Shri Shivaji Mofat Education Society's

Shri Shivaji College Of Art's, Commerce & Science, Kandhar

Coordination Compound

Presented By

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Welcome

Bonding in coordination compounds

1) Valence Bond Theory (VBT)

2) Crystal field theory (CFT)

3) Ligand field theory (LFT)

4) Molecular Orbital Theory (MOT)

Valance Bond Theory

❖ **Postulates of Valance Bond Theory:**

1) Metal ion in complex provides definite no. of vacant orbital s, p and d to form cordanate bond with ligands.
2) Number of vacant orbitals provided by metal atom is its co. no.
3) The metal atom or ion under the influence of ligands can use its (n-1)*d*, n*s*, n*p* or n*s*, n*p*, n*d* orbitals for hybridization to yield a set of equivalent orbitals of definite geometry.
4) These hybridised orbitals are allowed to overlap with ligand orbitals that can donate electron pairs for bonding.
5) If (n-1) d orbitals are used for hybridization called inner complexes.
6) If nd orbitals are used for hybridization called outer complexes.

Valance Bond Theory

Types of Hybridisations

Coordination number	Type of hybridisation	Distribution of hybrid orbitals in space
4	sp^3	Tetrahedral
4	dsp^2	Square planar
5	sp^3d	Trigonal bipyramidal
6	sp^3d^2	Octahedral
6	d^2sp^3	Octahedral

Valance Bond Theory

Common Geometries of Complexes

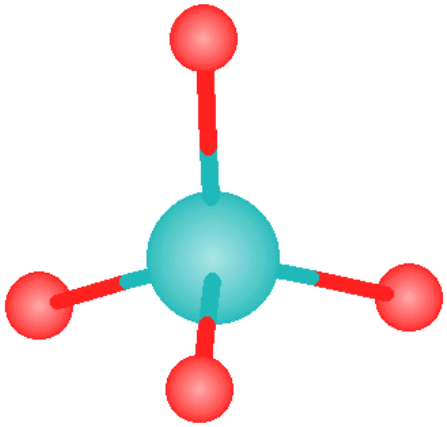
Coordination Number	Geometry
2	 Linear

Example: $[Ag(NH_3)_2]^+$

Common Geometries of Complexes

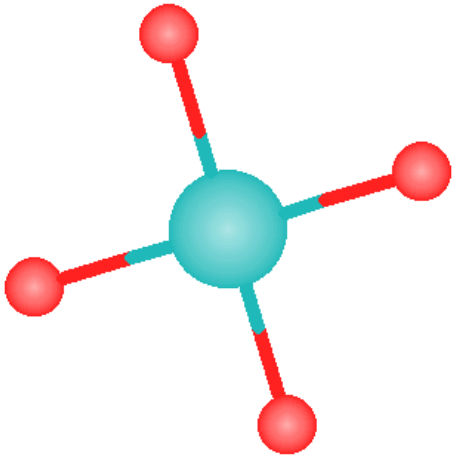
Coordination Number	Geometry
4	tetrahedral

