Chemical bonding

- **Ionic bond :-** b/w electropositive & electronegative element
  Covalent :- b/w 2 -ve elements
  Metallic = b/w 2 +ve elements
  Gain 1 e^- :- @ electro -ve , Loss e^- = electro +ve

★ **% ionic character** $= 16(x_A - x_B) + 3.5(x_A - x_B)^2$,
  in a molecule.

→ **Lattice energy (U) :-** Energy released when no. of +ve and
  -ve ions combine to form one mole of ionic compound
  $(U = -ve)$

- Energy required to break apart an ionic solid and
  convert its components into gaseous ions $(U = +ve)$
  ↑ Lattice Energy, ↑ Stability, ↑ MP & B.P.
  ↓ Solubility

★ **Born Haber Cycle :-** Application of Hess's law
  ① Calculate lattice energy
  ② Determine the electron affinity
  ③ determine bonding in compound is truly ionic

$$\Delta H = \Delta H + I.E + \frac{1}{2} \Delta H + \Delta H + \Delta H$$
$$\quad\ \text{Sublimation} \qquad\qquad\ \text{B.D.E} \quad\ \text{E.G.} \quad \text{Lattice}$$
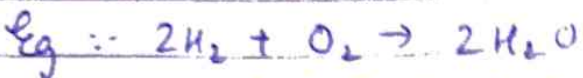
★ **Covalent B-E changes.**
  B.E can be used to estimate energy change of chemical
  rxn
  in reactant
  When bond broken , $\Delta H = +ve$
  When bond form in products , $\Delta H = -ve$

B.E.( )

NF_3 NH_3 because of differ...
$\angle 102.4°$ $107.48°$ polarity of N in these indicate
                                F more electronegative than H

$$Eg :- 2H_2 + O_2 \rightarrow 2H_2O.$$
$$2H-H + O-O \rightarrow 2H-O.H$$
Energy required to break.   Energy required to form
$2H-H = 2(+436 \, kJ/mol)$ $4(O-H) = 4(465)$
$1O-O = (+498 \, kJ/mol$ $1852 \, kJ/mol$
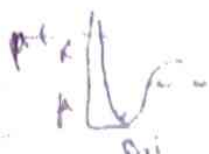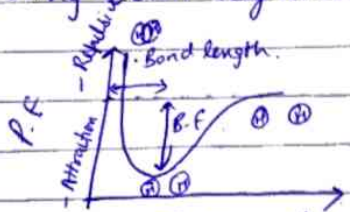$1370 \, kJ/mol$ $O=H-H \cdot H-H=O$

Net energy change = $1370 - 1852 = 482 \, kJ/mol$

* Potential Energy curve for H_2 molecule
When H atoms separated by large distance (∞) we
take this energy to O.
$\downarrow$Energy , $\uparrow$ Stability
For H_2, Bond length = 74 pm.
moving atoms together $\uparrow$ P.E

Bond length.

P.E vs Distance.

moving
atoms P.E

Internuclear distance (pm)   strong bonds, over d...

* Props of Covalent bond. (MP $\downarrow$, BP $\downarrow$, Electricity X, Soluble $\downarrow$)
① Does not result in formation of new e's. bond only pairs them
② Very powerful chemical bonds exist b/w atoms
③ Most compounds with covalent bond have $\downarrow$MP, $\downarrow$BP
④ Compounds don't conduct electricity due to lack of free e's
⑤ Not soluble in water   covalent bond
• Bond order :- Total e pairs b/w 2 atoms. BO $\propto$ Stability
→ Bond angle :- Angle b/w 2 covalent bonds. originate from
   same atom
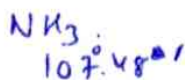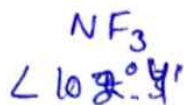   B.A. $\propto$ Electronegativity
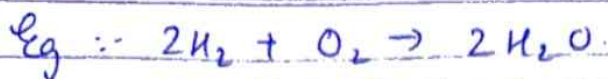 $104.5°C$
→ Bond length:-
Distance b/w nuclei of 2 chemically bonded atoms in
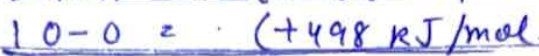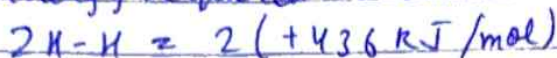a molecule.   B.L $\propto \dfrac{1}{Bond \, order}$
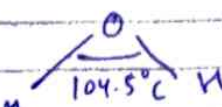
NF_3 NK_3 be cause of difference in
$\angle 102.4'$ $107.48°1$ polarity of N in these molecules
                         F more electronegative than H.
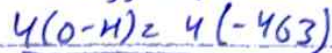
$Eg :- 2H_2 + O_2 \rightarrow 2H_2O.$

