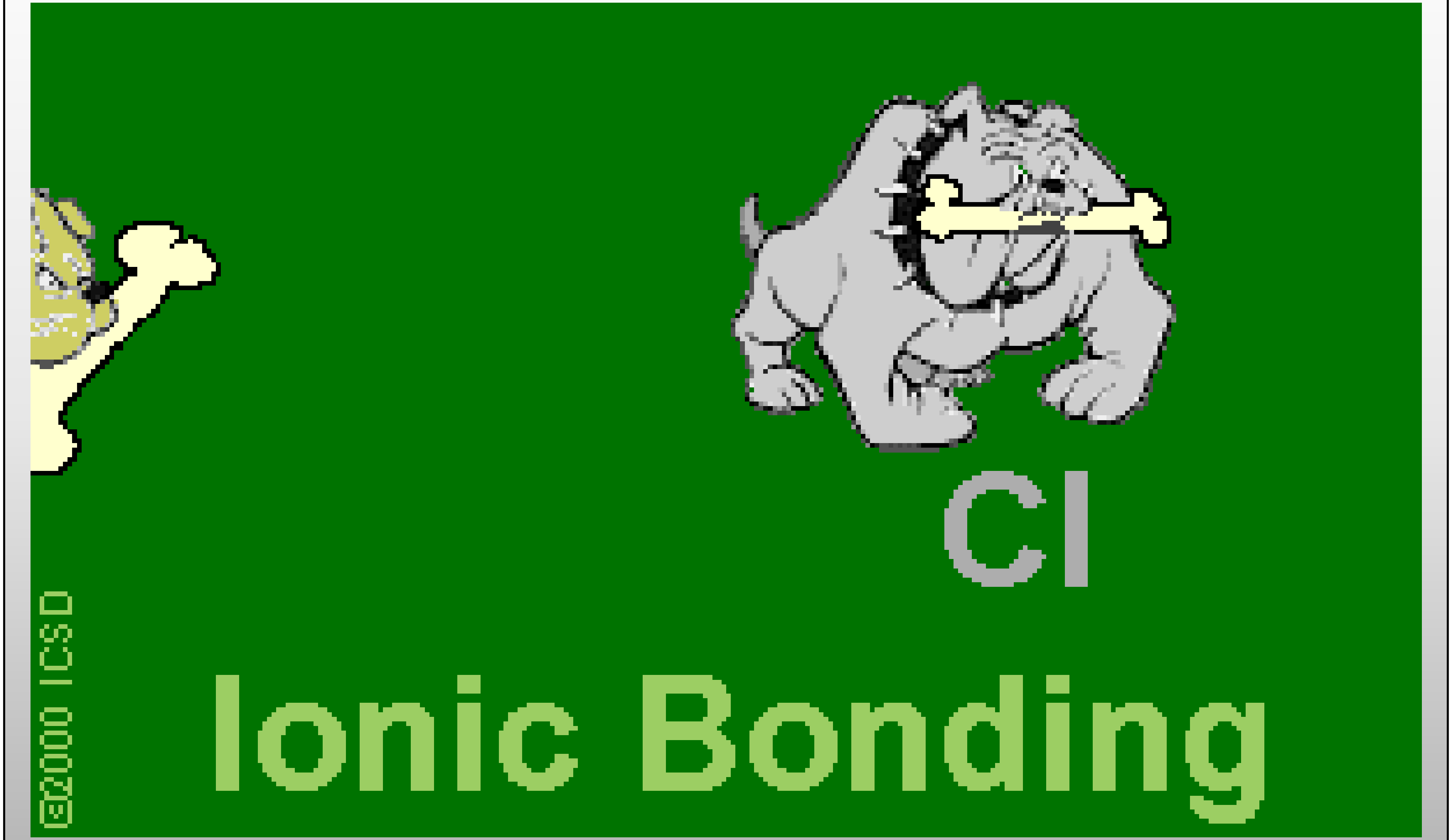
$$\mathrm{Na}^{+} + \mathrm{Cl}^{-} \rightarrow \mathrm{NaCl} \text{ or } \mathrm{Na}^{+}\mathrm{Cl}^{-}$$



1) Ionic bond – electron from Na is transferred to Cl, this causes a charge imbalance in each atom. The Na becomes (Na^+) and the Cl becomes (Cl^-), charged particles or ions.


Cl
Na

Ionic Bonds: One Big Greedy Thief Dog!



Ionic Bond

- Between atoms of metals and nonmetals with very different electronegativity
- Bond formed by transfer of electrons
- Produce charged ions all states. Conductors and have high melting point.
- Examples; $NaCl$, $CaCl_2$, K_2O

Electrovalent bond

- **The bond formed, as a result of the electrostatic attraction between the positive and negative ions was termed as the electrovalent bond.**

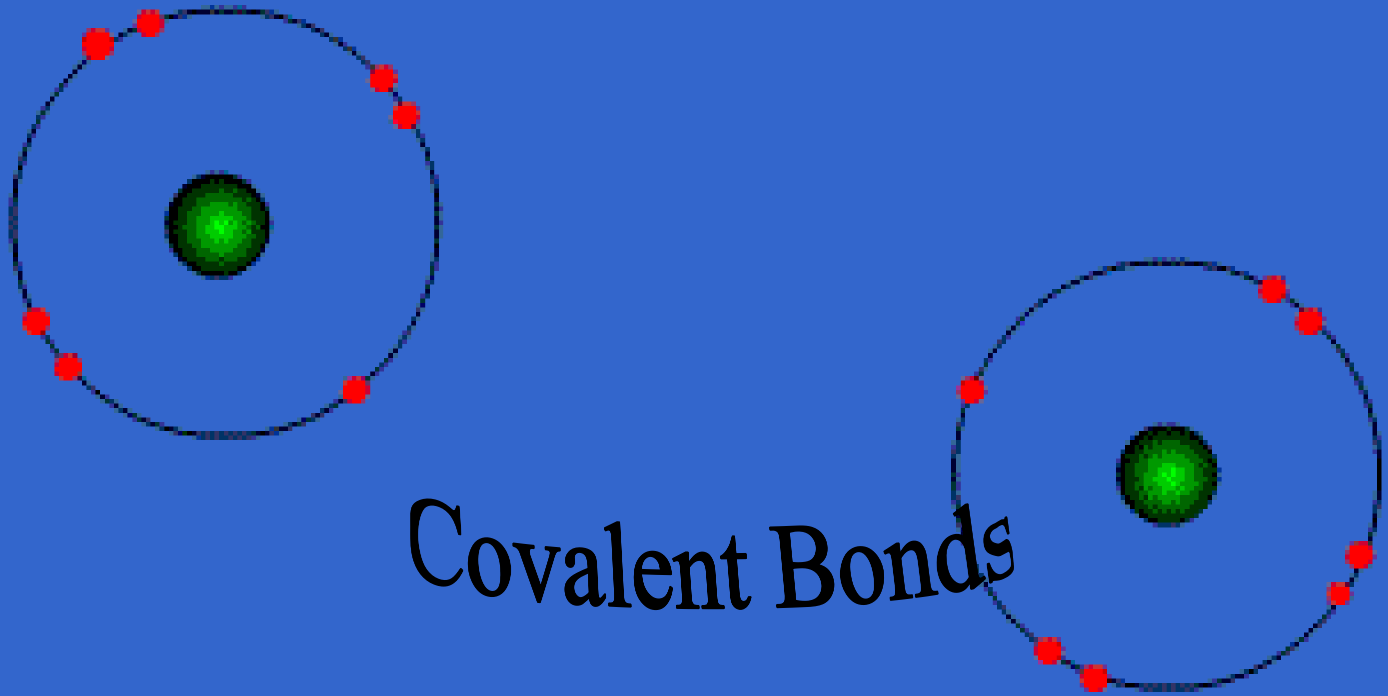
- **The electrovalence is thus equal to the number of unit charge(s) on the ion.**

- **Thus, calcium is** assigned a positive electrovalence of two, while chlorine a negative electrovalence of one.

Covalent Bond

- Between nonmetallic elements of similar electronegativity.
- Formed by sharing electron pairs
- Stable non-ionizing particles, they are not conductors at any state
- Examples; O_2, CO_2, C_2H_6, H_2O, SiC

Covalent Bonds



COVALENT BOND

bond formed by the *sharing* of electrons

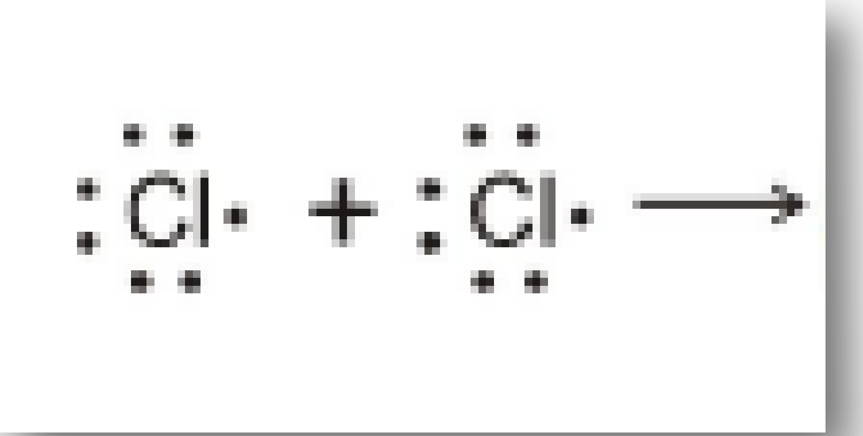
Bonds in all the polyatomic ions and diatomics are all covalent bonds

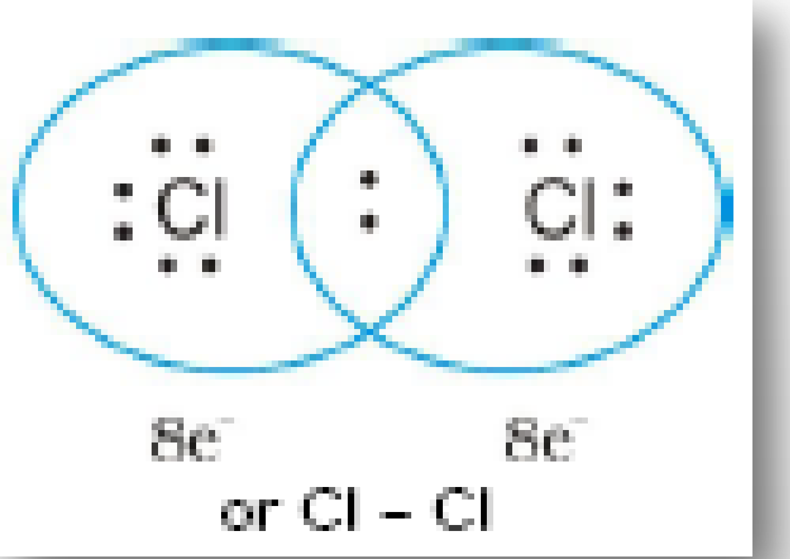
Covalent Bond in Cl_2 molecule

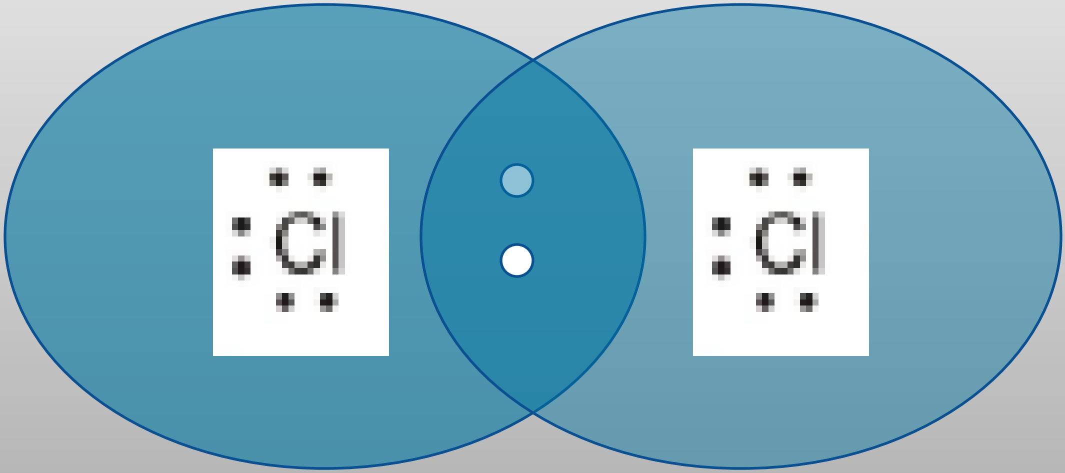
- The formation of the Cl_2 molecule can be understood in terms of the sharing of a pair of electrons between the two chlorine atoms, each chlorine atom contributing one electron to the shared pair.

- In the process both chlorine atoms attain the outer shell octet of the nearest noble gas (i.e., argon).

Covalent bond between two Cl atoms

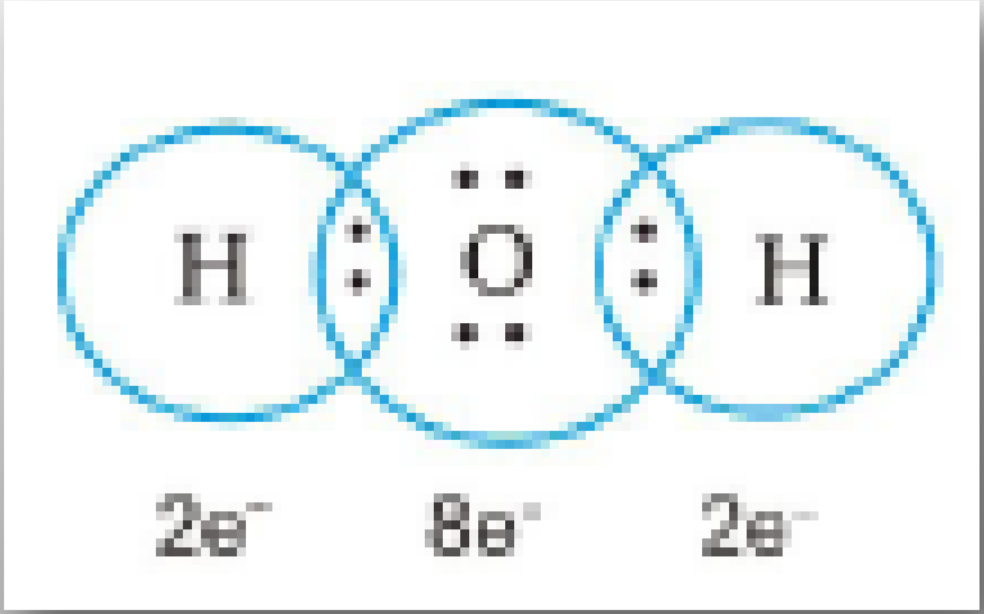




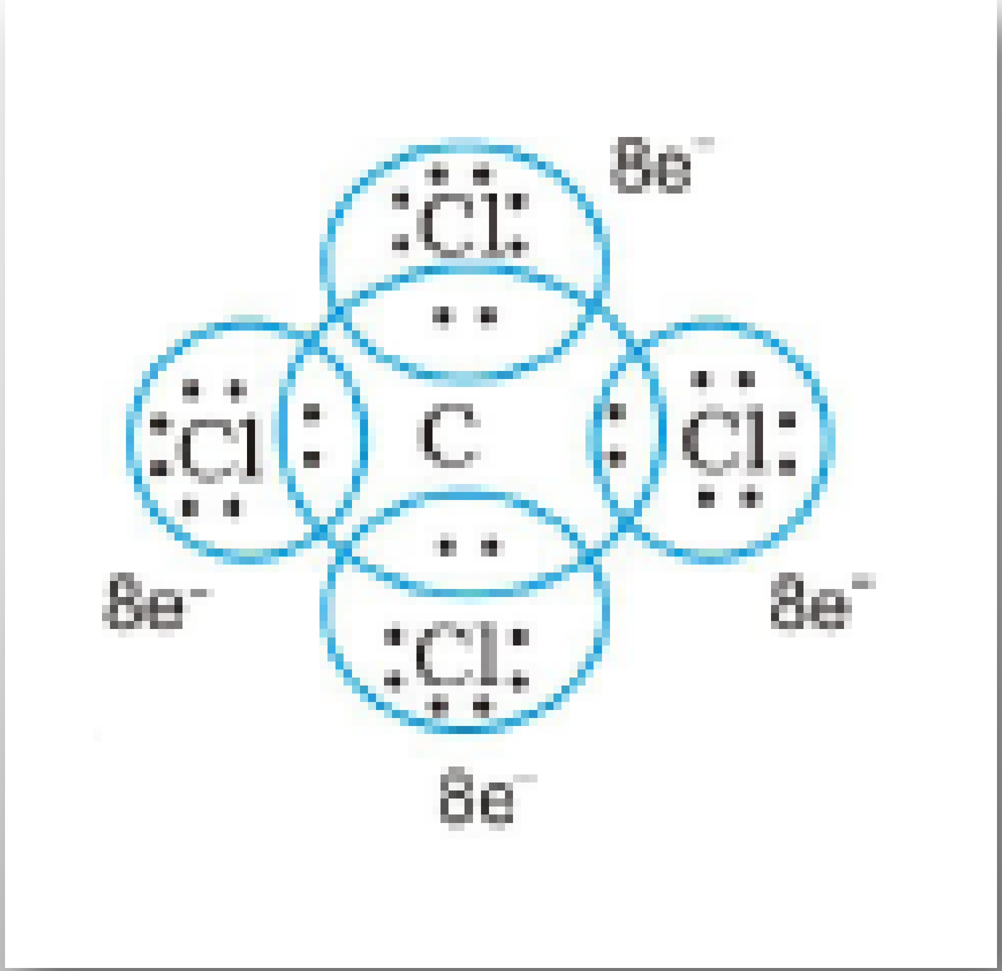


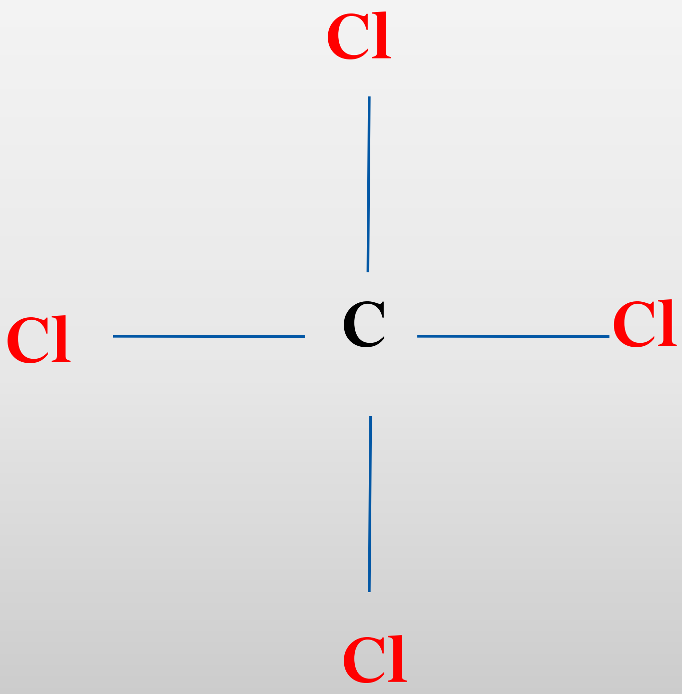
Lewis dot structures

- **The dots represent electrons.**
- **Such structures are referred to as Lewis dot structures.**



Lewis dot structure for CCl_4



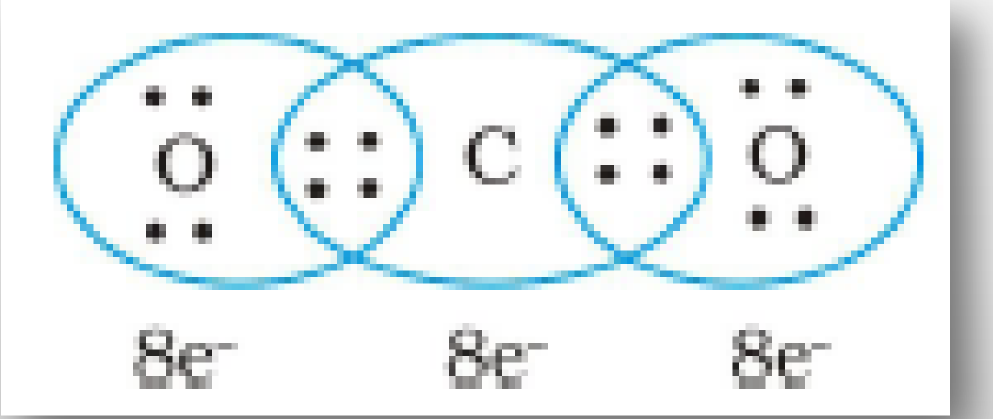

Cl

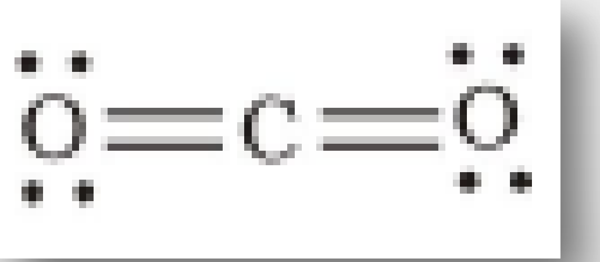
Cl C Cl

Cl

Thus, when two atoms share one electron pair they are said to be joined by a single covalent bond.

