HSAB Theory [Hard & Soft Acid Base Theory]

1. Metal-Ligand Bond :-

(A) (B)

↓ ↓ $A \leftarrow :B$

e^- acceptor e^- donor

Case 1 :- If A → strong e^- acceptor, B → weak e^- donor ⇒ strong complex (stable complex)

Case 2 :- If either A or B are strong/weak acceptor/donor ⇒ weak complex (unstable complex)

2. Hard/Soft Acid Base

A < Hard Lewis Acid / Soft Lewis Acid & B < Hard Lewis Base / Soft Lewis Base

Properties of :-

(i) Hard Acid :-
- Small ionic radius
- High +ve charge
- Low electron affinity & High electronegativity
- Empty orbitals in their valence shell
- Low polarisability
- High Ionisation Potential

Eg :- Alkali & Alkaline light metals :- Na^+, K^+, Ca^{2+}, H^+
(G1) (G2)

Examples of complex/molecules :- BF_3, $AlCl_3$, CO_2, ~~SO_2~~

* Hard Lewis Acid —prefers→ Hard Lewis Base
(But)
Hard Lewis Acid —does not prefer→ ~~Soft~~ Lewis Base

In transition metals,

↳ Examples :- Fe^{3+}, Cr^{3+}, Al^{3+}

(ii) Soft Acid :- • Large ionic radius
• Low +ve charge
• High electron affinity & low electronegativity
• Completely filled atomic orbitals
• High polarizability
• Low Ionisation Potential

Eg :- Transition metals (Gr 10, Gr 11, Gr 12) :- Cu^+, Ag^+, Au^+, Pt^{2+}, Pd^{2+}, Hg^+

Example of complex/molecules :- BH_3, Br_2, I_2, ...

(iii) Hard Base :- • Small ionic radius
• High -ve charge
• Low electron affinity & High electronegativity
• Empty orbitals in their valence shell
• Low polarisability
• High Ionisation potential

Eg :- F^-, NH_3, H_2O, SO_4^{2-}, PO_4^{3-}, OH^-, etc

Example of complex/molecule :- H_2O, NH_3

(iv) Soft Base :- • Large ionic radius
• Low -ve charge
• High electron affinity & Low electronegativity (Intermediate)
• Completely filled atomic orbitals
• High polarizability
• Low Ionisation Potential

Eg :- I^-, S^{2-}, NCS^-

Example of complex/molecule :- PPh_3, PR_3, CO, C_6H_6

3 According to HSAB Theory, hard acids prefer to bind with hard bases to give rise to ionic complex whereas soft acid prefer binding with soft base to give rise to covalent complex.