$2H-H + O-O \rightarrow 2H-O-H$ 4OH bonds

Energy required to break.   Energy required to form

$2H-H = 2(+436 kJ/mol)$ $4(O-H) = 4(-463)$

$1 O-O = (+498 kJ/mol$ $-1852 kJ/mol$

        $1370 kJ/mol.$ $O=H-H-H-H=O$

                                ,(OH)(2H)
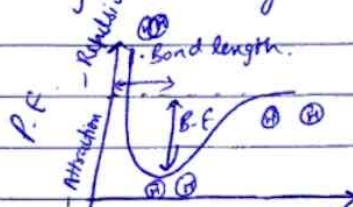
       Net energy change ⟹ $1370-1852 = -482 kJ/mol$

★ Potential Energy curve for H_2 molecule.

When H atoms separated by large distance (∞) we
take this energy to 0.

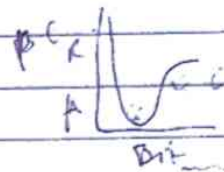 $\downarrow$ Energy , $\uparrow$ Stability.

For H_2 , Bond length $= 74$ pm.

moving atoms together $\uparrow$ P.E.

P.E vs Distance

           $\infty \rightarrow E < 0$

Internuclear distance (pm).   strong bonds, sharing

★ Props of Covalent bond. (MP $\downarrow$, BP $\downarrow$, Electricity ✗, Soluble $\downarrow$)

① Does not result in formation of new e^-s. bond only pairs them

② Very powerful chemical bonds exist b/w atoms

③ Most compounds with covalent bond have $\downarrow$MP, $\downarrow$BP

④ Compounds don't conduct electricity due to lack of free e^-s

⑤ Not soluble in water

• Bond order :- Total e^- pairs b/w 2 atoms. BO $\propto$ Stability
                 covalentey bond

→ Bond angle :- Angle b/w 2 covalent bonds originate from
same atom

                      O

                     $104.5°$ B.A. $\propto$ Electronegativity.
                 H   H

→ Bond length :-

• Distance b/w nucles of 2 chemically bonded atoms in
a molecule.   B.L. $\propto \dfrac{1}{Bond\ order}$

Werner

$$B.E \propto \frac{1}{BL} \propto BO \propto Electronegativity \propto \frac{1}{size\ of\ anion}$$

'BL ↑ with size of anion.

BL :- $sp^3 > sp^2 > sp$.

→ Bond Energy :- Strength of chemical bond / Energy required to break all covalent bonds in one mole of a chemical compound (gaseous)

$$\checkmark\ B.E \propto \frac{1}{BL} \propto Bond\ order. \propto Electronegativity$$

★ EAN :- Total no. of e^-s surrounding nucleus of a metal atom in a metal complex.

✓ EAN :- Atomic number(Z) — Oxidation no. (x) + 2× Coordination No.

C.N = No. of ligands × No. of coordinate bonds formed by ligand.

Eg :- $[Cu(NH_3)_4]^{2+}$

EAN = 29 − 2 + 2(4) = 35 (Exception due to odd no. of e^-s)

★ VSEPR :- Whenever there is repulsion b/w pairs of valence e^-s in all atoms, atoms will rearrange themselves in a geometric shape so as to minimize e^- pair repulsion.
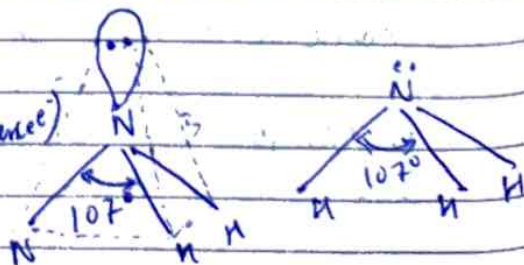
Postulates.