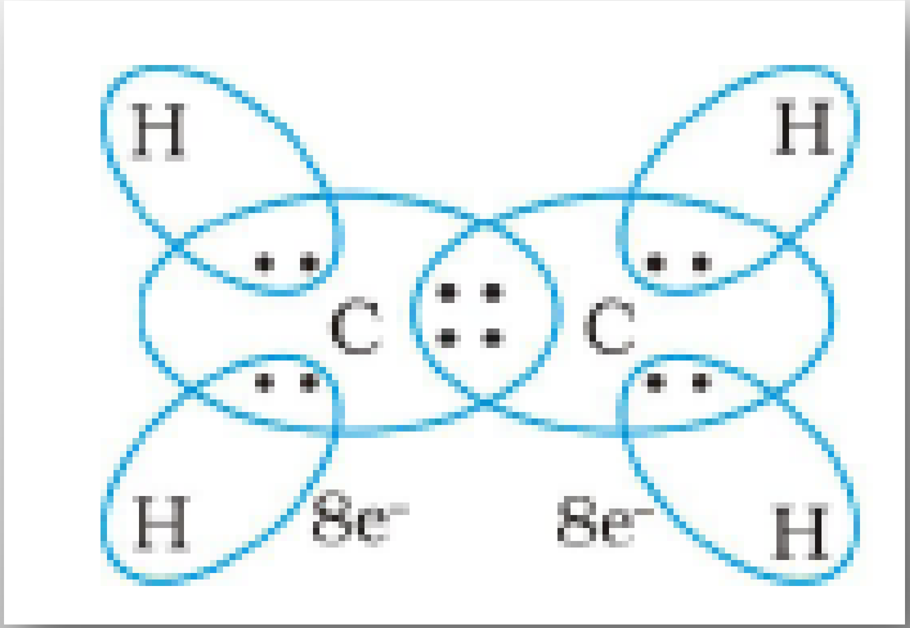
Double bond

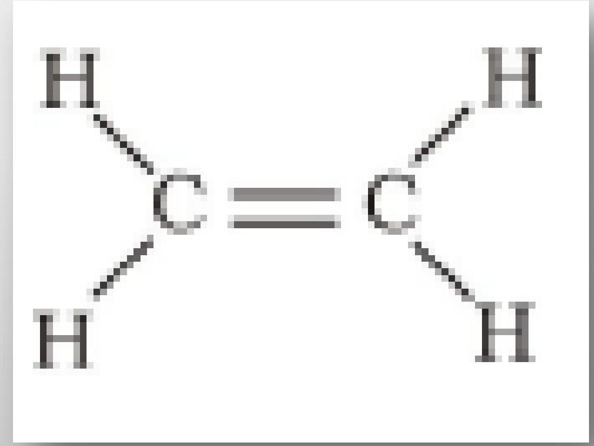




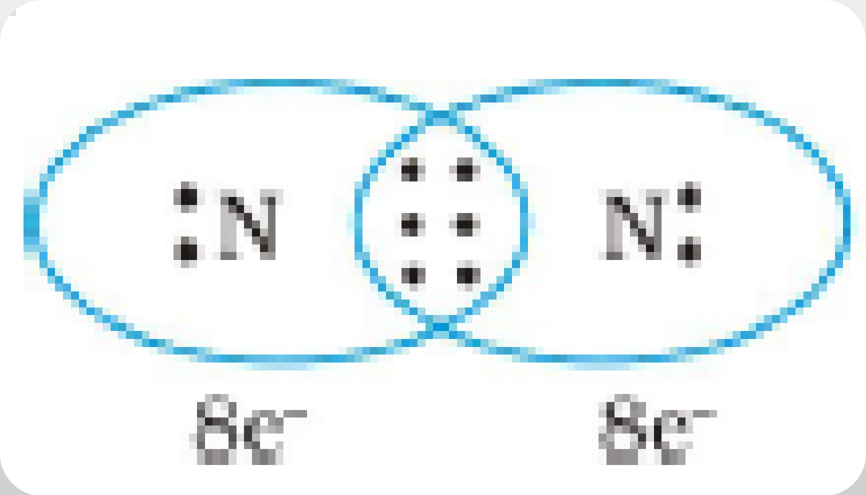
Double bonds in CO_2 molecule

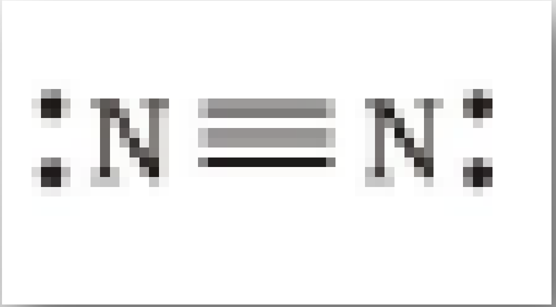
C_2H_4 molecule



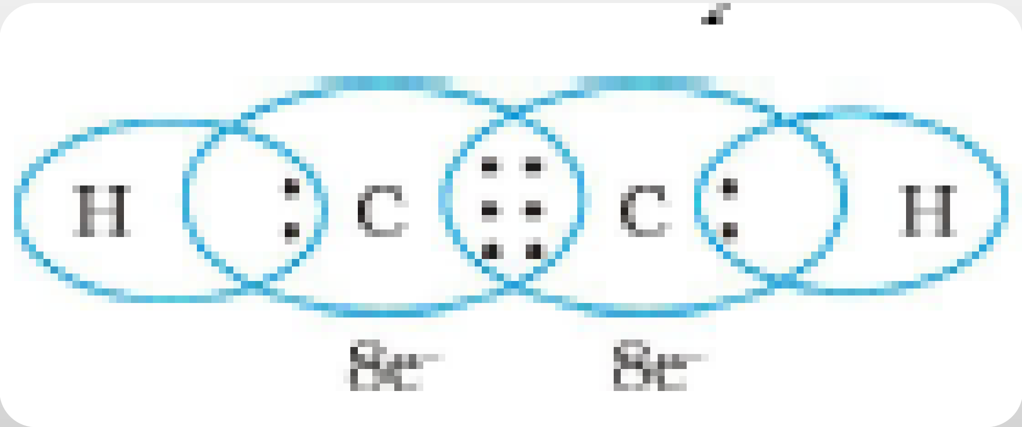


Triple bond in N_2 molecule



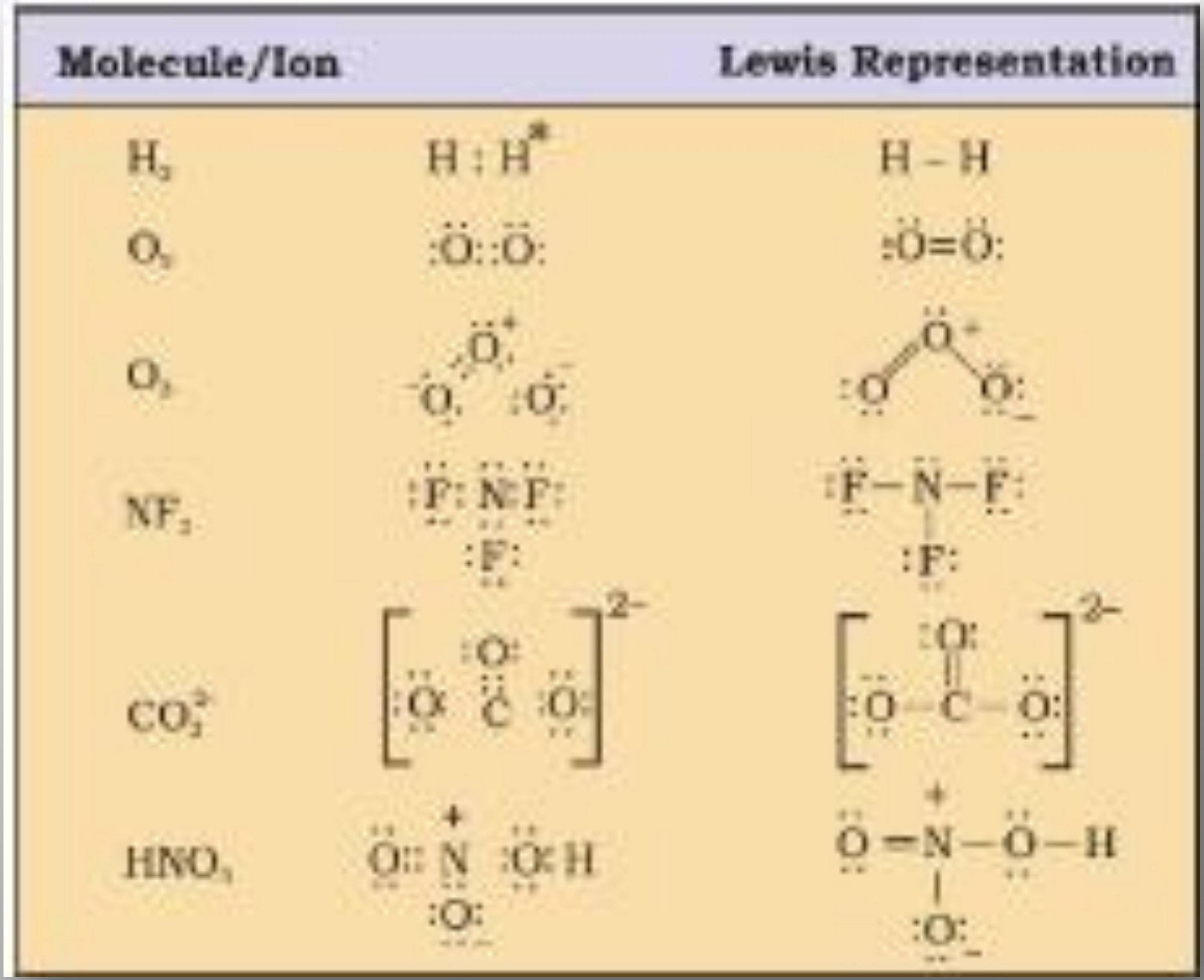


Ethyne Molecule



$H-C\equiv C-H$

The Lewis Representation of Some Molecules



Molecule/Ion		Lewis Representation
H_2	H : H*	H - H
O_2	:Ö::Ö:	:Ö=Ö:
O_3		
NF_3		
CO_3^{2-}		
HNO_3		

Limitations of the Octet Rule

There are three types of exceptions to the octet rule.

1. *The incomplete octet of the central atom*

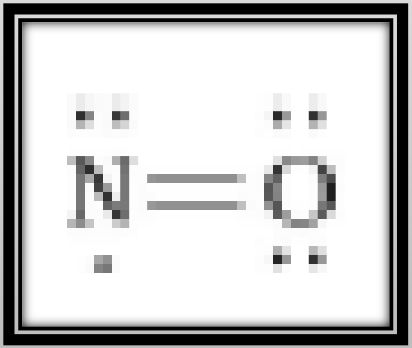
Examples are LiCl, BeH_2 and BCl_3.

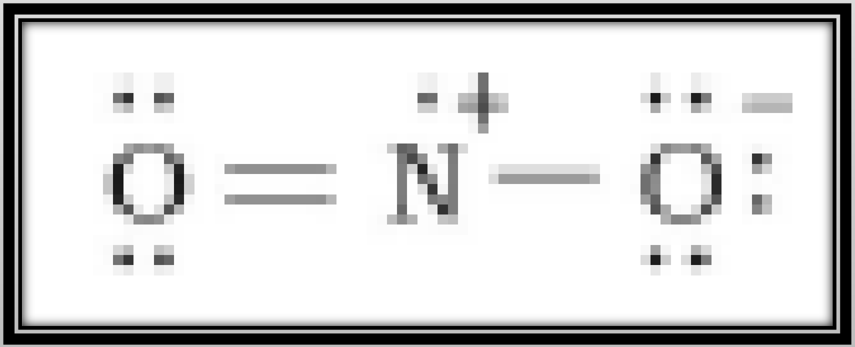
Li, Be and B have 1,2 and 3 valence electrons only.
Some other such compounds are $AlCl_3$ and BF_3.

Limitations of the Octet Rule

2. *Odd-electron molecules*

- In molecules with an odd number of electrons like nitric oxide, NO and nitrogen dioxide, NO_2, the octet rule is not satisfied for all the atoms





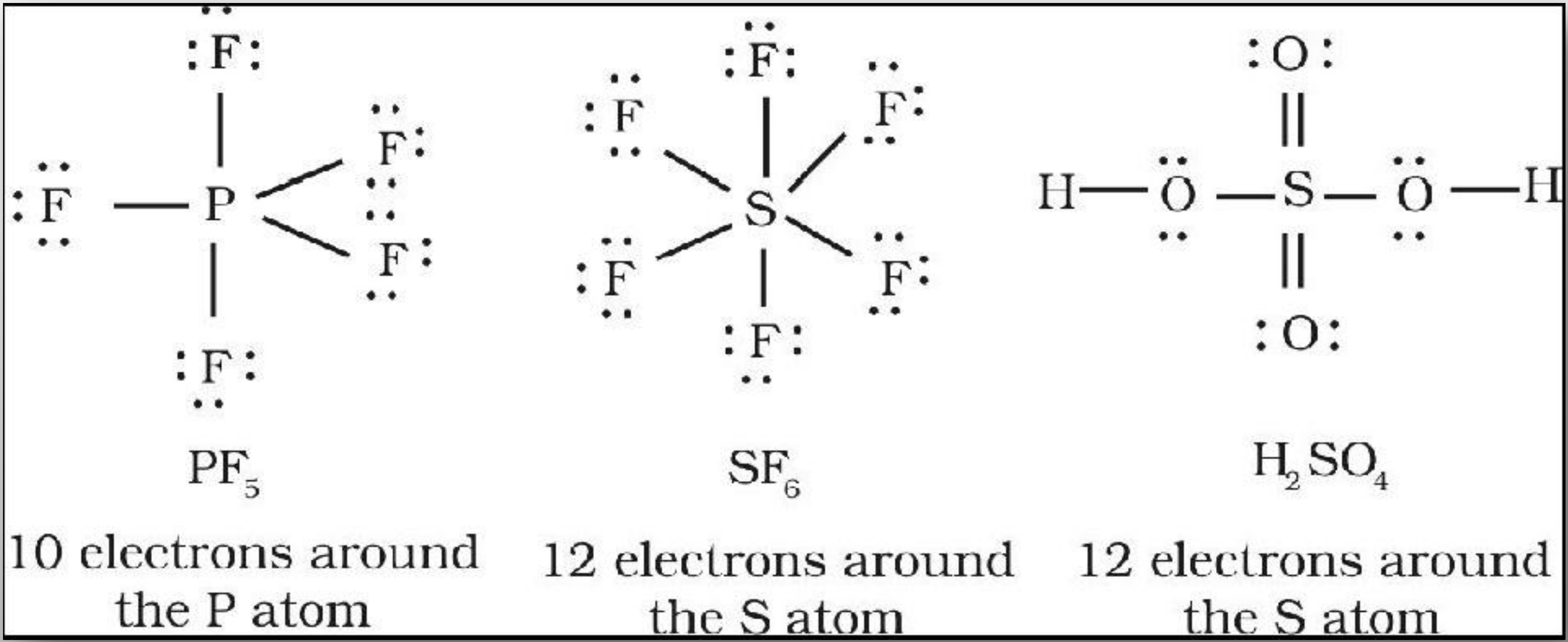
Limitations of the Octet Rule

3. *The expanded octet*

- The octet rule does not apply in the expanded octet.
- Some of the examples of such compounds are:
- PF_5, SF_6, H_2SO_4 and a number of coordination compounds.

Limitations of the Octet Rule

3. *The expanded octet*



PF_5

10 electrons around the P atom

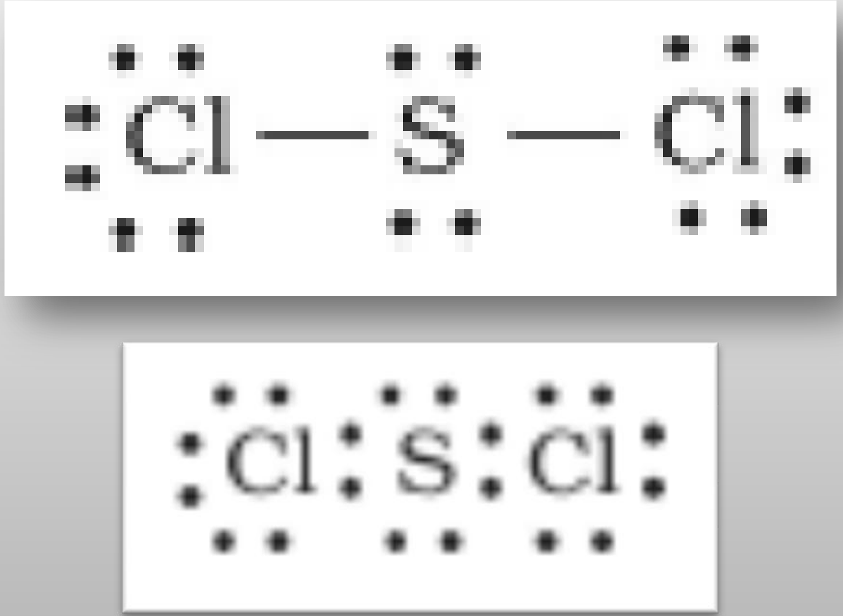
SF_6

12 electrons around the S atom

H_2SO_4

12 electrons around the S atom

- Interestingly, sulphur also forms many compounds in which the octet rule is obeyed.
- In sulphur dichloride, the S atom has an octet of electrons around it.



Other drawbacks of the octet theory

- It is clear that octet rule is based upon the chemical inertness of noble gases.
- However, some noble gases *(for example xenon and krypton)* also combine with oxygen and fluorine to form a number of compounds like XeF_2, KrF_2, $XeOF_2$ etc.,
- This theory does not account for the shape of molecules.
- It does not explain the relative stability of the molecules being totally silent about the energy of a molecule.

IONIC OR ELECTROVALENT BOND

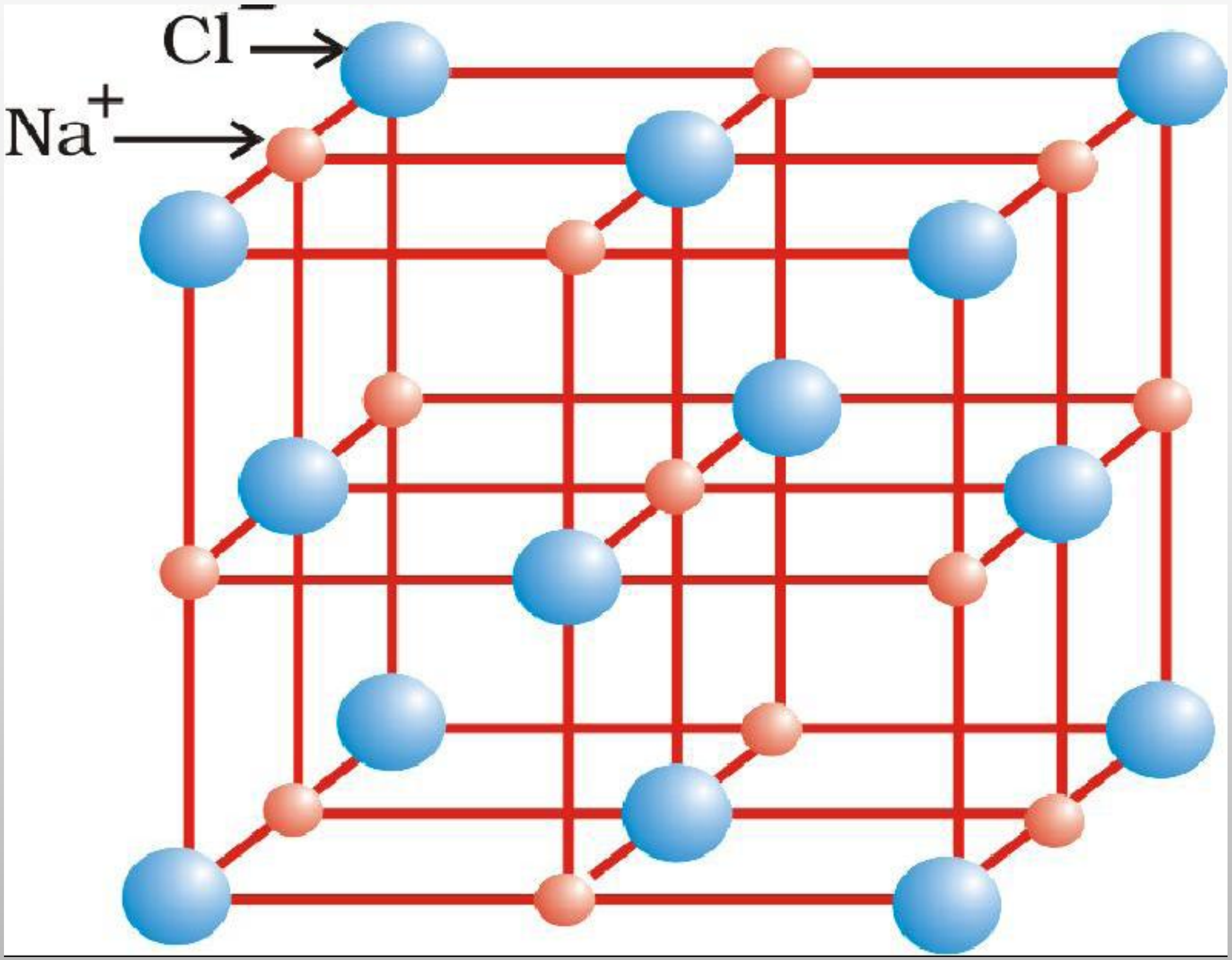
formation of ionic compounds would primarily depend upon:

1. The ease of formation of the positive and negative ions from the respective neutral atoms;

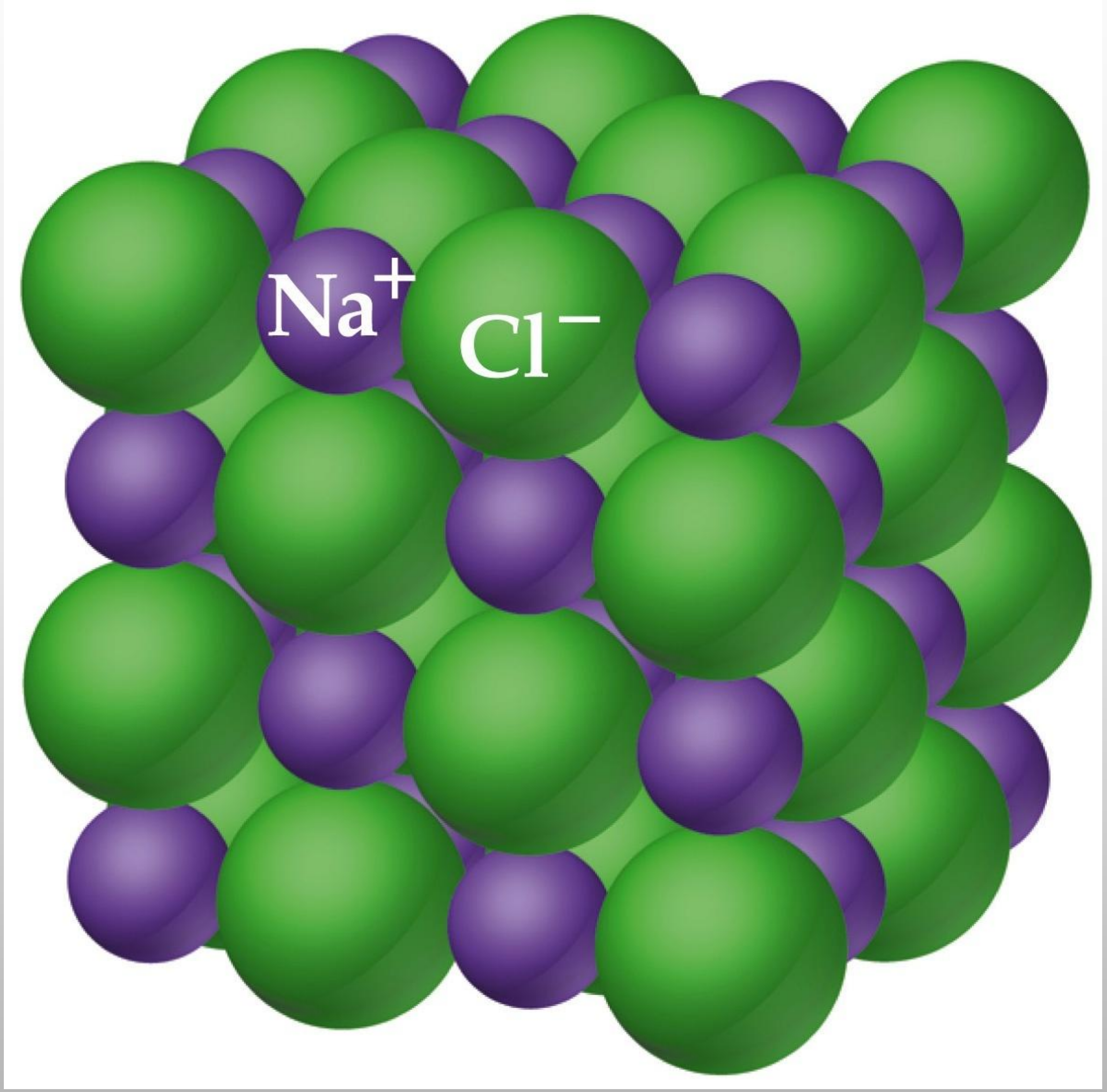
2. The arrangement of the positive and negative ions in the solid, that is, the lattice of the crystalline compound.

- Ionic bonds will be formed more easily between elements with comparatively low ionization enthalpies and elements with comparatively high negative value of electron gain enthalpy.

Rock salt structure



Rock salt structure



Lattice Enthalpy

The Lattice Enthalpy of an ionic solid is defined as the energy required to completely separate one mole of a solid ionic compound into gaseous constituent ions.

- For example, the lattice enthalpy of NaCl is 788 kJ mol^{-1}.
- This means that 788 kJ of energy is required to separate one mole of solid NaCl into one mole of Na^+ (g) and one mole of Cl^- (g) to an infinite distance.

BOND PARAMETERS

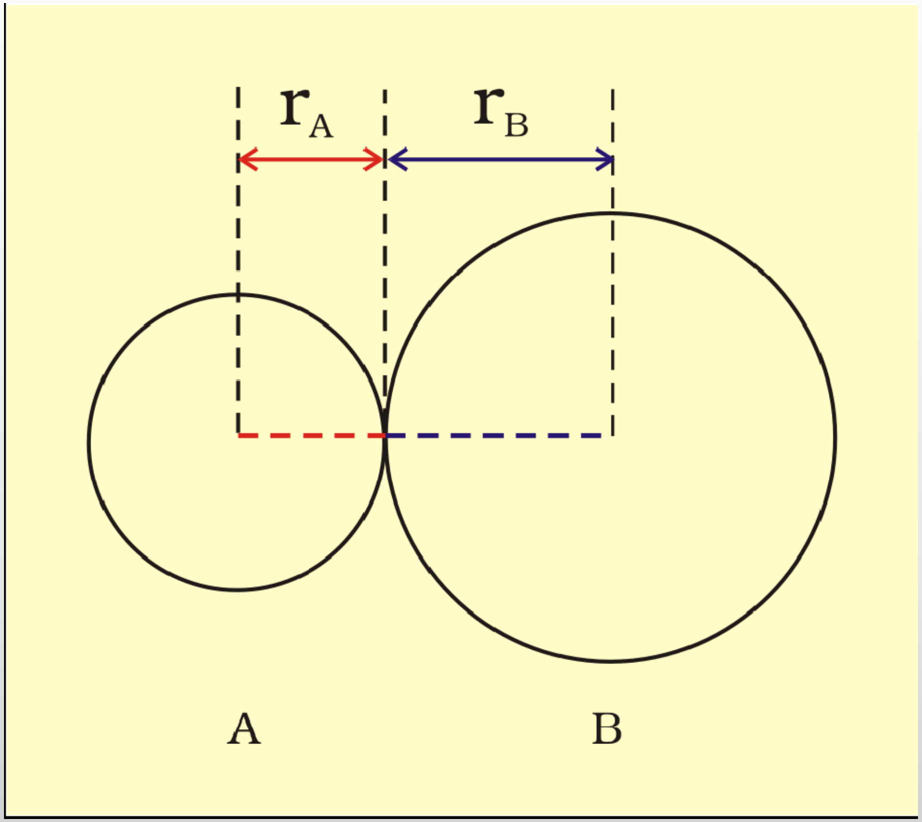
1. Bond Length
2. Bond Angle
3. Bond Enthalpy
4. Bond Order
5. Resonance Structures
6. Polarity of Bonds

Bond Length

- ***Bond length is defined as the equilibrium distance between the nuclei of two bonded atoms in a molecule*.**

- Bond lengths are measured by spectroscopic, X-ray diffraction and electron-diffraction techniques

Bond Length



The bond length in a covalent molecule AB.

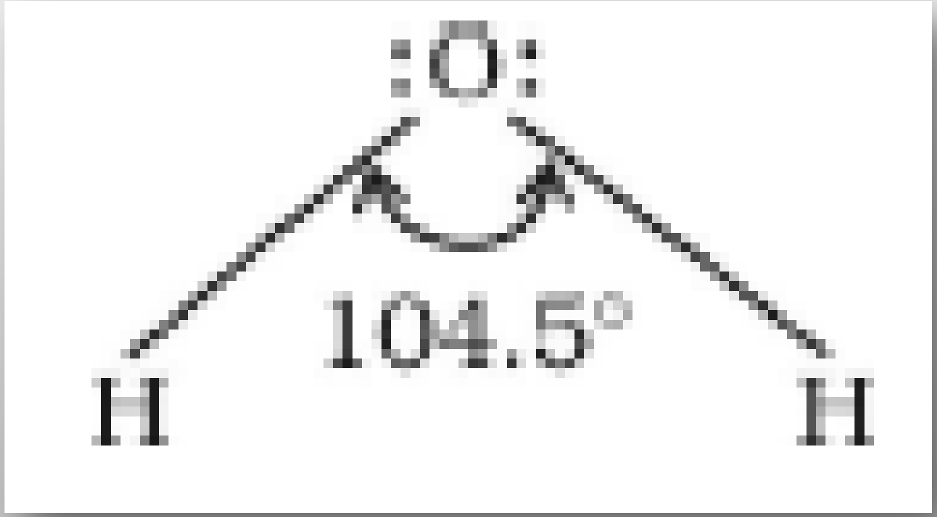
R = rA + rB (*R is the bond length and rA and rB are the covalent radii of atoms A and B respectively*)

Bond Angle

- *It is defined as the angle between the orbitals containing bonding electron pairs around the central atom in a molecule/complex ion.*
- Bond angle is expressed in degree which can be
- experimentally determined by spectroscopic methods.
- It gives some idea regarding the distribution of orbitals around the central atom in a molecule/complex ion
- and hence it helps us in determining its shape.

Bond Angle

- For example H–O–H bond angle in water can be represented as under :



Bond Enthalpy

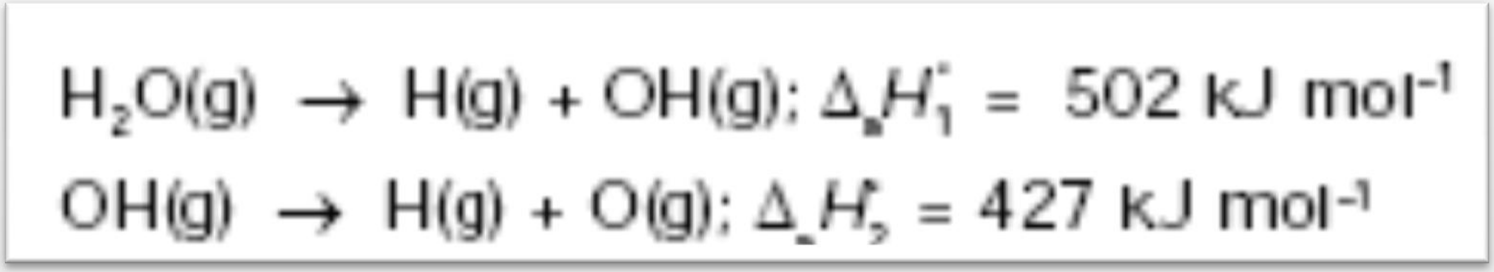
- *It is defined as the amount of energy required to break one mole of bonds of a particular type between two atoms in a gaseous state.*
- The unit of bond enthalpy is kJ mol^{-1}.
- For example, the H – H bond enthalpy in hydrogen molecule is 435.8 kJ mol^{-1}
- It is important that larger the bond dissociation enthalpy, stronger will be the bond in the molecule.

Bond Enthalpy

- In case of polyatomic molecules, the measurement of bond strength is more complicated.
- *For example in case of* H_2O *molecule, the enthalpy needed to break the two* $O-H$ *bonds is not the same.*
- Therefore in polyatomic molecules the term **mean or average bond enthalpy is** used.
- It is obtained by dividing total bond dissociation enthalpy by the number of bonds broken

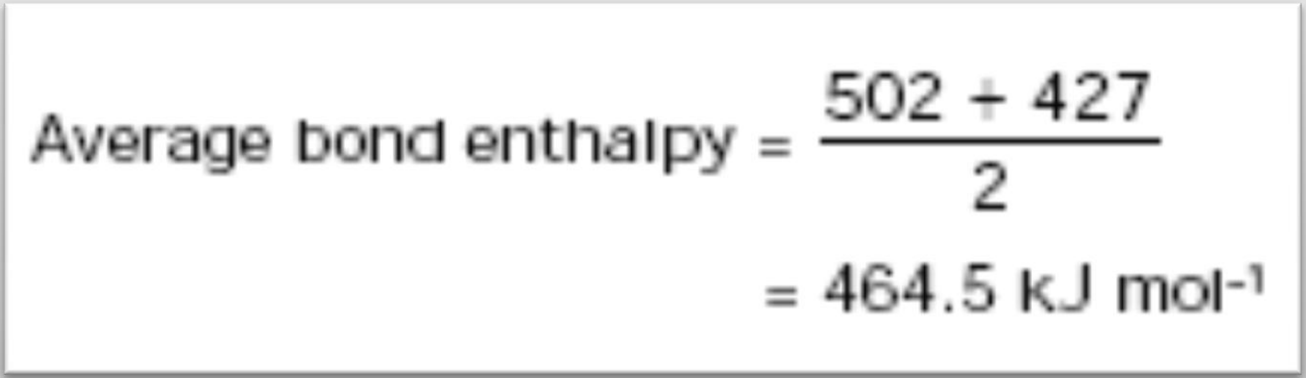
Bond Enthalpy

- **For example in case of H_2O**



$$H_2O(g) \rightarrow H(g) + OH(g);\ \Delta_a H_1^\circ = 502\ \text{kJ mol}^{-1}$$

$$OH(g) \rightarrow H(g) + O(g);\ \Delta_a H_2^\circ = 427\ \text{kJ mol}^{-1}$$



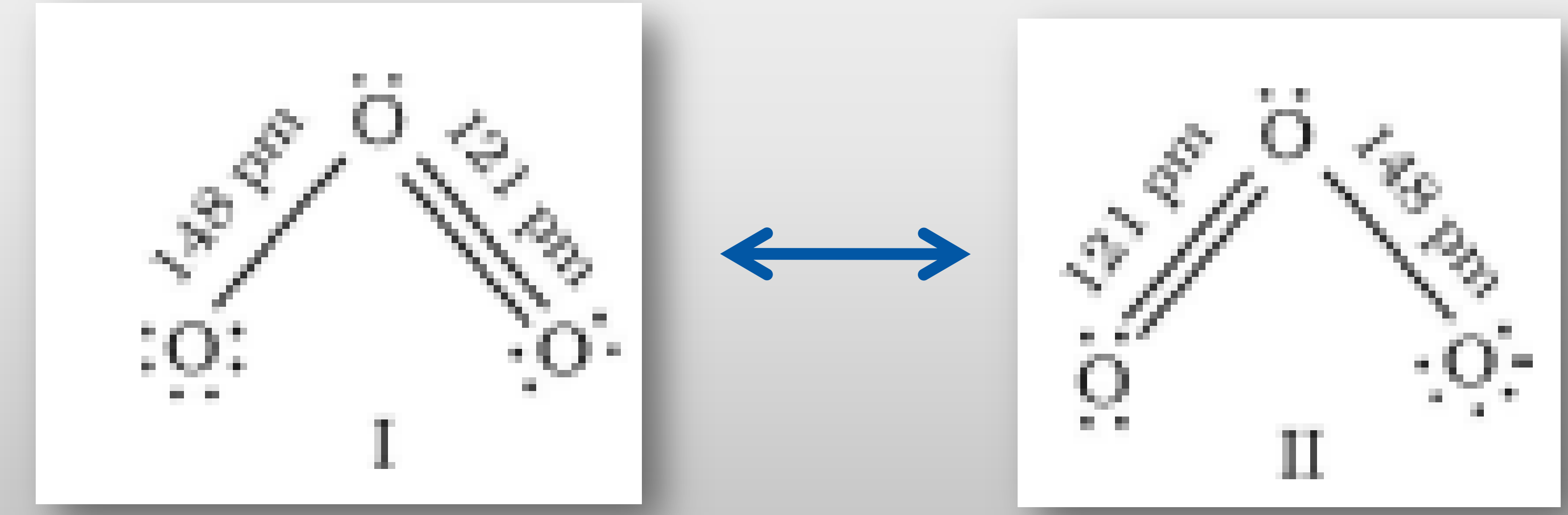
$$\text{Average bond enthalpy} = \frac{502 + 427}{2} = 464.5\ \text{kJ mol}^{-1}$$

Bond Order

- *In the Lewis description of covalent bond, the Bond Order is given by the number of bonds between the two atoms in a molecule*.
- The bond order, for example in H_2 , O_2 , and N_2 is 1,2,3 respectively.
- Similarly in CO *(three shared electron pairs between C and O)* the bond order is 3.
- Isoelectronic molecules and ions have identical bond orders; for example, $\mathbf{F_2}$ and $\mathbf{O_2}^{2-}$ have bond order **1**.
- **with increase in bond order, bond enthalpy increases and bond length decreases.**

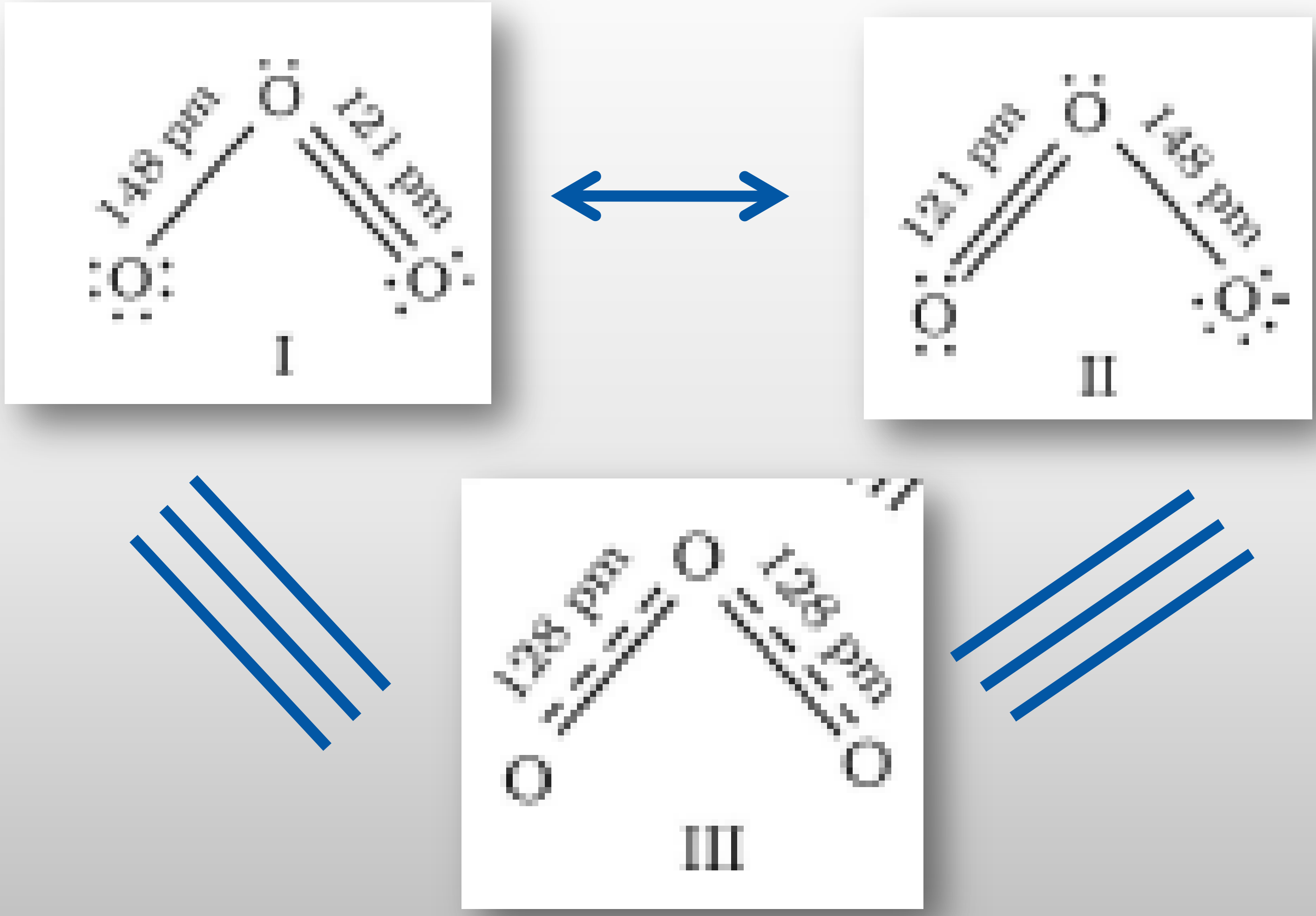
Resonance Structures

The ozone, O_3 molecule can be equally represented by the structures I and II shown below:



Resonance is represented by a double headed arrow.

Resonance Structures



(structures I and II represent the two canonical forms while the structure III is the resonance hybrid)

Resonance

In general, it may be stated that

- Resonance stabilizes the molecule as the energy of the resonance hybrid is less than the energy of any single canonical structure; and,

- Resonance averages the bond characteristics as a whole.

- Thus the energy of the O_3 resonance hybrid is lower than either of the two canonical forms I and II

Note: The cannonical forms have no real existence.