Examples: $[Zn(NH_3)_4]^{2+}$, $[FeCl_4]^-$

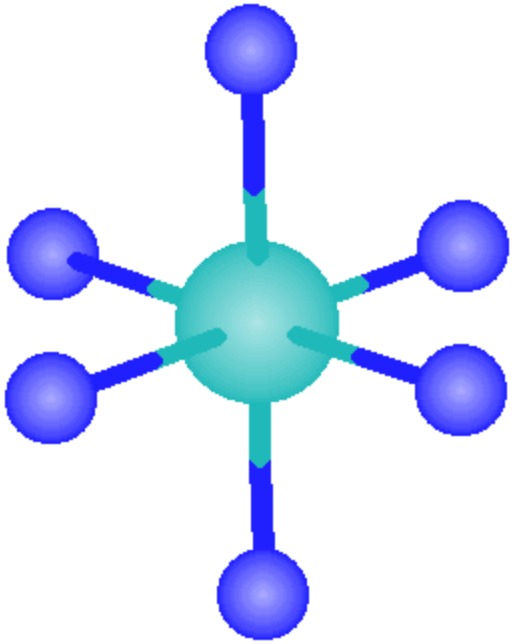


square planar

Example: $[Ni(CN)_4]^{2-}$



Common Geometries of Complexes

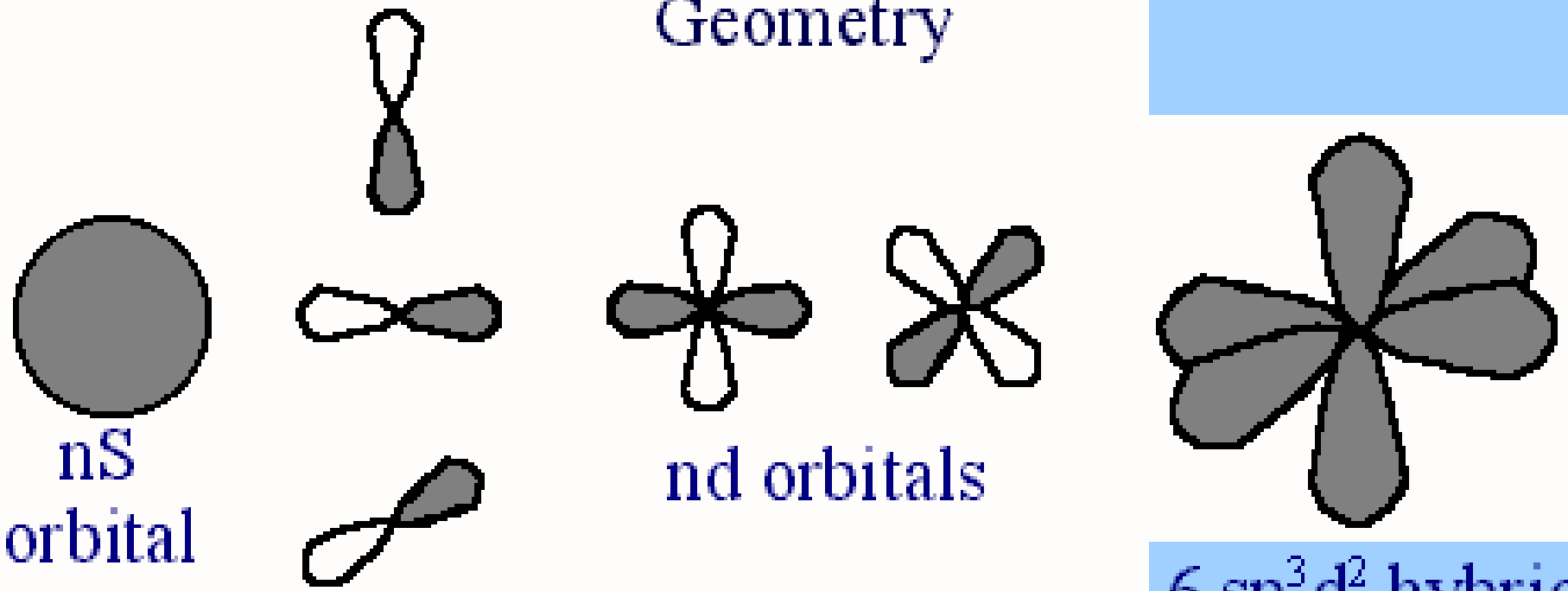