① Triple bond > Double bond > Single bond -- Order of repulsion.
② Strength :- $lp-lp > lp-bp > bp-bp$.
③ Decides shape of molecule
④ In polyatomic molecules, one of constituent atom is identified as central atom to which all other atoms belonging to molecule are linked
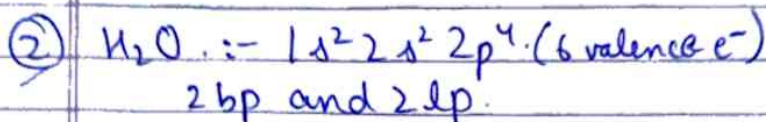
★ Structure.
① NH_3 :- $1s^2 2s^2 2p^3$ (5 valence)
   3 bp and 1 lp.
   Geometry :- Pyramidal
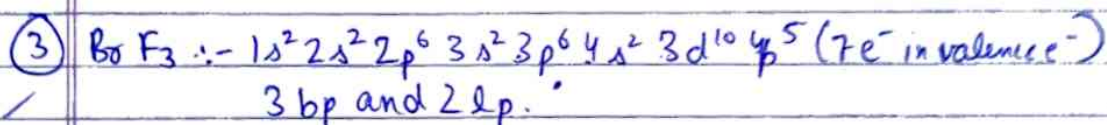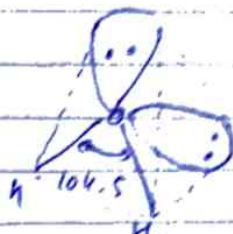
$107°$

$107°$

Presence of l.p on N will repel the bp more than bp - bp. repulsions. Leads to decrease in H - N - H bond angle from $109°28'$ to $107°48'$

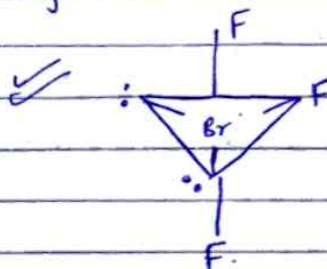② H_2O :- $1s^2 2s^2 2p^4$ (6 valence e^-)
   2 bp and 2 lp.

❖ Geometry :- Bent/Angular/V shaped.

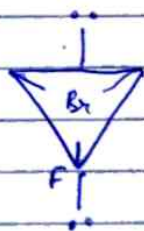Due to presence of 2 lps on O, Repulsion will be b/w both lp's, lp - bp and both bp's.
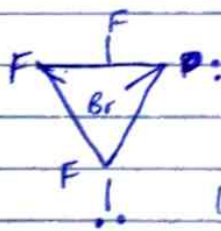   Repulsion b/w lps is more ↑, H_2O is more deviated from symetrical tetrahedral geometry resulting in bent shape

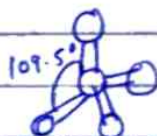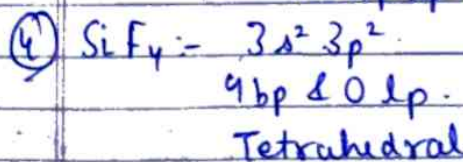③ BrF_3 :- $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$ (7 e^- in valence e^-)
   3 bp and 2 lp.
   Geometry :- T.B.P

4 90° repulsions b/w lp - bp
No lp - lp at 40°.

∴ Most symmetrical
6 90° repulsions
b/w lp - bp
No lp - lp at 40°

3 90° repulsion
b/w lp - bp
1 lp - lp at 40°

④ SiF_4 :- $3s^2 3p^2$
   4 bp & 0 lp.
   Tetrahedral

* VBT :- Covalent bonds form when.
• an orbital one one atom overlaps an orbital on 2nd atom
• Single e's in each orbital combine to form an e⁻ pair

$$(C_1 \psi_A + C_2 \psi_B)^2$$

→ * Limitations of VBI.
Many molecules such as methane (tetrahedral, B A= 105°)
cannot be explained by half filled atomic orbitals

→ Hybridization :- Concept of mixing 2 atomic orbitals to give
rise to a new type of hybridized orbitals.

① sp :- 1s and 1p orbital
Shape = Linear

Eg BeF$_2$

	1s	2s	2p
g.s	⇅	⇅	☐ ☐ ☐
e.s	⇅	↑	↑ ☐ ☐
2 bonds with F atoms	⇅	⇅	⇅ ☐ ☐

→ g-s overlap :-   ◯ + ◯ → ◖◗
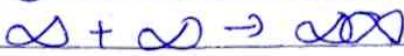
⊙ s-p overlap :-   ◯ + ∞ → ∞◯
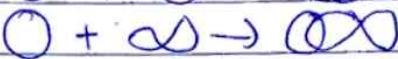
⊙ p-p overlap :-   ∞ + ∞ → ∞∞

                    Describe
* MOT :- "Structure and properties of diff. molecules.
1. Use LCAO to form molecular Orbital concept.

Postulates :

1. Atomic orbitals overlap to form new orbitals called
molecular orbitals

• e⁻'s in molecules filled in new energy states.