Polarity of Bonds

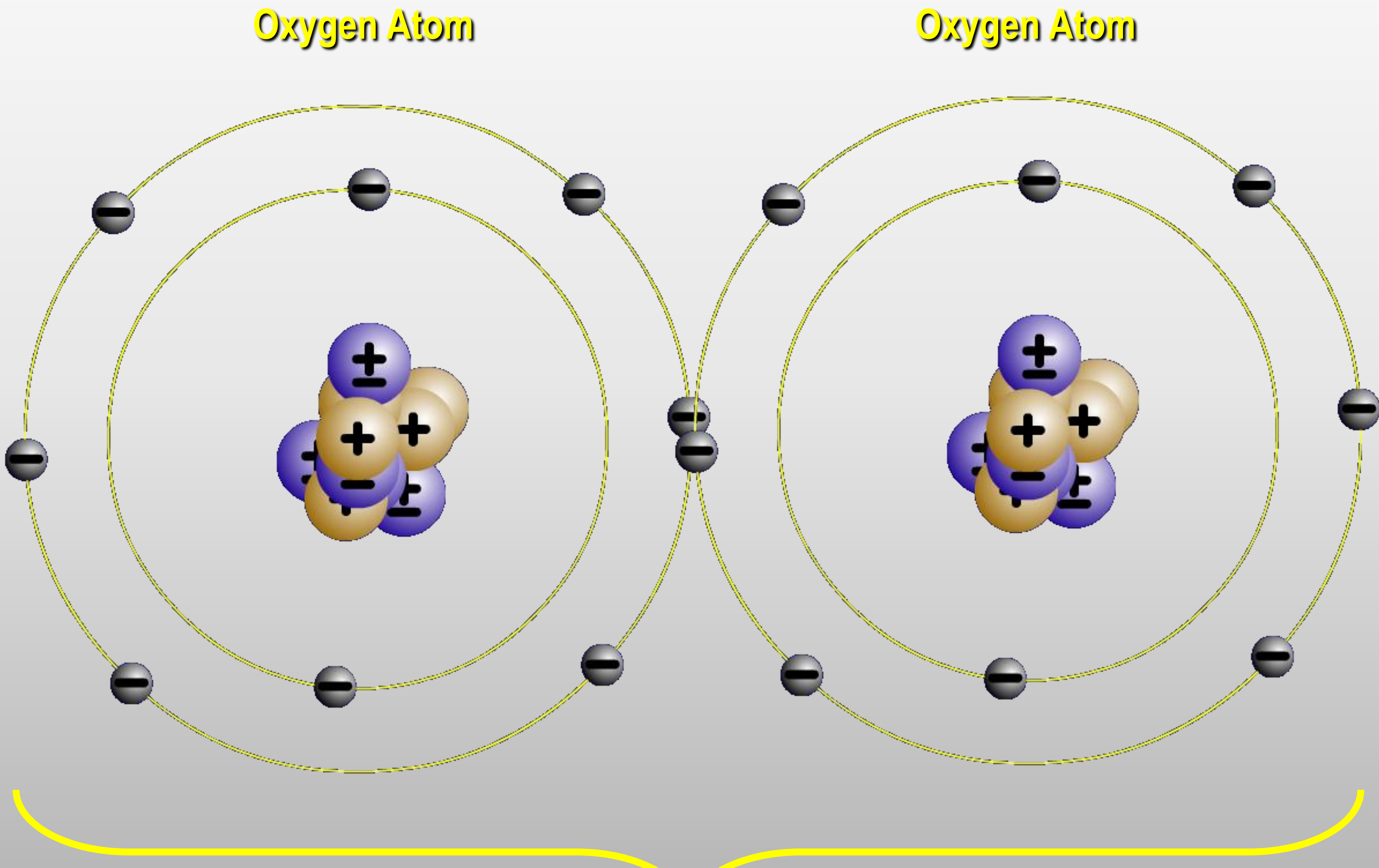
1. Polar &
2. Non-Polar Covalent bonds.

NONPOLAR COVALENT BONDS

when electrons are shared *equally*

H_2 or Cl_2

Two atoms share one or more pair of outer-shell electrons.



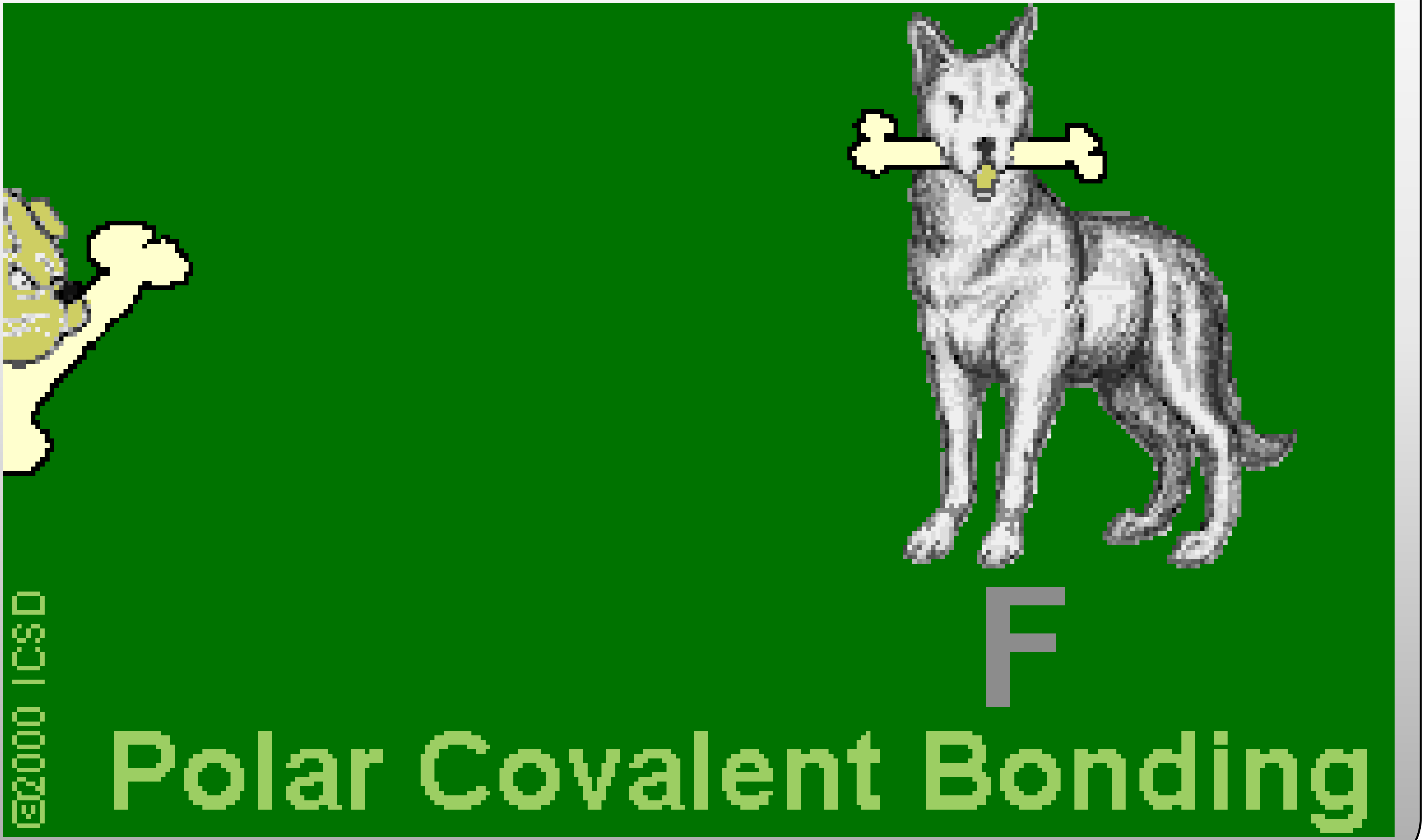
Oxygen Molecule (O_2)

POLAR COVALENT BONDS

when electrons are shared but shared *unequally*

HF

Polar Covalent Bonds: Unevenly matched, but willing to share.



dipole moment

- As a result of polarisation, the molecule possesses the **dipole moment** which can be defined *as the product of the magnitude of the charge and the distance between the centres of positive and negative charge.*
- It is usually designated by a Greek letter 'μ'. Mathematically, it is expressed as follows :

Dipole moment (μ) = charge (Q) × distance of separation (r)

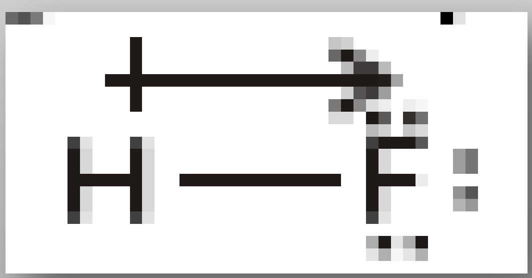
dipole moment a vector quantity

- Dipole moment is usually expressed in Debye units (**D**).

The conversion factor is **1 D = 3.33564 × $\mathbf{10^{-30}}$ C m**

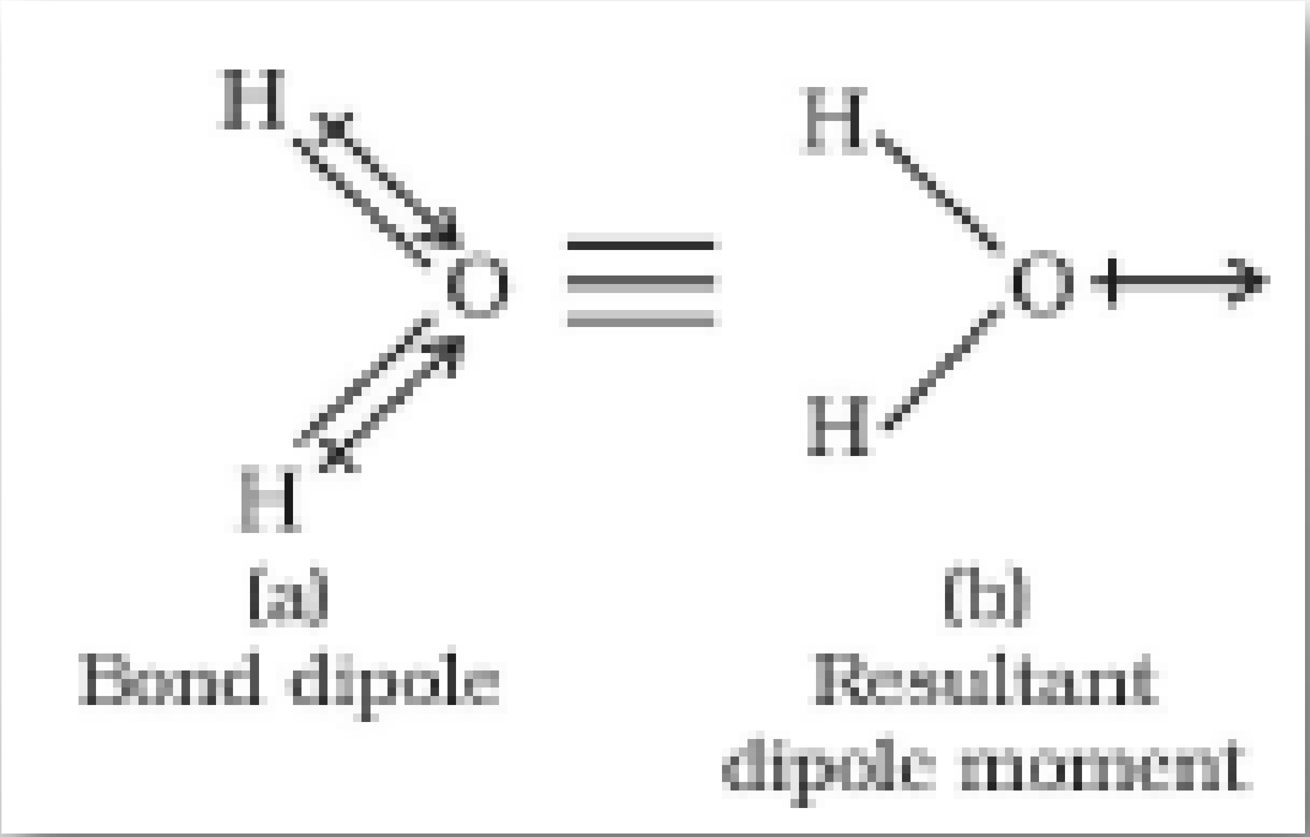
where **C** is coulomb and **m** is meter.

- **dipole moment is** depicted by a small arrow with tail on the positive centre and head pointing towards the negative centre.



dipole moment in polyatomic molecules

- The dipole moment of a molecule is the vector sum of the dipole moments of various bonds.
- For example in H_2O molecule, which has a bent structure, the two O–H bonds are oriented at an angle of 104.5^0.
- Net dipole moment of 6.17×10^{-30} C m (1D = 3.33564×10^{-30} C m) is the resultant of the dipole moments of two O–H bonds.

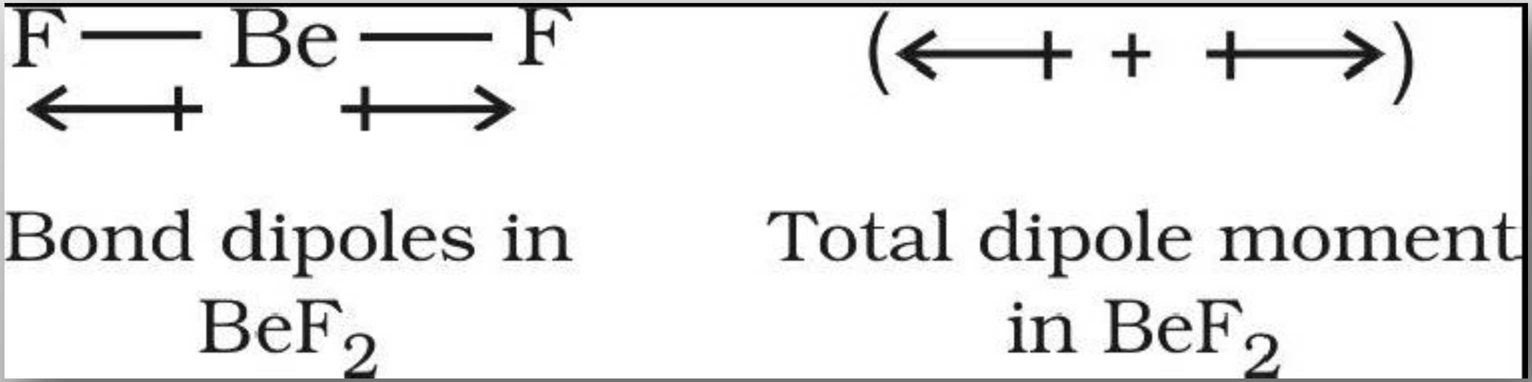


Net Dipole moment, μ = 1.85 D

$= 1.85 \times 3.33564 \times 10^{-30}$ C m $= 6.17 \times 10^{-30}$ C m

dipole moment in BeF_2

- The dipole moment in case of BeF_2 is zero.
- This is because the two equal bond dipoles point in opposite directions and cancel the effect of each other.

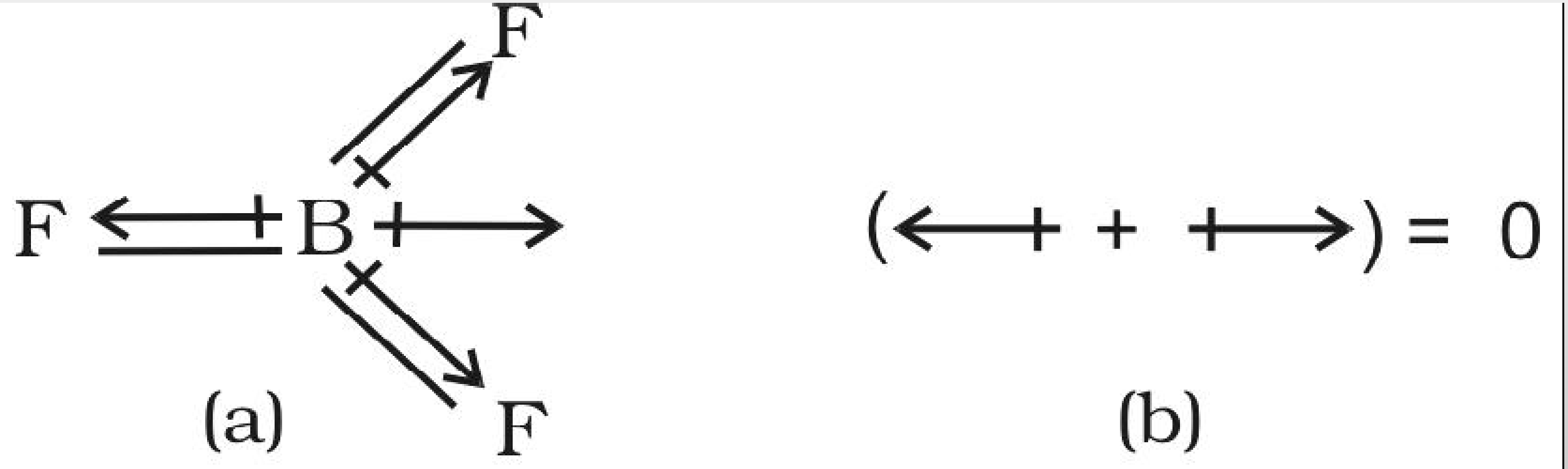


Bond dipoles in BeF_2

Total dipole moment in BeF_2

dipole moment in BF_3

- In BF_3, the dipole moment is zero although the B – F bonds are oriented at an angle of 120° to one another, the three bond moments give a net sum of zero as the resultant of any two is equal and opposite to the third.



BF_3 molecule; representation of (a) bond dipoles and (b) total dipole moment

dipole moment in NH_3 and NF_3 molecule.

- Both the molecules have pyramidal shape with a lone pair of electrons on nitrogen atom.

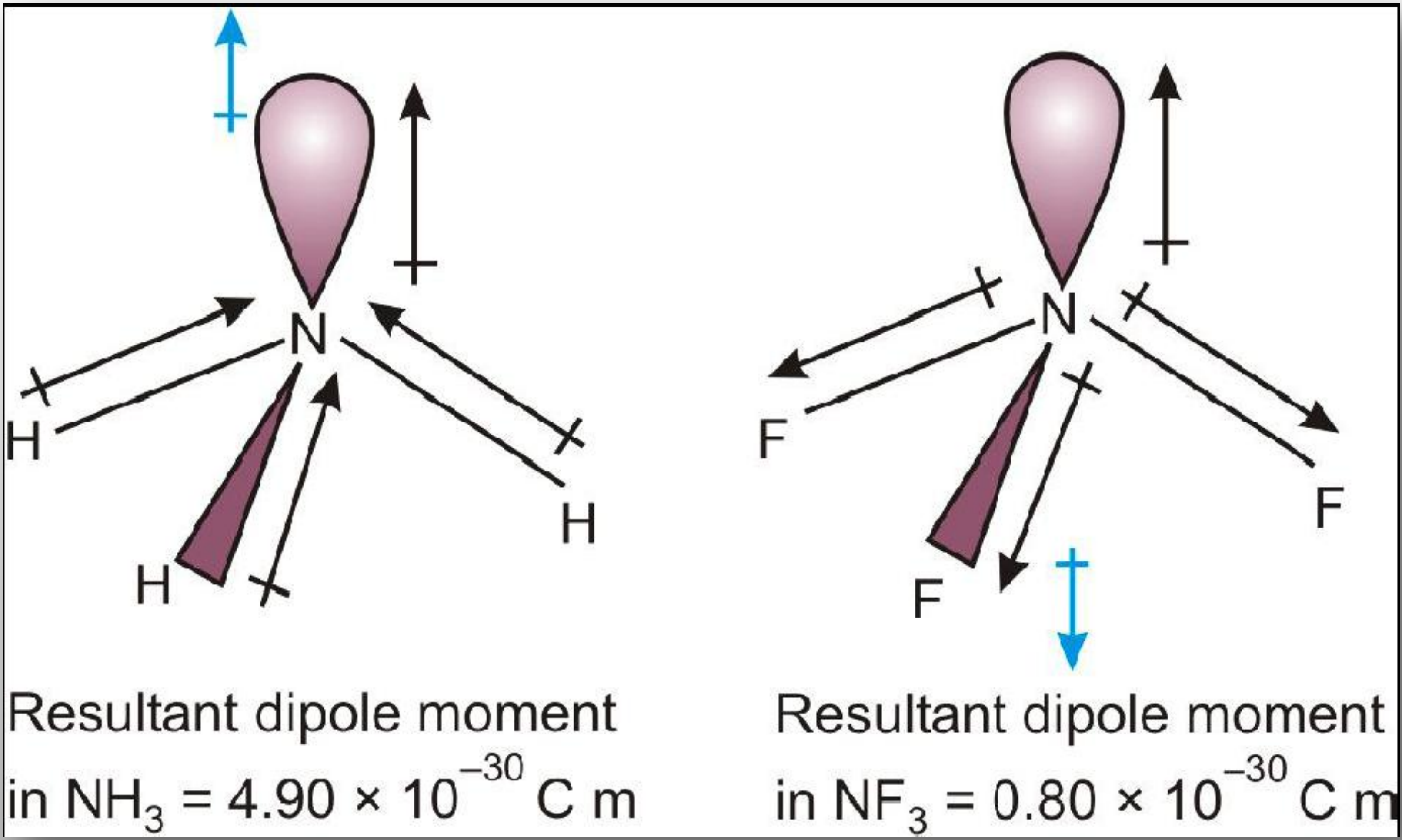
- Although fluorine is more electronegative than nitrogen, the resultant dipole moment of NH_3 (4.90×10^{-30} C m) is greater than that of NF_3 (0.8×10^{-30} C m).

dipole moment in NH_3 and NF_3 molecule.