Coordination Number	Geometry
6	

Examples: $[Co(CN)_6]^{3-}$, $[Fe(en)_3]^{3+}$

octahedral

Valence Bond Theory

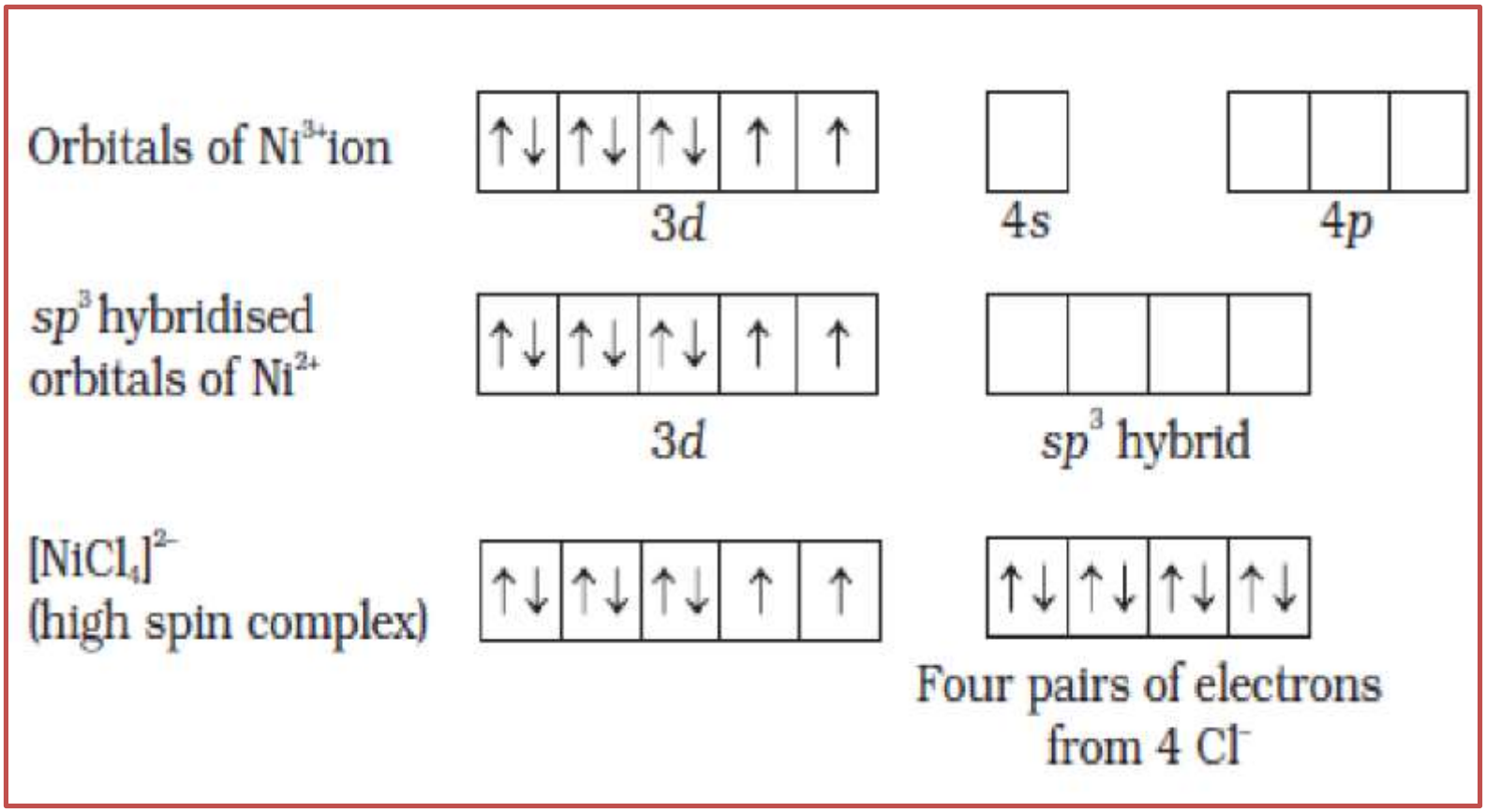
Example of hybrid orbital formation: Octahedral Geometry



