Charge Transfer Transitions

*Some transition metal compounds **with no d-electrons** are colored.

This is because there can be electronic transitions in the visible region that do not involve d-electrons.

It called **Charge transfer**

*The colour is a result of the transfer of an electron from the ligands into the d-orbitals of the central atom (**LMCT**), **or vice versa (MLCT)**.

LMCT (Ligand to Metal Charge Transfer): excitation of an electron in a **ligand-based** orbital into an empty **metal-based** orbital.

LMCT transition is a partial transfer of electrons from the **ligand** to the **metal**.
This is common when the **metal** has a **high oxidation state** (e.g., Mn^{7+} in MnO_4^-, Cr^{6+} in CrO_4^{2-} and V^{5+} in V_2O_5)

$KMnO_4$ $K_2Cr_2O_7$

MnO_4^- : In this case, electrons in filled **O** based orbitals are **excited** into empty **Mn d-orbitals** gives the **intense purple color of permanganate.**

In this **oxo-anion**, the electron migrates from an orbital that is largely limited to the **O** atom ligands to an orbital that is largely limited to the **Mn** atom.

Conditions for LMCT

1. Presence of pi donor ligands:

   F^-, Cl, Br-, I^-, H_2O, OH^-, RS^-, S_2^-, NCS^-, NCO.

2. Metal ions are devoid of d- electrons.

MLCT transition is a partial transfer of electrons from the **metal** to the **ligand**.

Usually this occurs for metals with highly-filled d orbitals capable of donating electrons into the **antibonding** orbitals of the aromatic entity (ligand).

The non-bonding d orbitals must match the antibonding orbitals in terms of size, shape, and symmetry

Conditions for MLCT

1. Presence of pi accepting ligands

CO, NO, CN^-, N_2, bipy, phen, RNC, $C_5H_5^-$, $C{=}C$, $C{\equiv}C$

2. Metal in 0,+1,+2 oxidation states (low oxidation state).

****MLCT** Transitions or **LMCT** transitions resulted in strong intensity of colour**