- This is because, in case of NH_3 the orbital dipole due to lone pair is in the same direction as the resultant dipole moment of the N – H bonds, whereas in NF_3 the orbital dipole is in the direction opposite to the resultant dipole moment of the three N–F bonds.

- The orbital dipole because of lone pair decreases the effect of the resultant N – F bond moments, which results in the low dipole moment of NF_3 as represented below

dipole moment in NH_3 and NF_3 molecule.



Resultant dipole moment in $NH_3 = 4.90 \times 10^{-30}$ C m

Resultant dipole moment in $NF_3 = 0.80 \times 10^{-30}$ C m

- Just as all the covalent bonds have some partial ionic character,

  the ionic bonds also have partial covalent character.

(VSEPR) THEORY

THE VALENCE SHELL ELECTRON PAIR REPULSION THEORY

Lewis concept is unable to explain the shapes of molecules.

- Sidgwick and Powell in 1940, proposed a simple theory based on the repulsive interactions of the electron pairs in the valence shell of the atoms.
- This theory provides a simple procedure to predict the shapes of covalent molecules.
- It was further developed and redefined by Nyholm and Gillespie

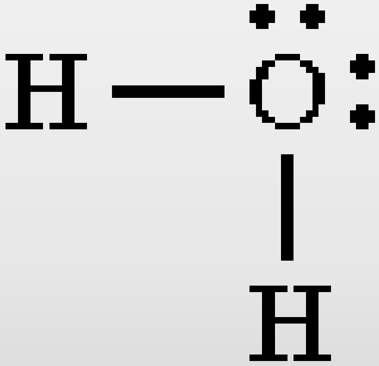
Postulates of VSEPR theory

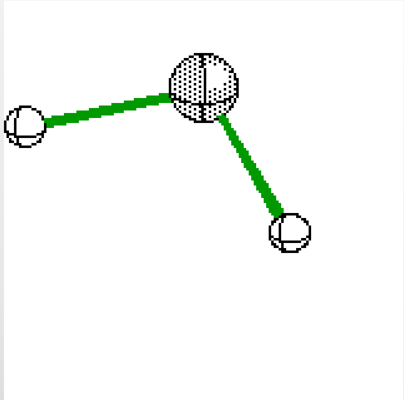
- The shape of a molecule depends upon the number of valence shell electron pairs (bonded or nonbonded) around the central atom.
- Pairs of electrons in the valence shell repel one another since their electron clouds are negatively charged.
- These pairs of electrons tend to occupy such positions in space that minimise repulsion and thus maximise distance between them.

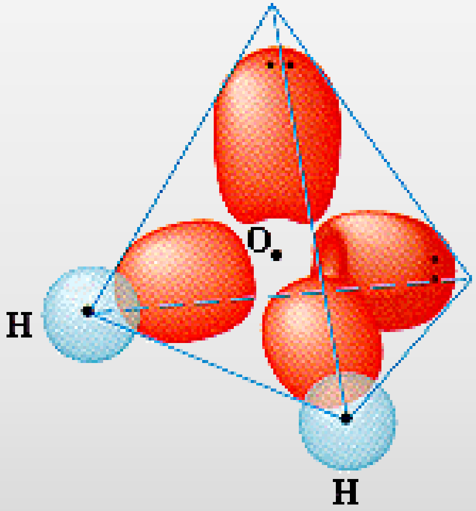
Postulates of VSEPR theory

- The valence shell is taken as a sphere with the electron pairs localising on the spherical surface at maximum distance from one another.
- A multiple bond is treated as if it is a single electron pair and the two or three electron pairs of a multiple bond are treated as a single super pair.
- Where two or more resonance structures can represent a molecule, the VSEPR model is applicable to any such structure.

Lone Pair & Bond Pair







Repulsive interaction

The repulsive interaction of electron pairs decrease in the order:

- Lone pair (lp) – Lone pair (lp) > Lone pair (lp) – Bond pair (bp) > Bond pair (bp) – Bond pair (bp)

- That is Lone pair (lp) – Lone pair (lp) (**Maximum**)
- Lone pair (lp) – Bond pair (bp) (**Internediate**)
- Bond pair (bp) – Bond pair (bp) (**Minimum**)

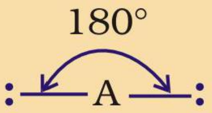
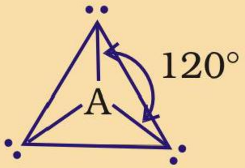
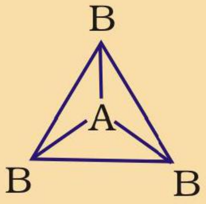
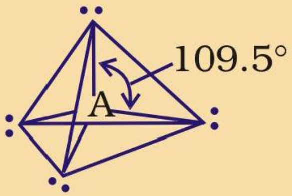
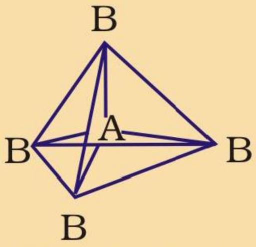
Geometrical shapes of molecules

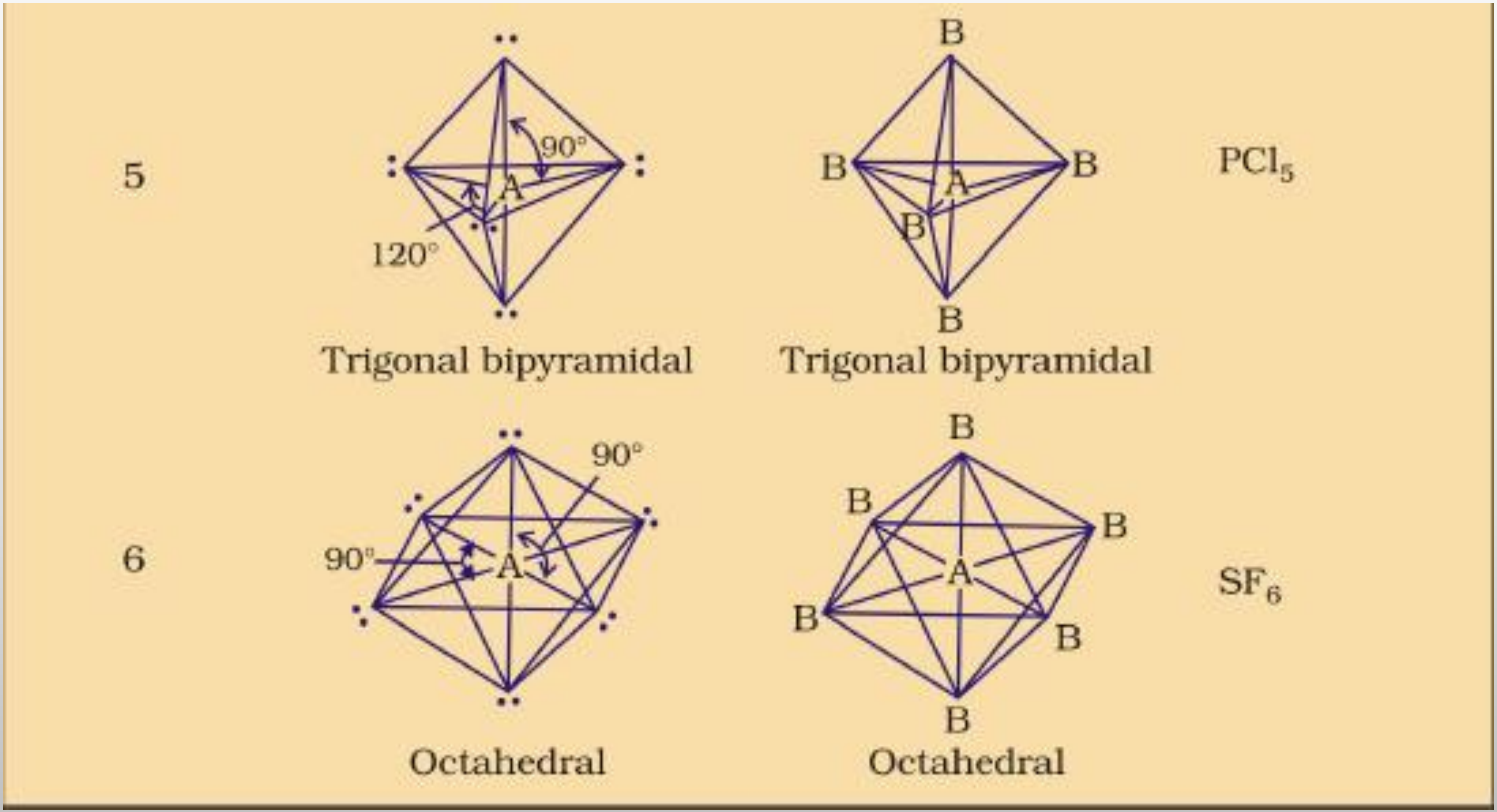
with the help of VSEPR theory,

It is convenient to divide molecules into two categories as

- **(i) molecules in which the central atom has no lone pair and**
- **(ii) molecules in which the central atom has one or more lone pairs.**

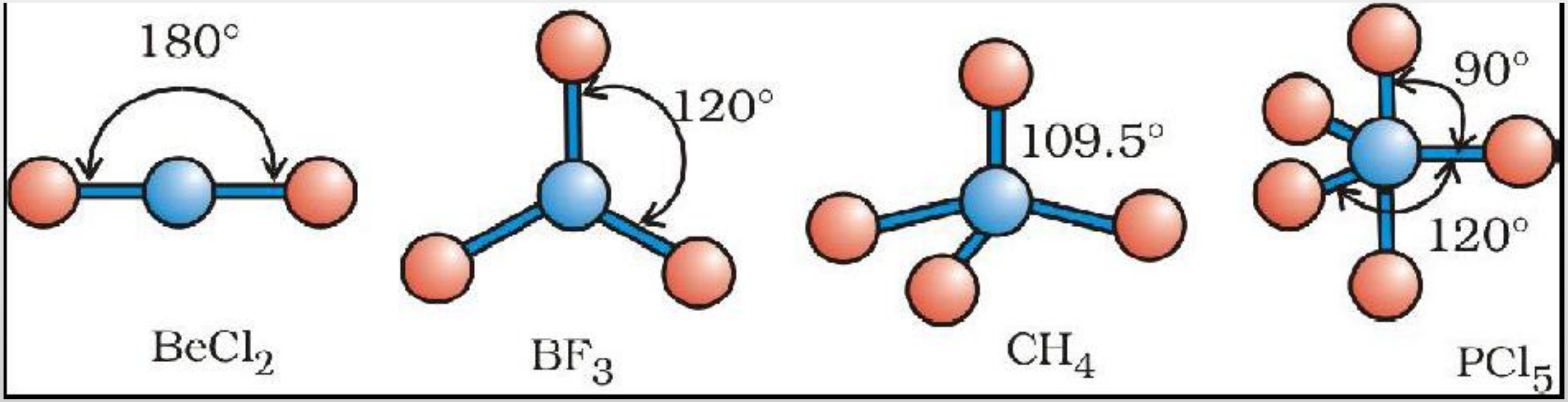
Geometry of Molecules in which the Central Atom has No Lone Pair of Electrons

Number of electron pairs	Arrangement of electron pairs	Molecular geometry	Examples
2	 Linear	B—A—B Linear	$BeCl_2$, $HgCl_2$
3	 Trigonal planar	 Trigonal planar	BF_3
4	 Tetrahedral	 Tetrahedral	CH_4, NH_4^+



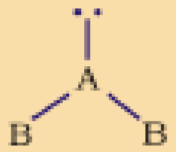
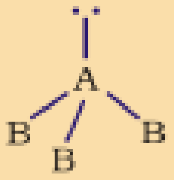
5	Trigonal bipyramidal	Trigonal bipyramidal	PCl_5
6	Octahedral	Octahedral	SF_6

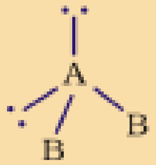
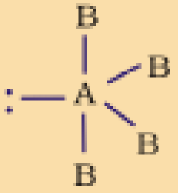
Molecules like BF_3 (AB_3), CH_4 (AB_4) and PCl_5 (AB_5)

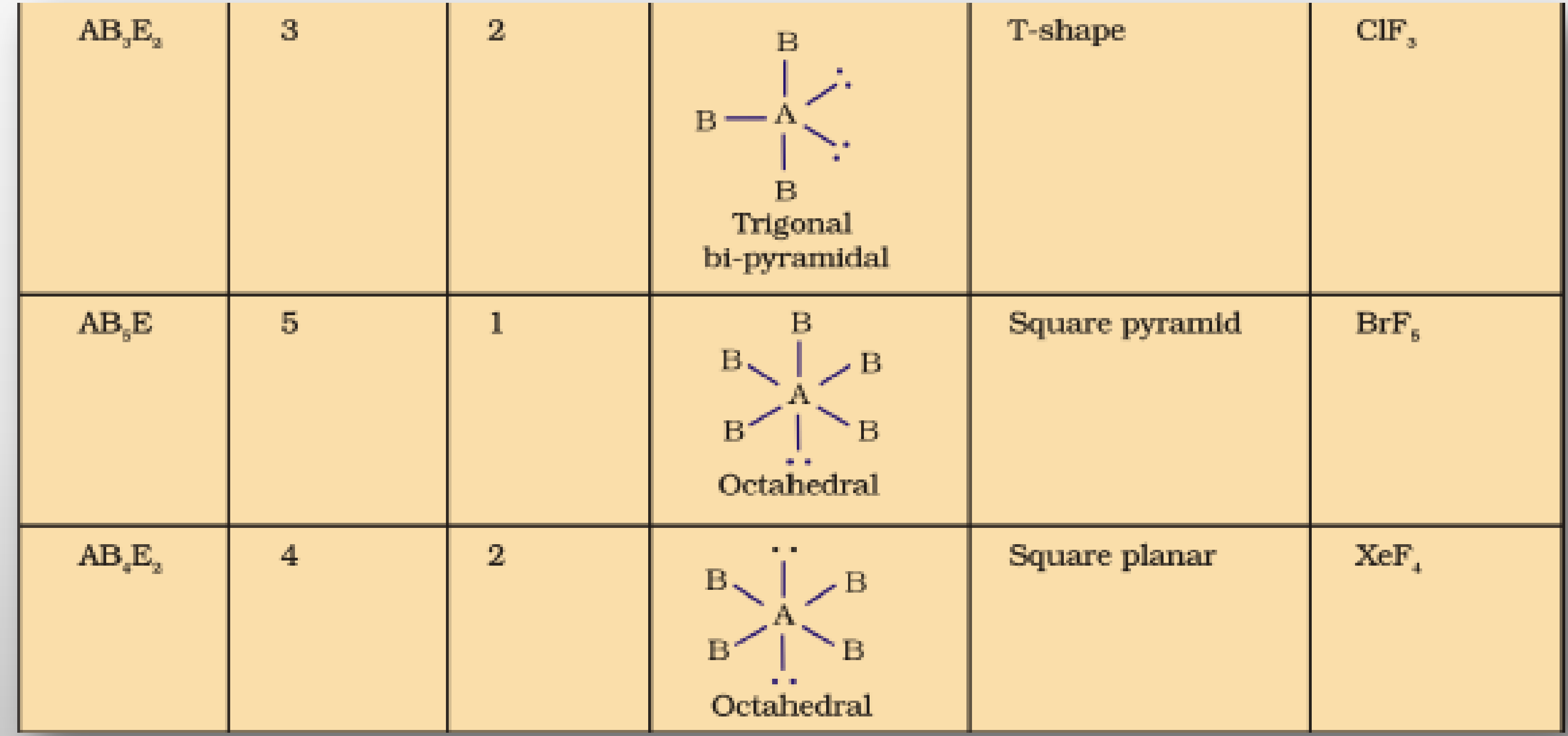


The shapes of molecules in which central atom has no lone pair

Shape (geometry) of Some Simple Molecules/Ions with Central Ions having One or More Lone Pairs of Electrons(E).

Molecule type	No. of bonding pairs	No. of lone pairs	Arrangement of electron pairs	Shape	Examples
AB_2E	2	1	 Trigonal planar	Bent	SO_2, O_3
AB_3E	3	1	 Tetrahedral	Trogonal pyramidal	NH_3

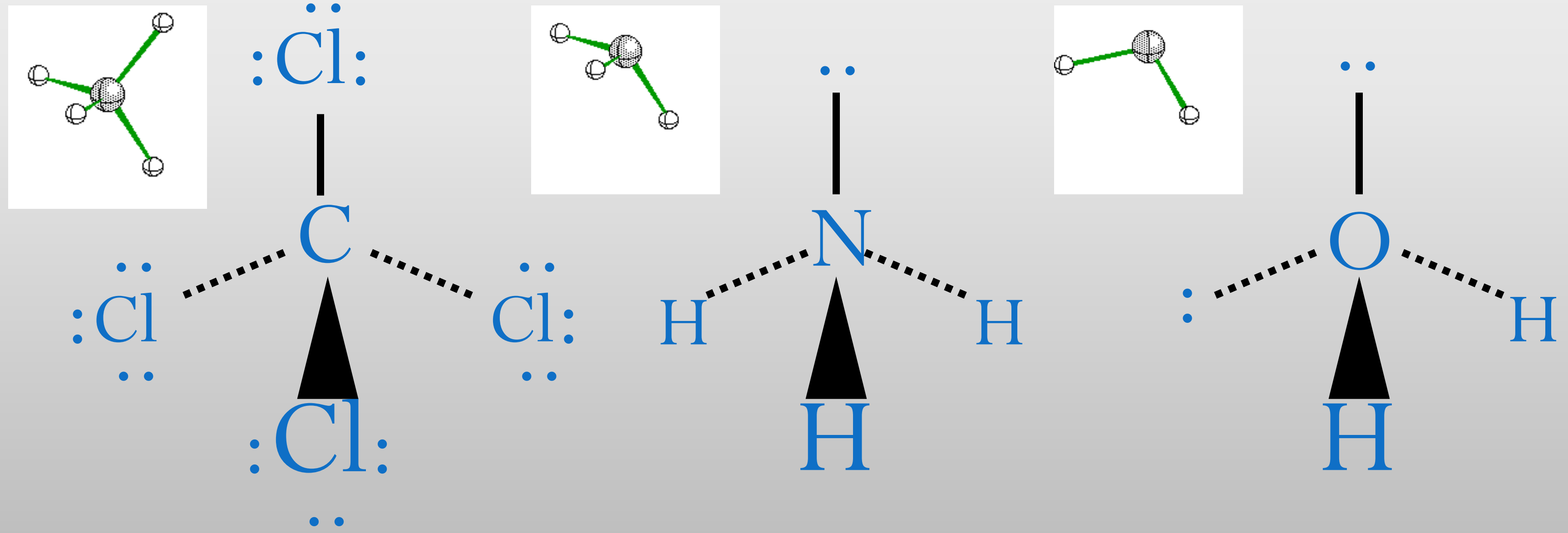
AB_2E_2	2	2	 Tetrahedral	Bent	H_2O
AB_4E	4	1	 Trigonal bi-pyramidal	See saw	SF_4



AB_3E_2	3	2	Trigonal bi-pyramidal	T-shape	ClF_3
AB_5E	5	1	Octahedral	Square pyramid	BrF_5
AB_4E_2	4	2	Octahedral	Square planar	XeF_4

Predicting Molecular Geometry

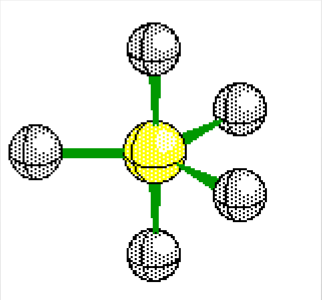
- Four electron pairs (**tetrahedral arrangement**).

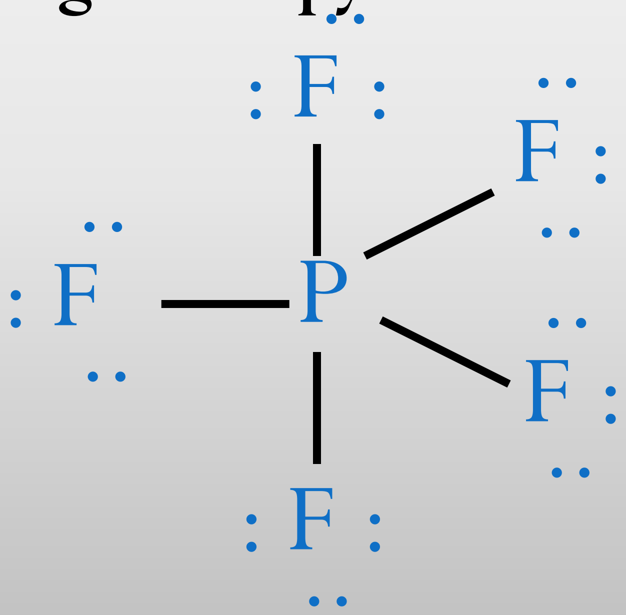


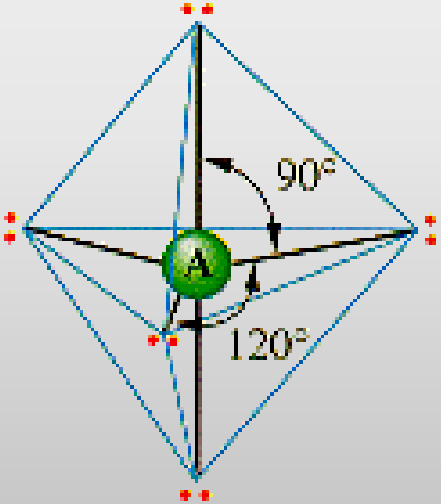
tetrahedral **trigonal pyramid** **bent**

Predicting Molecular Geometry

- Five electron pairs
- (trigonal bipyramidal arrangement).