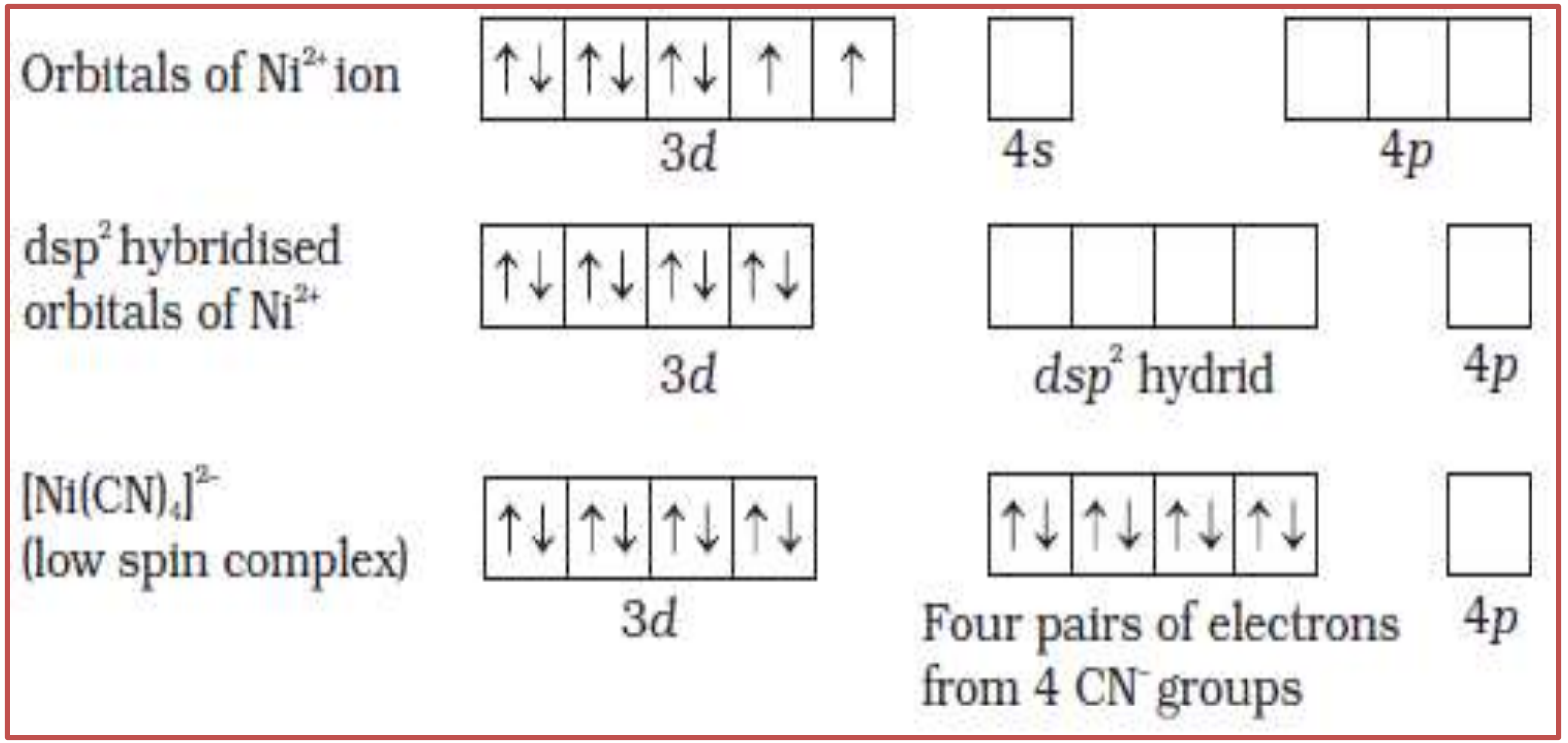
Mixing these 6 atomic orbitals of the metal ion together gives 6 equivalent hybrid orbitals.