• No. of molecular orbitals formed = no. of atomic orbitals

• Shape of molecular orbitals formed depends upon shape (combining)
of combining atomic orbitals.

→ LCAO :- An atomic orbital is an e⁻ wave; the waves of
2 atomic orbitals may be in phase or out phase.

Probability of finding an e⁻ in a given volume space

$$\psi^2_{AB} = (c_1^2 \psi^2_A + 2c_1 c_2 \psi_A \psi_B + c_2^2 \psi^2_B)$$
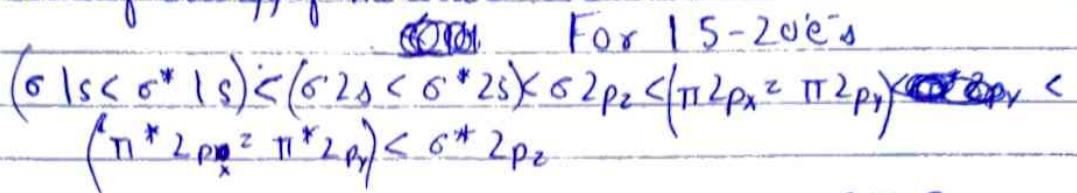
Prob. of finding an   Overlap   Prob. of finding an
e⁻ on atom A   Integral   e⁻ on atom B.

Conditions for LCAO.

- Atomic orbitals combining to form molecular orbitals should have comparable energy.
- Combining atoms should have same symmetry.
- 2 atomic orbitals will combine to form molecular orbital if overlap is proper. ↑ Overlap of Orbitals, ↑ Nuclear density b/w nuclei of 2 atoms

★ Order of energy of molecular orbitals

For 15-20 e⁻'s

$$(\sigma 1s < \sigma^* 1s) < (\sigma 2s < \sigma^* 2s) < \sigma 2p_z < (\pi 2p_x = \pi 2p_y) < \text{2p}_y <$$
$$(\pi^* 2p_x = \pi^* 2p_y) < \sigma^* 2p_z$$

< 14 e⁻'s

For molecules like Li, Be, B, C, N.   For ≤ 14 e⁻'s 15-20 e⁻
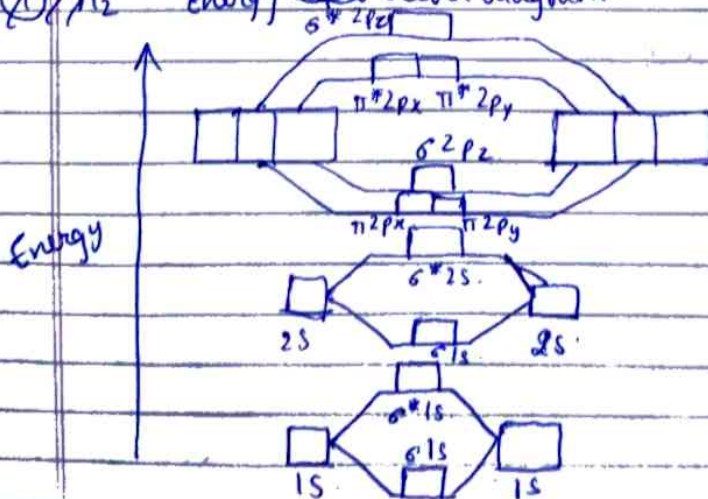
$$(\sigma 1s < \sigma^* 1s) < (\sigma 2s < \sigma^* 2s) < (\pi 2p_x = \pi 2p_y) < \sigma 2p_z < (\pi^* 2p_x = \pi^* 2p_y)$$
$$\sigma^* 2p_z$$

Reason :- sp mixing ; S is more stabalised than p.

★ Resonance :- It is way of describing the delocalization of e⁻'s within molecules.

★ MOT of H_2, N_2, O_2, F_2.

① H_2 Energy level diagram.

Energy
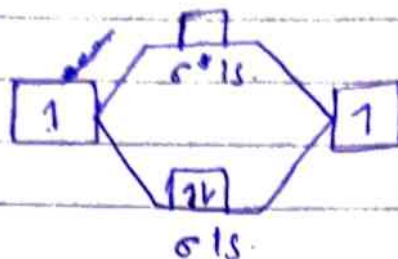
Werner bacha hai-

① $H_2 :- \sigma 1s^2$

② $N_2 :- \sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2 \pi 2p_x^2 z \pi 2p_y^2 \sigma 2p_z^2$

$N_{7e} - z 1s^2 2s^2 2p^3$