This structure results in both 90º and 120º bond angles.

Predicting Molecular Geometry

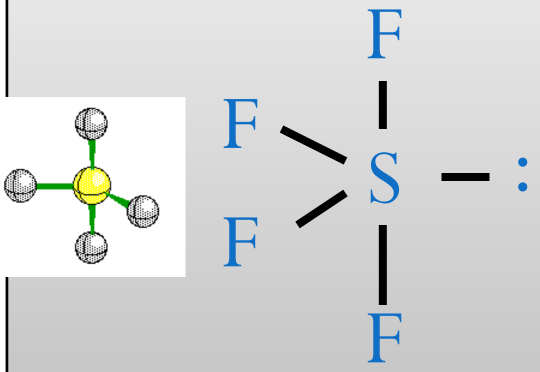
- Other molecular geometries are possible when one or more of the electron pairs is a lone pair.

SF_4 ClF_3 XeF_2

  - Let’s try their Lewis structures.

Predicting Molecular Geometry

- Other molecular geometries are possible when one or more of the electron pairs is a lone pair.



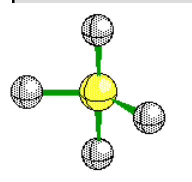
see-saw

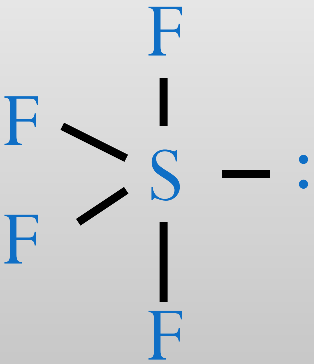
ClF_3

XeF_2

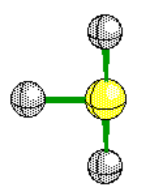
Predicting Molecular Geometry

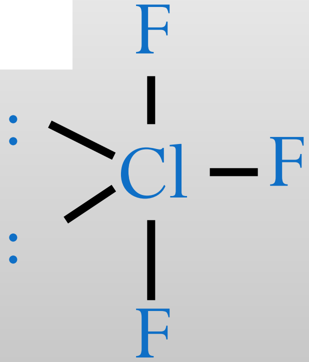
- Other molecular geometries are possible when one or more of the electron pairs is a lone pair.





see-saw



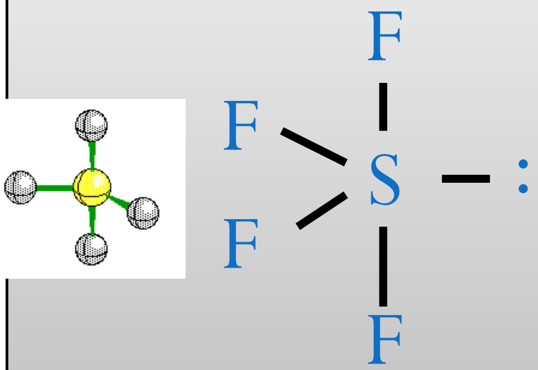


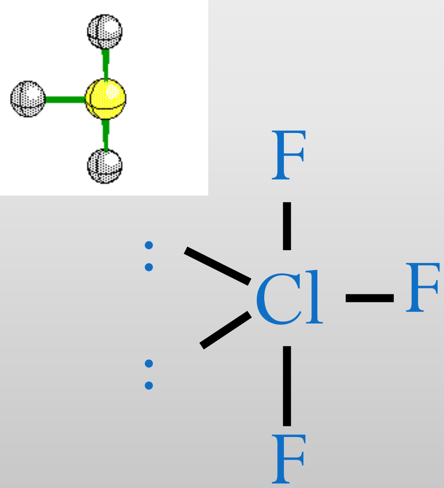
T-shape

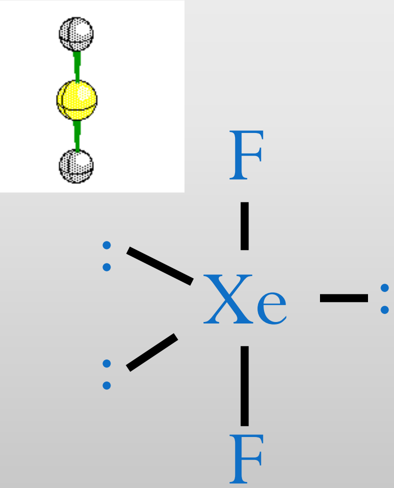
XeF_2

Predicting Molecular Geometry

- Other molecular geometries are possible when one or more of the electron pairs is a lone pair.







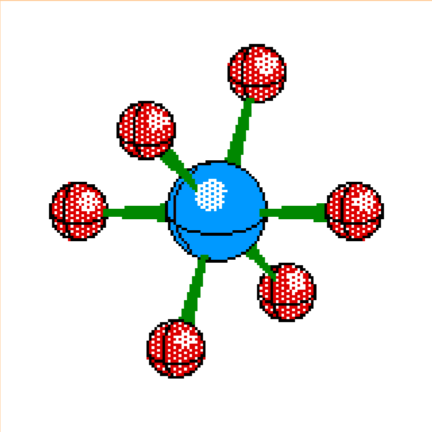
see-saw

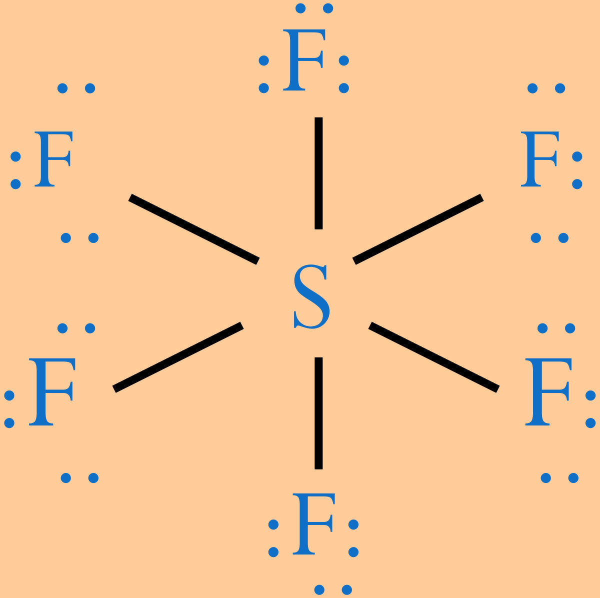
T-shape

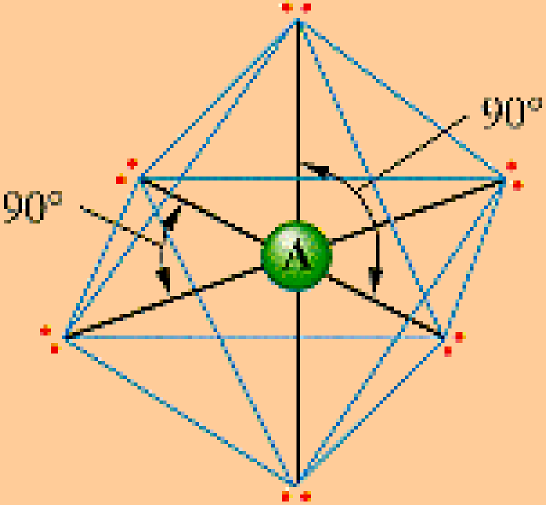
linear

Predicting Molecular Geometry

- Six electron pairs **(octahedral arrangement).**







  - This octahedral arrangement results in 90º bond angles.

Predicting Molecular Geometry

- Six electron pairs **(octahedral arrangement).**

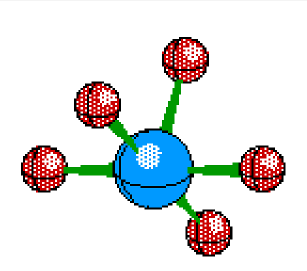
IF_5

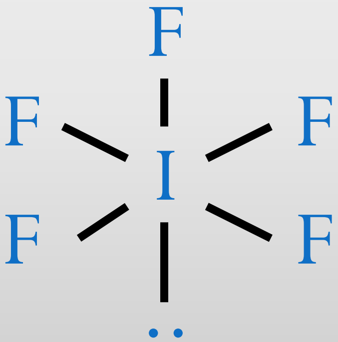
XeF_4

– Six electron pairs also lead to other molecular geometries.

Predicting Molecular Geometry

- Six electron pairs **(octahedral arrangement).**





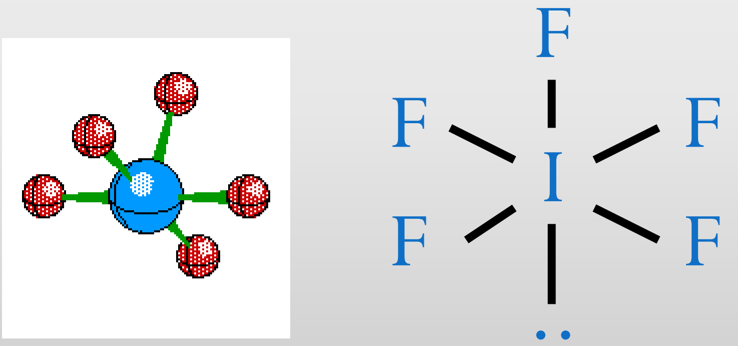
XeF_4

square pyramidal

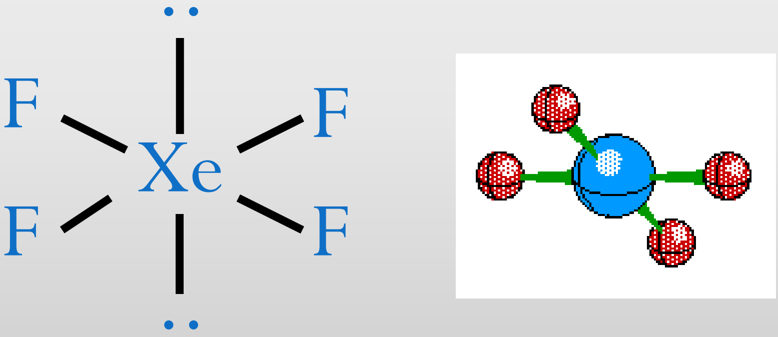
(See Animation: Iodine Pentafluoride Structure)

Predicting Molecular Geometry

- Six electron pairs **(octahedral arrangement).**



square pyramidal



square planar

  - Figures 10.2, 10.4, and 10.8 summarize all the possible molecular geometries.

- Lewis approach helps in writing the structure of molecules but it fails to explain the formation of chemical bond.
- It also gives no idea about the shapes of polyatomic molecules.
- Similarly the VSEPR theory gives the geometry of simple molecules but theoretically, it does not explain them and also it has limited applications.
- To overcome these limitations the two important theories based on quantum mechanical principles are introduced.

1. **Valence bond (VB) theory and**
2. **Molecular orbital (MO) theory.**

VALENCE BOND THEORY

- A discussion of the valence bond theory is based on
- **The knowledge of atomic orbitals,**
- **Electronic configurations of elements),**
- **The overlap criteria of atomic orbitals,**
- **The hybridization of atomic orbitals and**
- **The principles of variation and superposition**

VALENCE BOND THEORY

- Consider two hydrogen atoms A and B approaching each other having nuclei N_A and N_B and electrons present in them are represented by e_A and e_B.

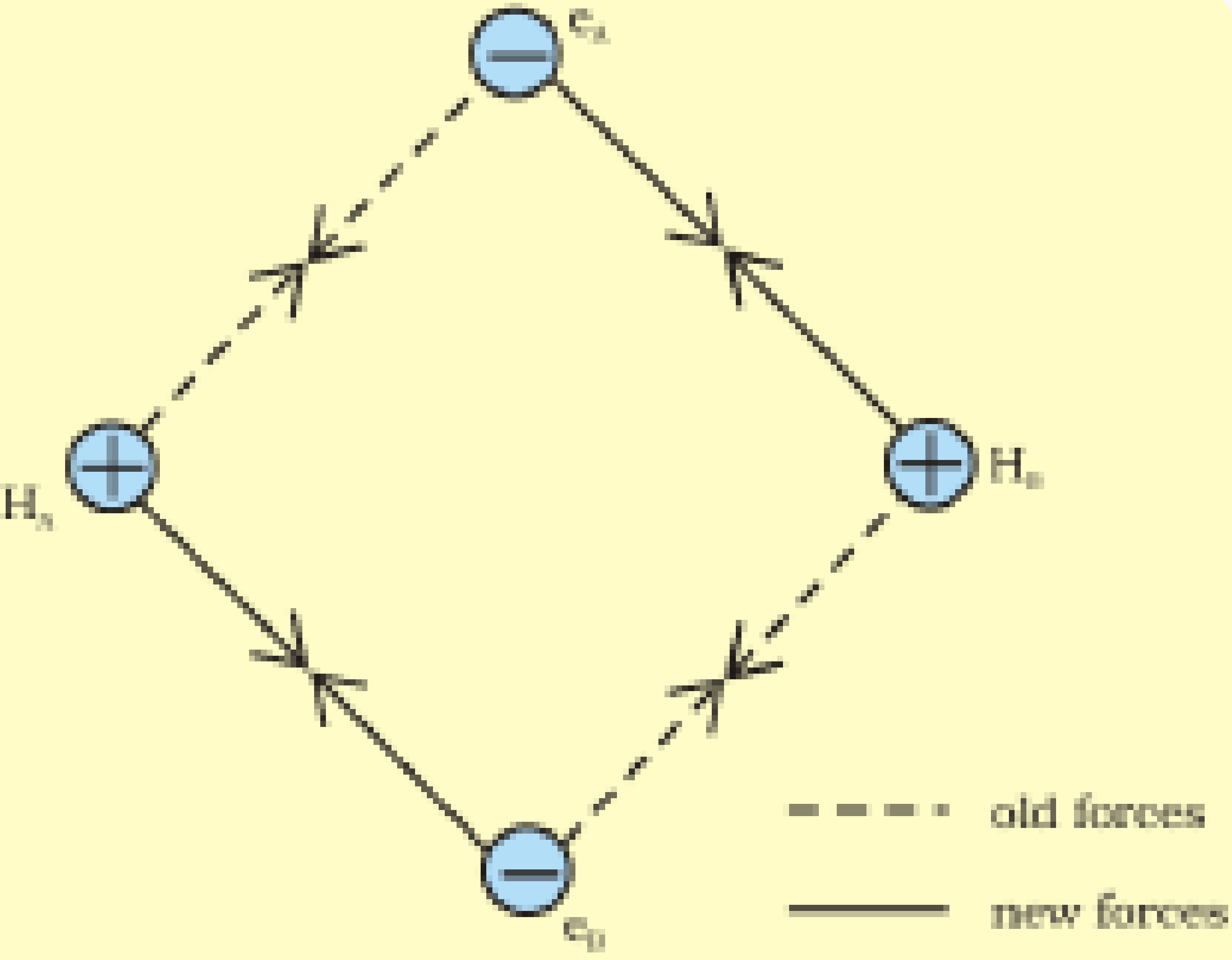
- When the two atoms are at large distance from each other, there is no interaction between them.

- As these two atoms approach each other, new attractive and repulsive forces begin to operate.

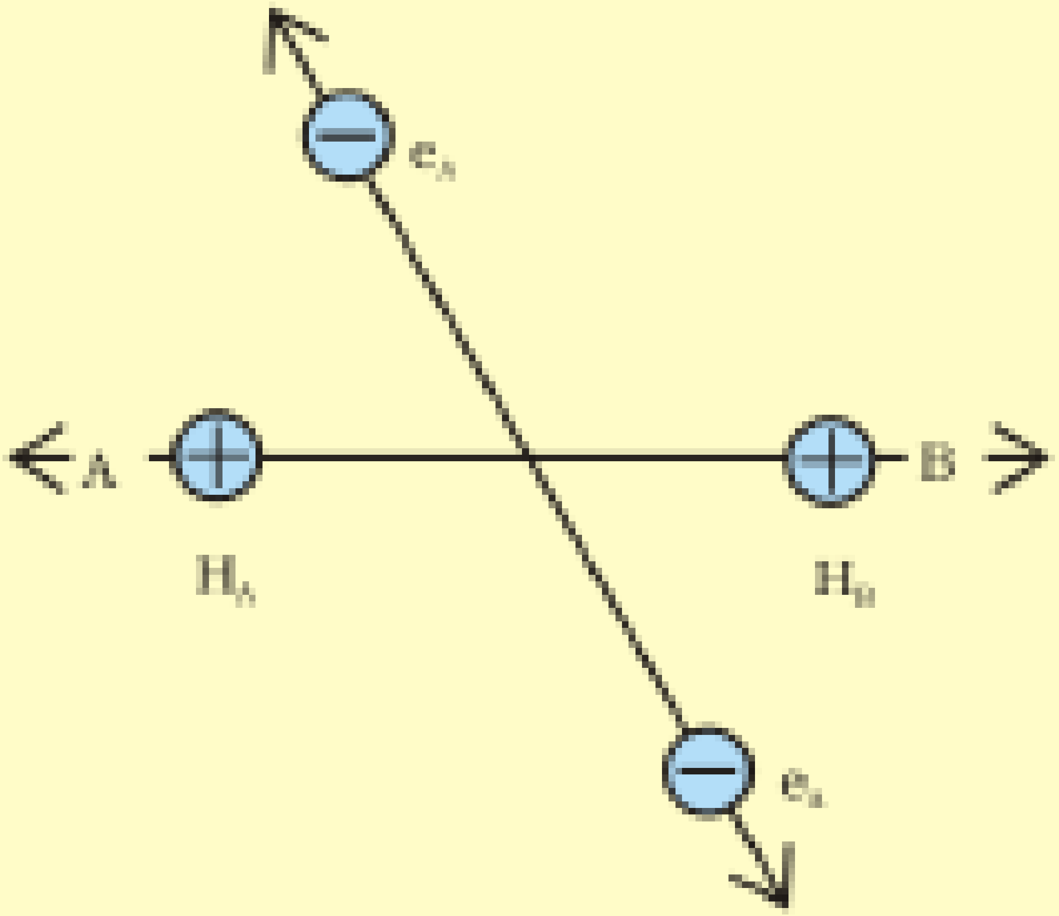
- Attractive forces arise between:
- (i) nucleus of one atom and its own electron that is
- $N_A - e_A$ and $N_B - e_B$.
- (ii) nucleus of one atom and electron of other atom
- i.e., $N_A - eB$, $N_B - e_A$.

- Similarly repulsive forces arise between
- (i) electrons of two atoms like $e_A - e_B$,
- (ii) nuclei of two atoms $N_A - N_B$.

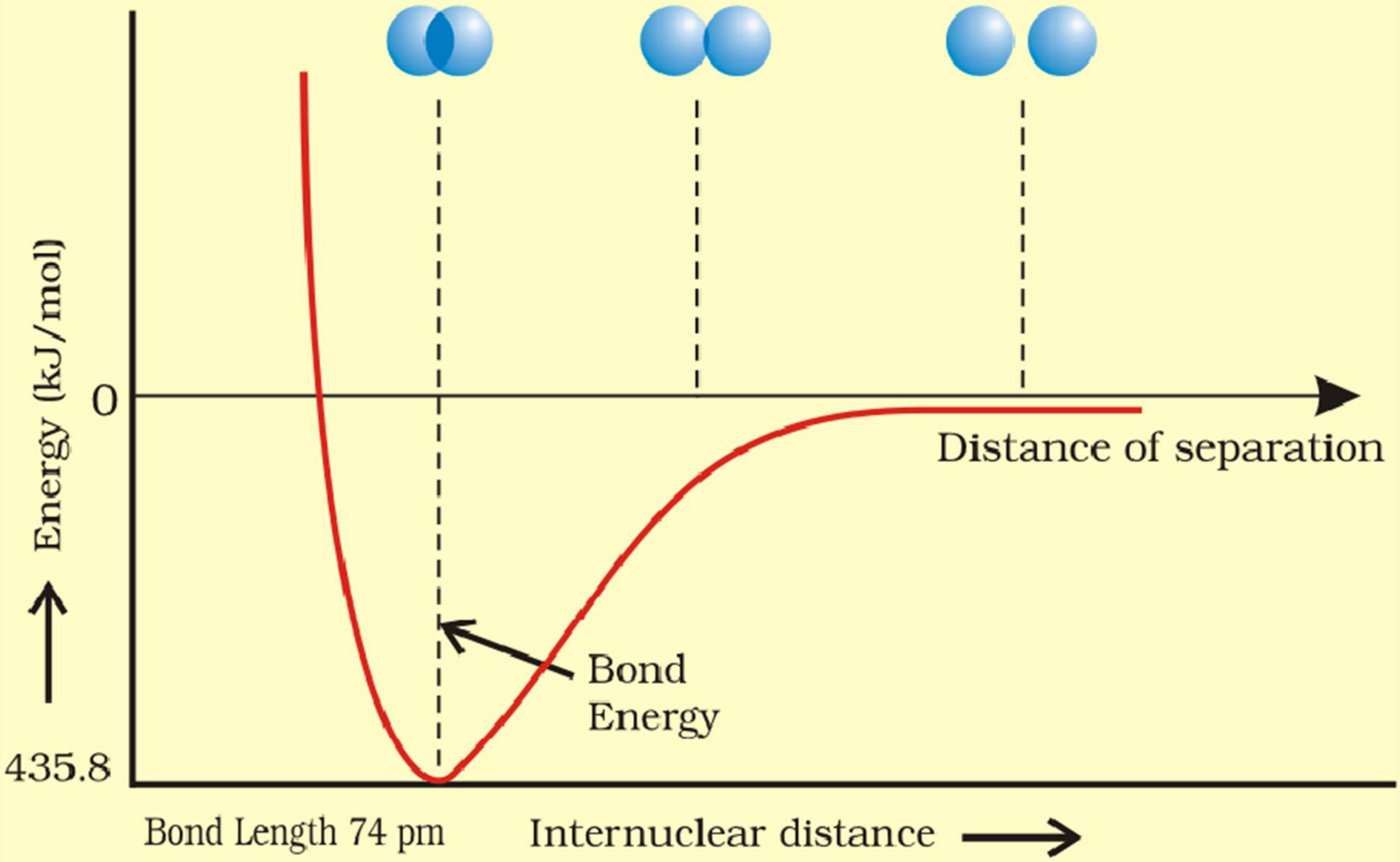
- Attractive forces tend to bring the two atoms close to each other whereas repulsive forces tend to push them apart



Attractive Forces



Repulsive Forces


Energy (kJ/mol)
0
435.8
Distance of separation
Bond
Energy
Bond Length 74 pm
Internuclear distance

Orbital Overlap Concept

- Minimum energy state is when two hydrogen atoms are so near that their atomic orbitals undergo partial interpenetration.