Tetrahedral complexes

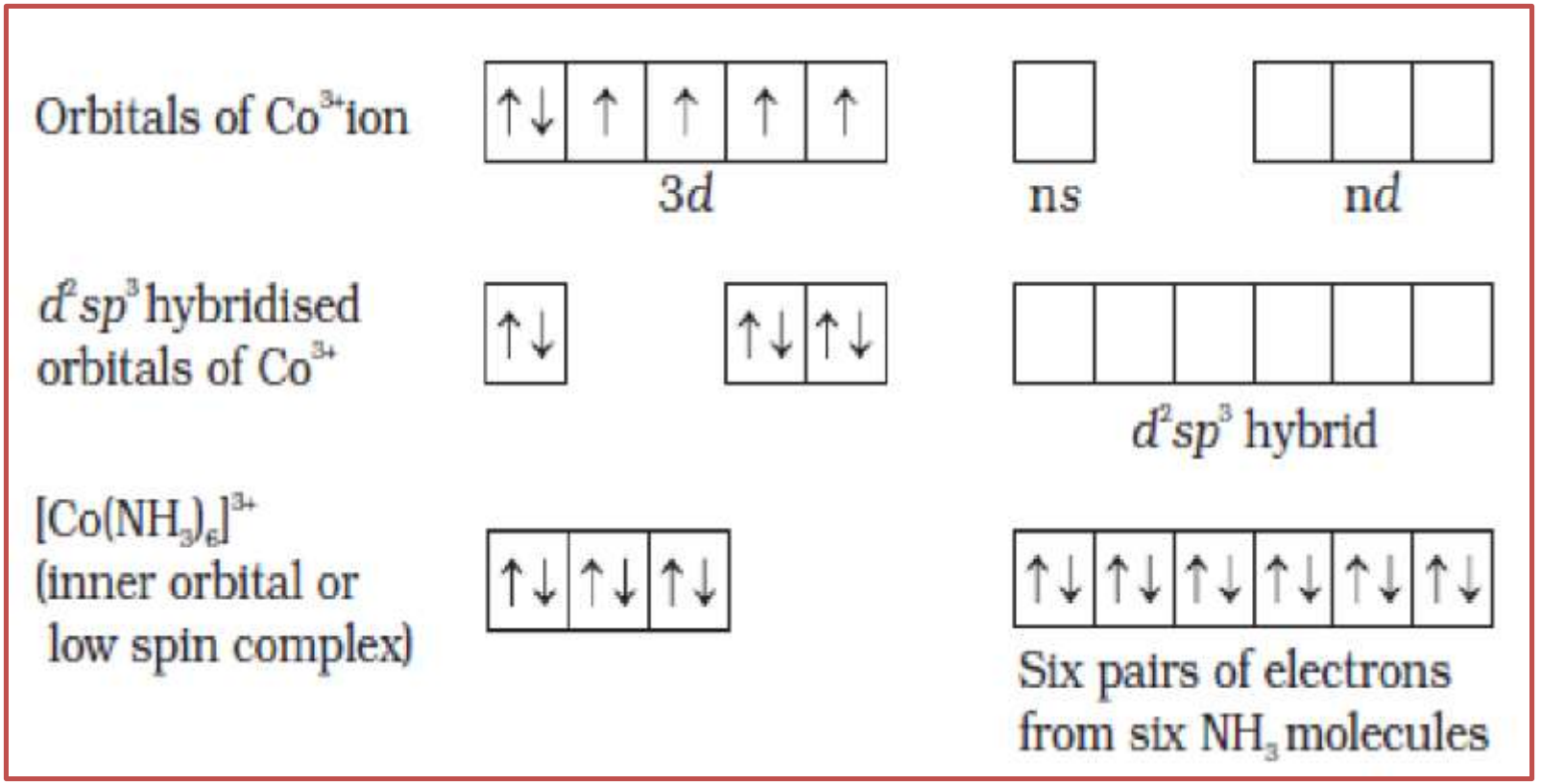
$[NiCl_4]^{2-}$



Square planar complexes $[Ni(CN)_4]^{2-}$