- This partial merging of atomic orbitals is called overlapping of atomic orbitals which results in the pairing of electrons.

- The extent of overlap decides the strength of a covalent bond.

Orbital Overlap Concept

- In general, greater the overlap the stronger is the bond formed between two atoms.

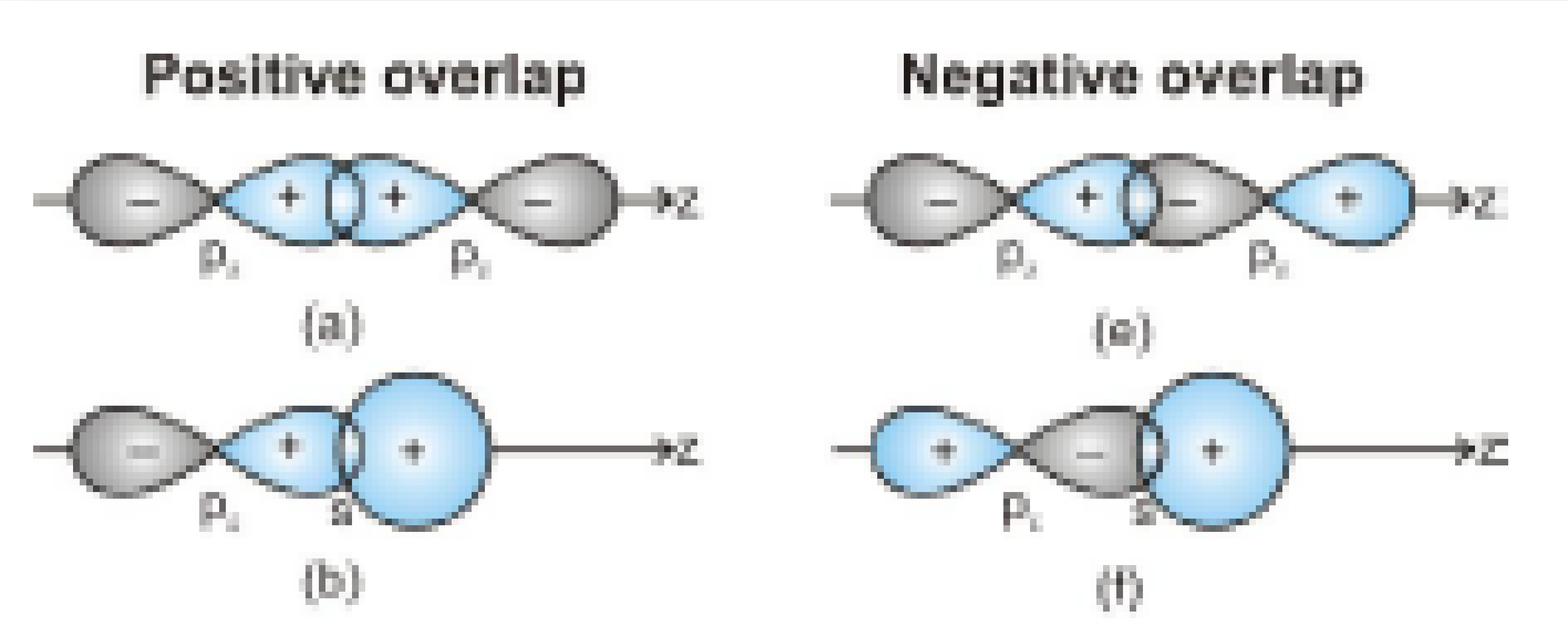
- Therefore, according to orbital overlap concept, the formation of a covalent bond between two atoms results by pairing of electrons present in the valence shell having opposite spins.

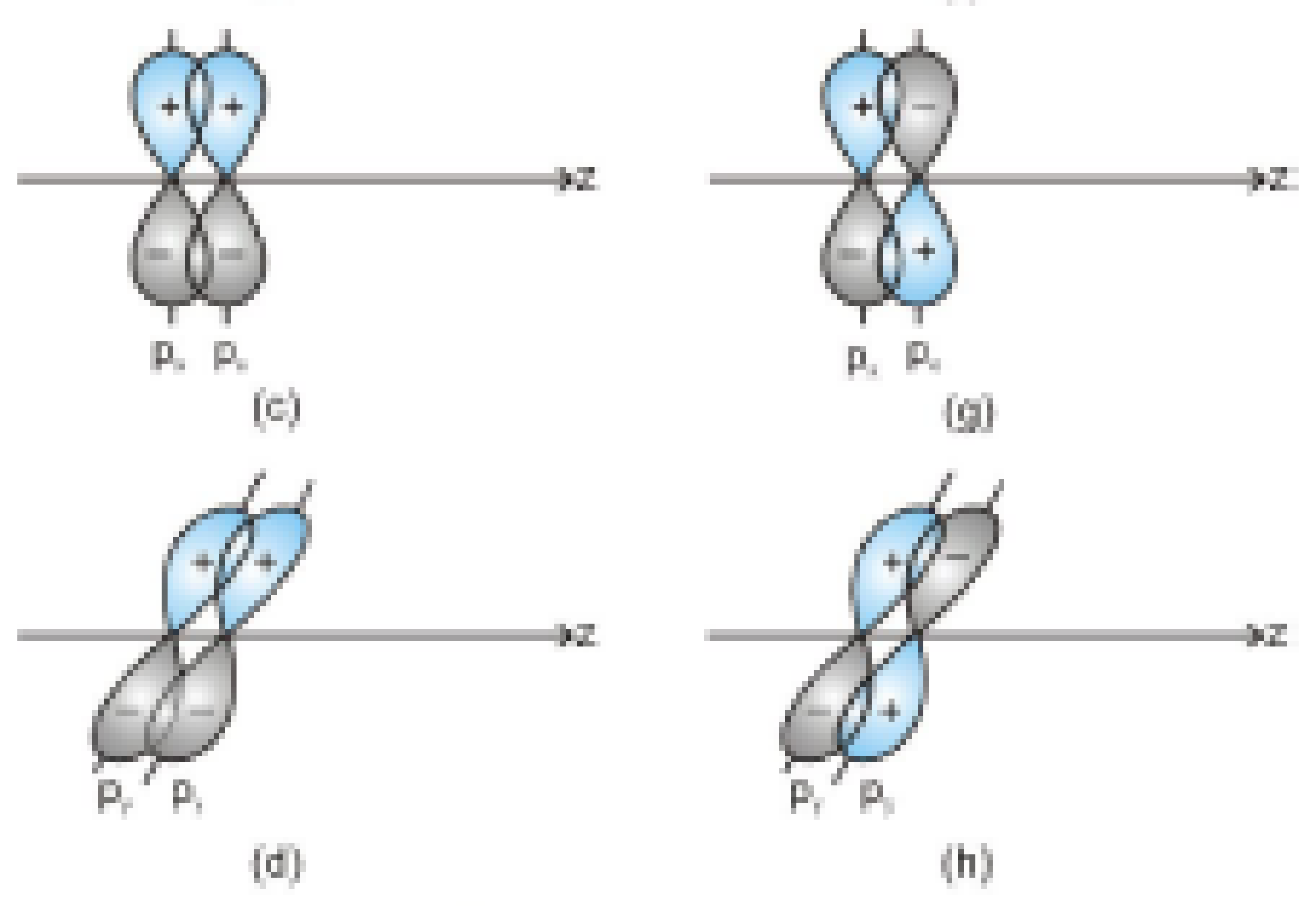
- The molecule of hydrogen is formed due to the overlap of 1*s-orbitals of* two H atoms,
- Why is it so that CH_4 molecule has tetrahedral shape and HCH bond angles are 109.5°?
- Why is the shape of NH3 molecule pyramidal ?
- The valence bond theory explains the formation and directional properties of bonds in polyatomic molecules like CH_4, NH_3 and H_2O, etc. in terms of overlap and hybridisation of atomic orbitals.

Overlapping of Atomic Orbitals

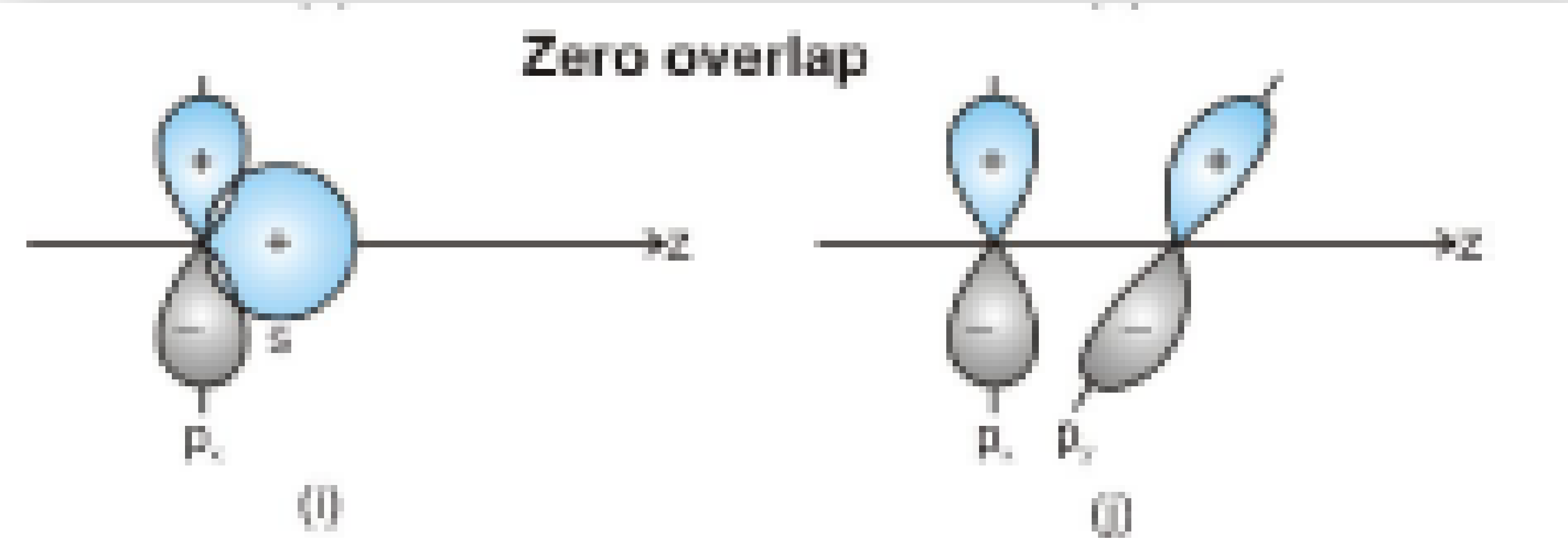
- When two atoms come close to each other, there is overlapping of atomic orbitals.
- This overlap may be positive, negative or zero
- depending upon the properties of overlapping of atomic orbitals

Overlapping of Atomic Orbitals



+
+
−
−
z
p_x p_x
(c)
+
−
−
+
z
p_x p_x
(g)
+
+
−
−
z
p_y p_y
(d)
+
−
−
+
z
p_y p_y
(h)

Zero Overlap



Types of Overlapping and Nature of Covalent Bonds

- The covalent bond may be classified into two types depending upon the types of overlapping:
- (i) Sigma(**σ**) bond, and
- (ii) pi(**π**) bond

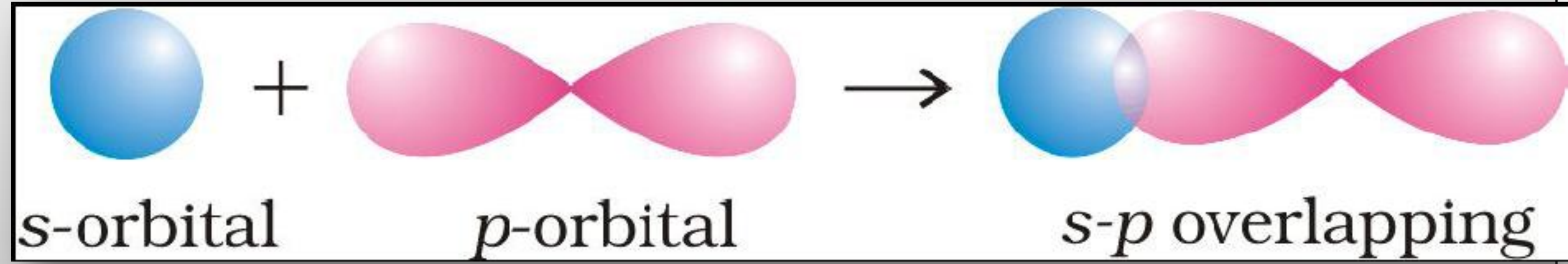
(i) Sigma (σ) bond

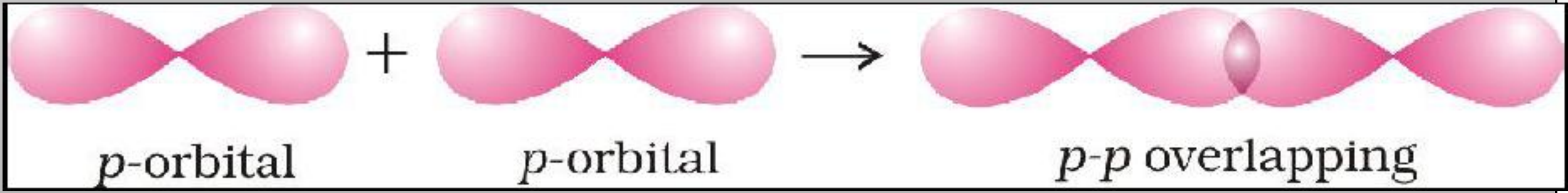
- This type of covalent bond is formed by the end to end (hand-on) overlap of bonding orbitals along the internuclear axis.
- This is called as head on overlap or axial overlap
- ***s-s overlapping***
- ***s-p overlapping:***
- ***p–p overlapping***

(ii) pi(**π**) bond

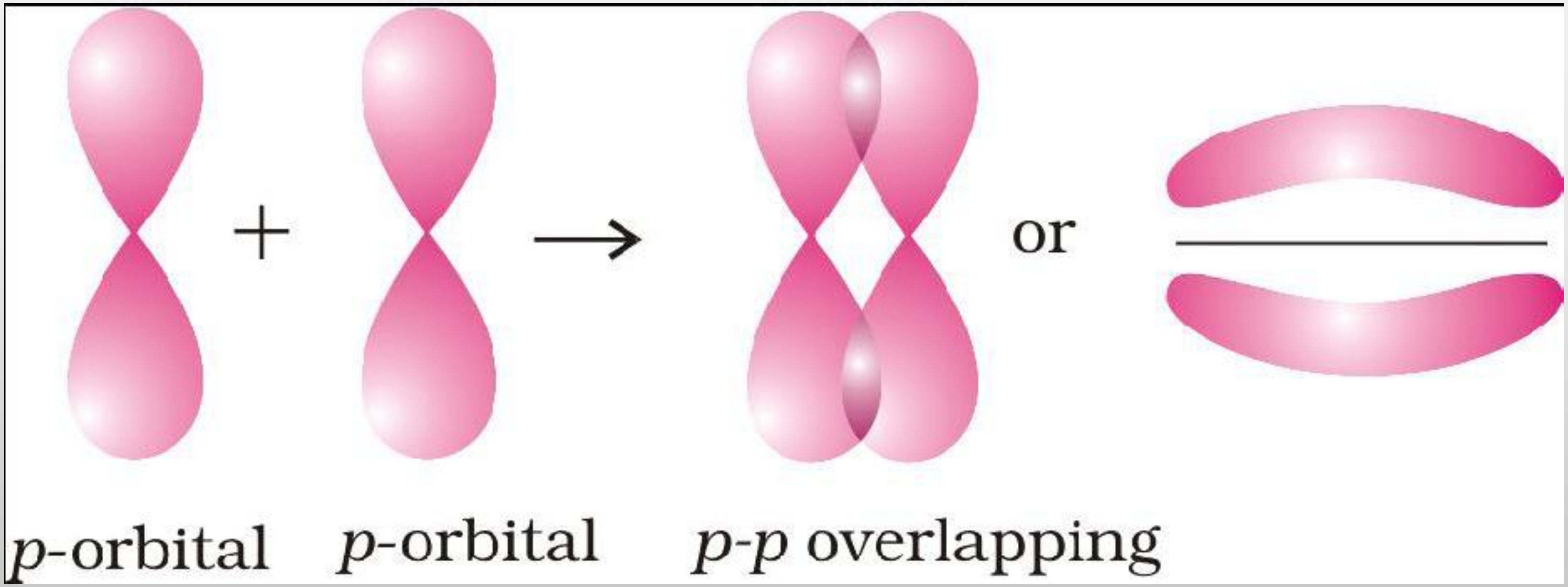
- In the formation of **π** bond the atomic orbitals overlap in such a way that their axes remain parallel to each other and perpendicular to the internuclear axis.
- The orbitals formed due to sidewise overlapping consists of two saucer type charged clouds above and below the plane of the participating atoms.

(i) Sigma (σ) bonds





(ii) pi(π) bond



Strength of Sigma and pi Bonds

HYBRIDISATION

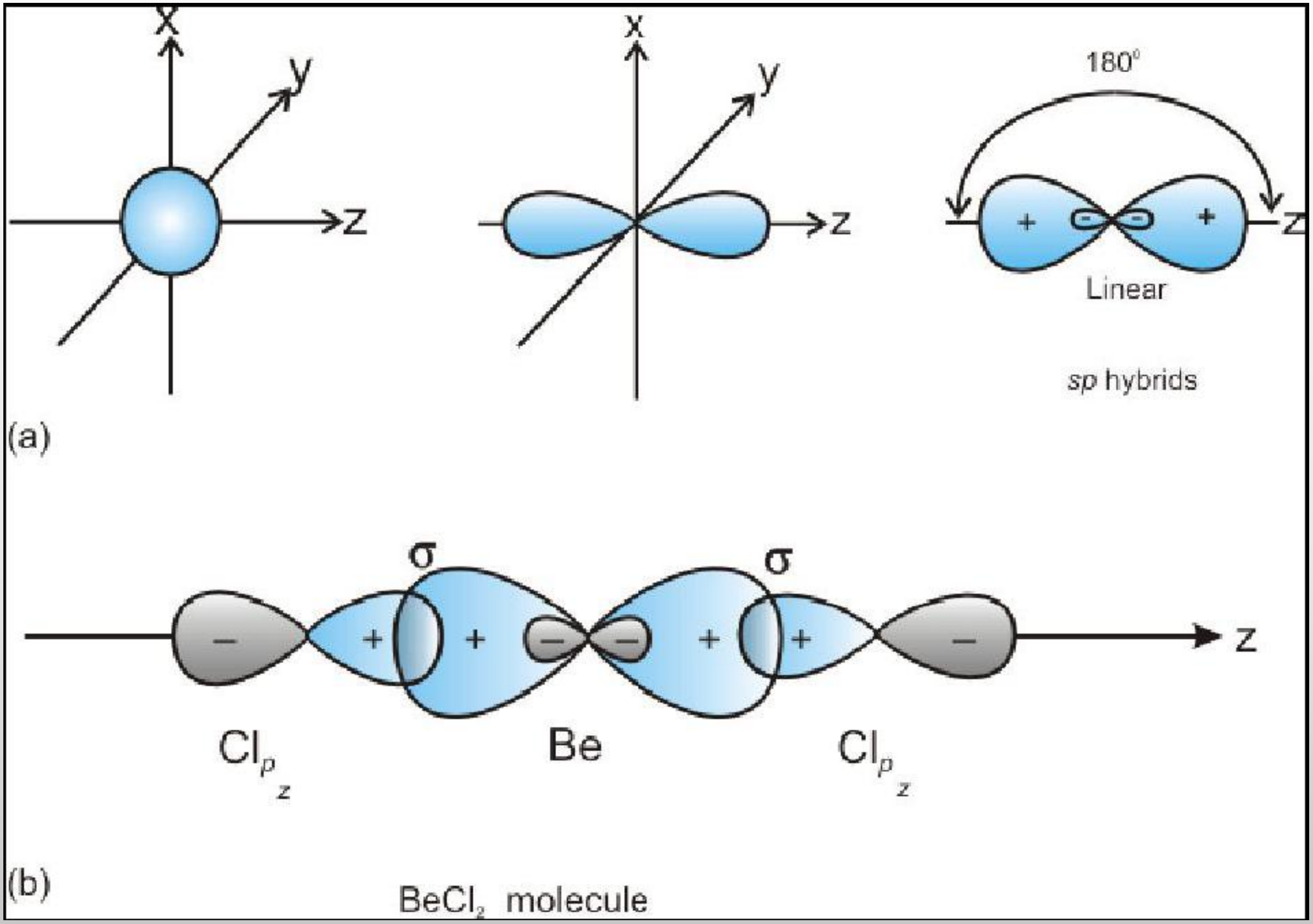
- According to Pauling the atomic orbitals combine to form new set of equivalent orbitals known as **hybrid orbitals.**
- **Unlike pure orbitals, the** hybrid orbitals are used in bond formation.
- The phenomenon is known as **hybridisation**
- ***Hybridisation*** *may be defined as the process of intermixing of the orbitals of slightly different energies so as to redistribute their energies, resulting in the formation of new set of orbitals of equivalent energies and shape*.

Types of Hybridisation

- There are various types of hybridisation involving ***s*, *p*** *and* ***d*** *orbitals.*

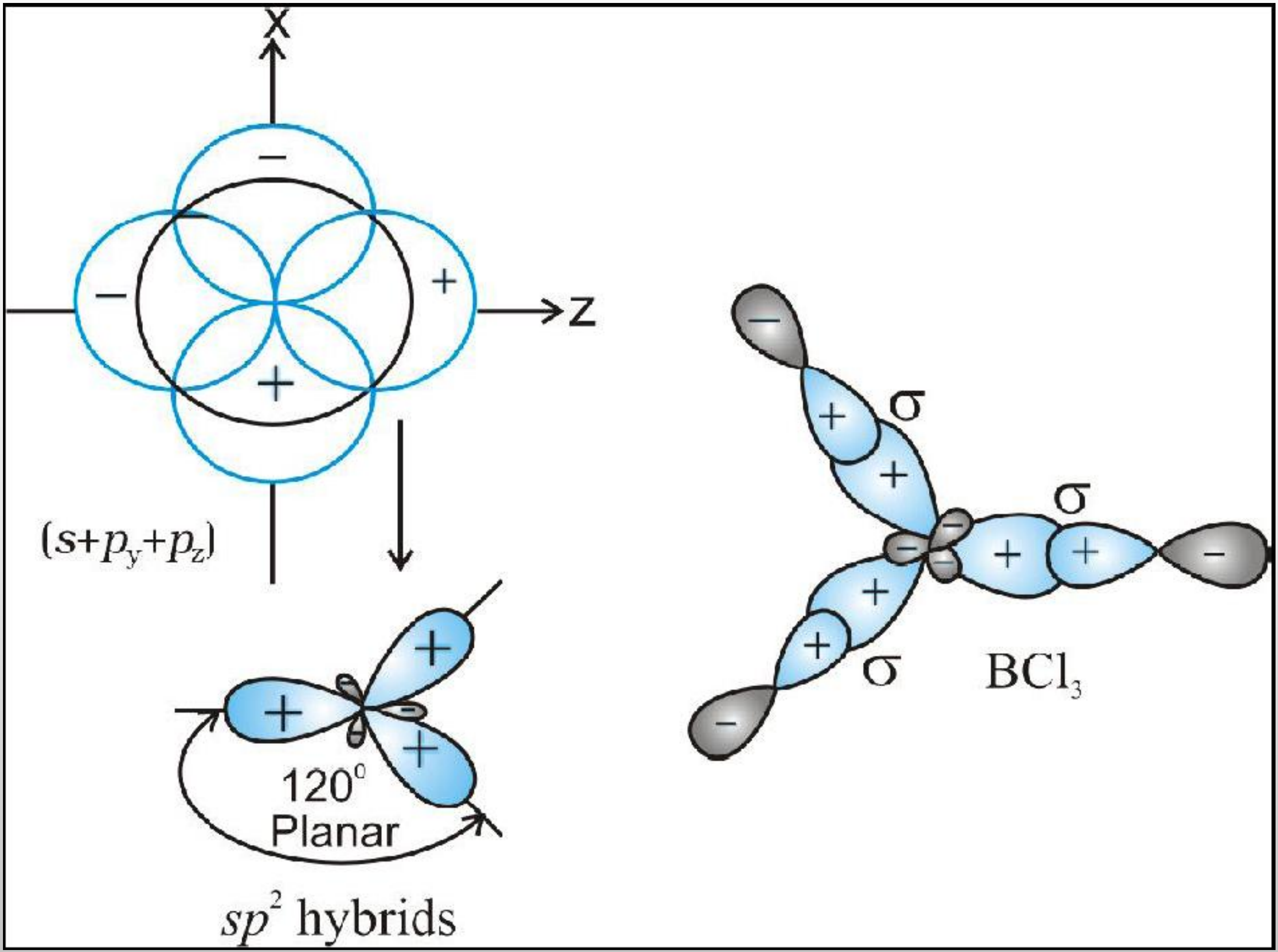
- **(I)** ***sp* hybridisation:**
- **(II)** ***sp^2* hybridisation**
- **(III)** ***sp^3* hybridisation:**

sp hybridisation



(a) Formation of sp hybrids from s and p orbitals;
(b) Formation of the linear $BeCl_2$ molecule

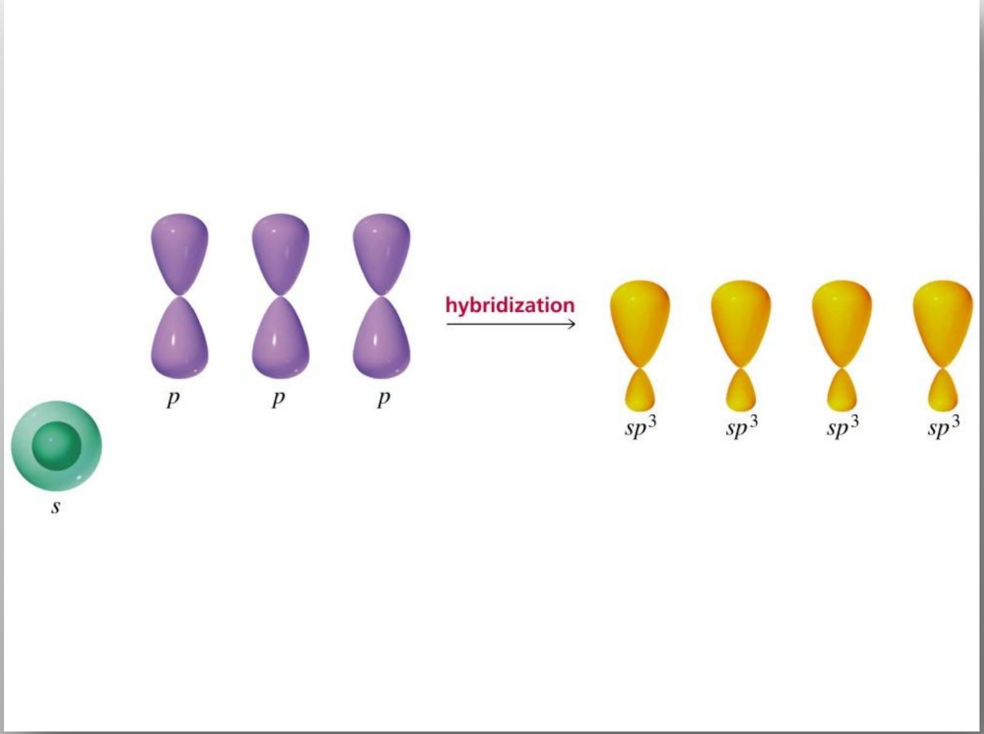
sp^2 hybridisation



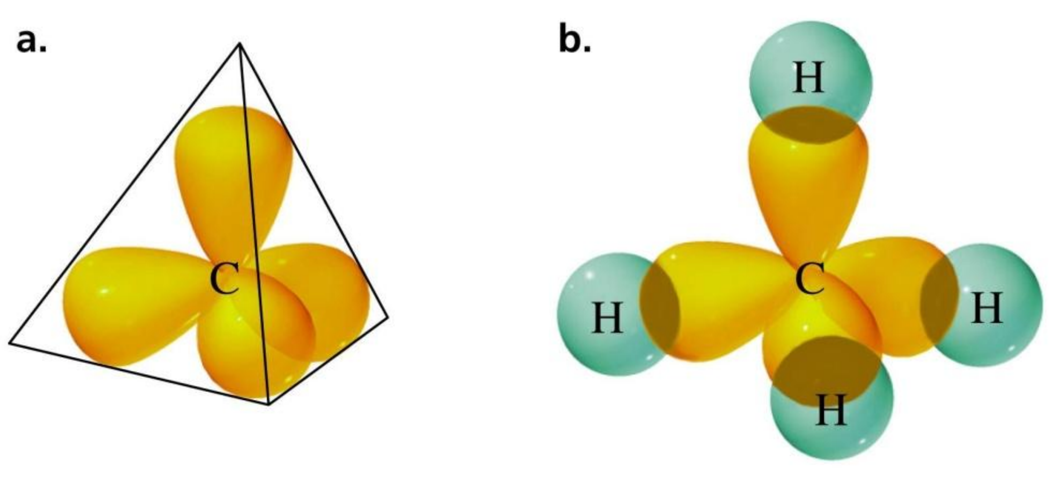
Formation of sp^2 hybrids and the BCl_3 molecule

sp^3 *hybrid* orbitals

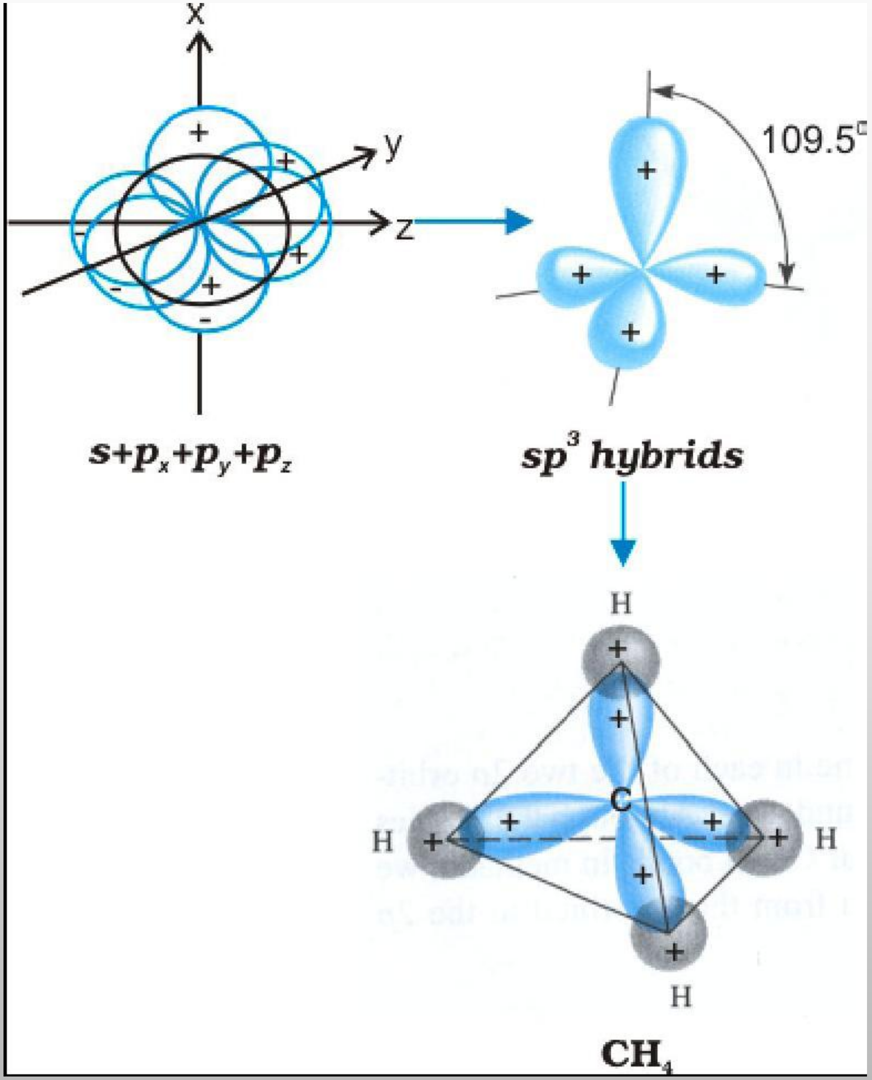
- For example when one 2*s and three 2p-orbitals of carbon* hybridise, there is the formation of **four** new ***sp^3 hybrid*** *orbitals.*



sp^3 hybridisation in Methane



sp^3 hybridisation Methane



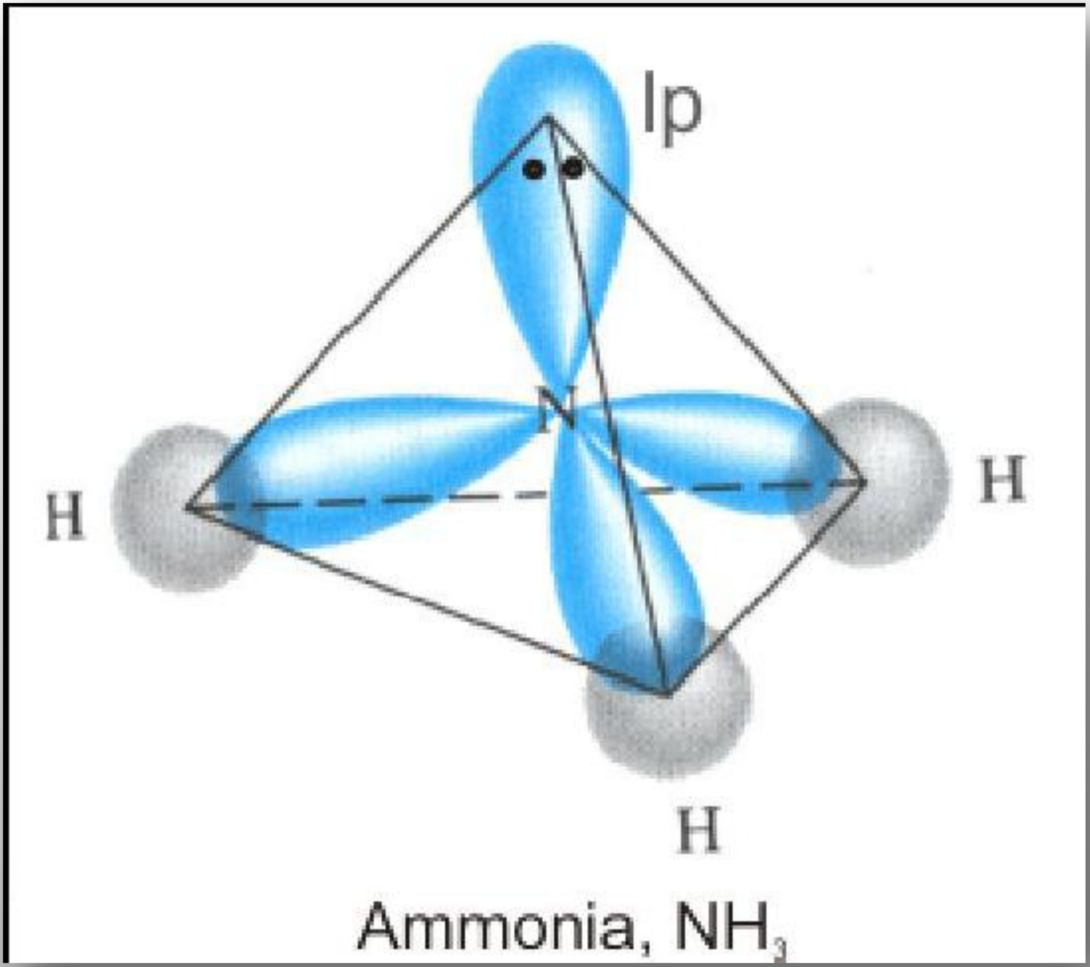
Salient features of hybridisation

1. The number of hybrid orbitals is equal to the number of the atomic orbitals that get hybridised.
2. The hybridised orbitals are always equivalent in energy and shape.
3. The hybrid orbitals are more effective in forming stable bonds than the pure atomic orbitals.
4. These hybrid orbitals are directed in space in some preferred direction to have minimum repulsion between electron pairs and thus a stable arrangement.
5. Therefore, the type of hybridisation indicates the geometry of the molecules.

Important conditions for hybridisation

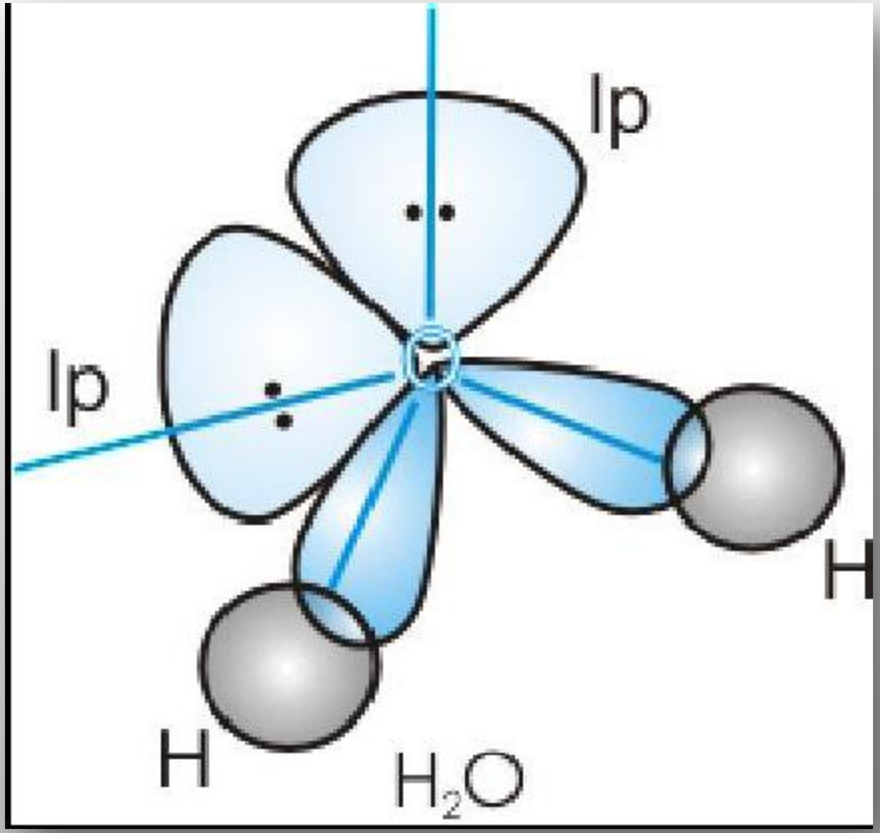
- (i) The orbitals present in the valence shell of the atom are hybridised.
- (ii) The orbitals undergoing hybridisation should have almost equal energy.
- (iii) Promotion of electron is not essential condition prior to hybridisation.
- (iv) It is not necessary that only half filled orbitals participate in hybridisation. In some cases, even filled orbitals of valence shell take part in hybridisation.

Formation of NH_3 molecule



Ammonia, NH_3

Formation of H_2O molecule



Types of H-Bonds

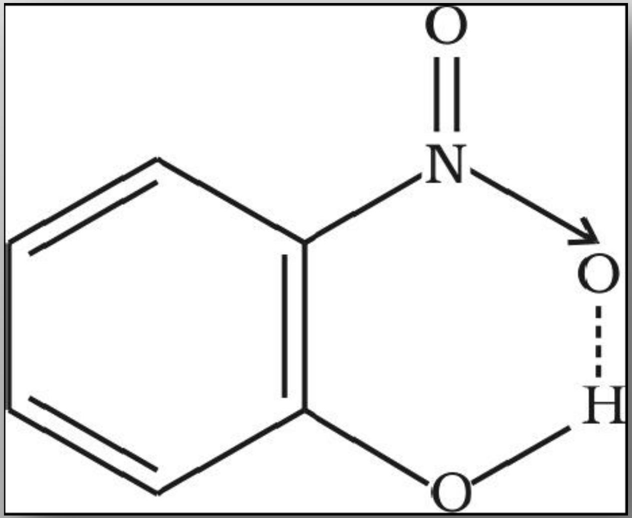
- There are two types of H-bonds
  - (i) Intermolecular hydrogen bond
  - (ii) Intramolecular hydrogen bond

Intermolecular hydrogen bond

- ***It is*** formed between two different molecules of the same or different compounds. For example, H-bond in case of HF molecule, alcohol or water molecules, etc.

Intramolecular hydrogen bond

- It is formed when hydrogen atom is in between the two highly electronegative (F, O, N) atoms present within the same molecule.
- For example, in *o-nitrophenol the hydrogen is in* between the two oxygen atoms.



Thank you

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