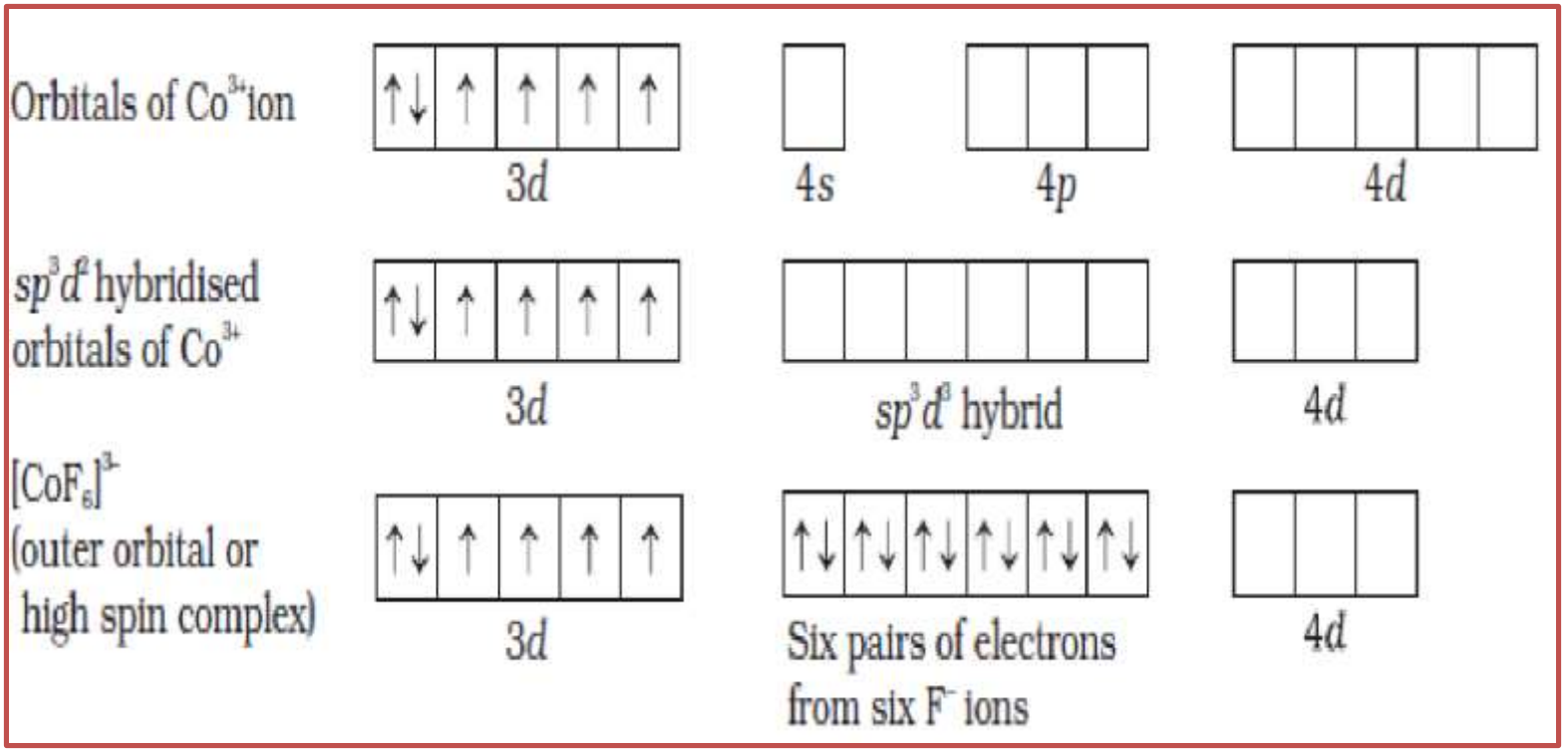


Octahedral complex $[Co(NH_3)_6]^{3+}$



low spin complex

Octahedral complex $[Co(NH_3)_6]^{3+}$

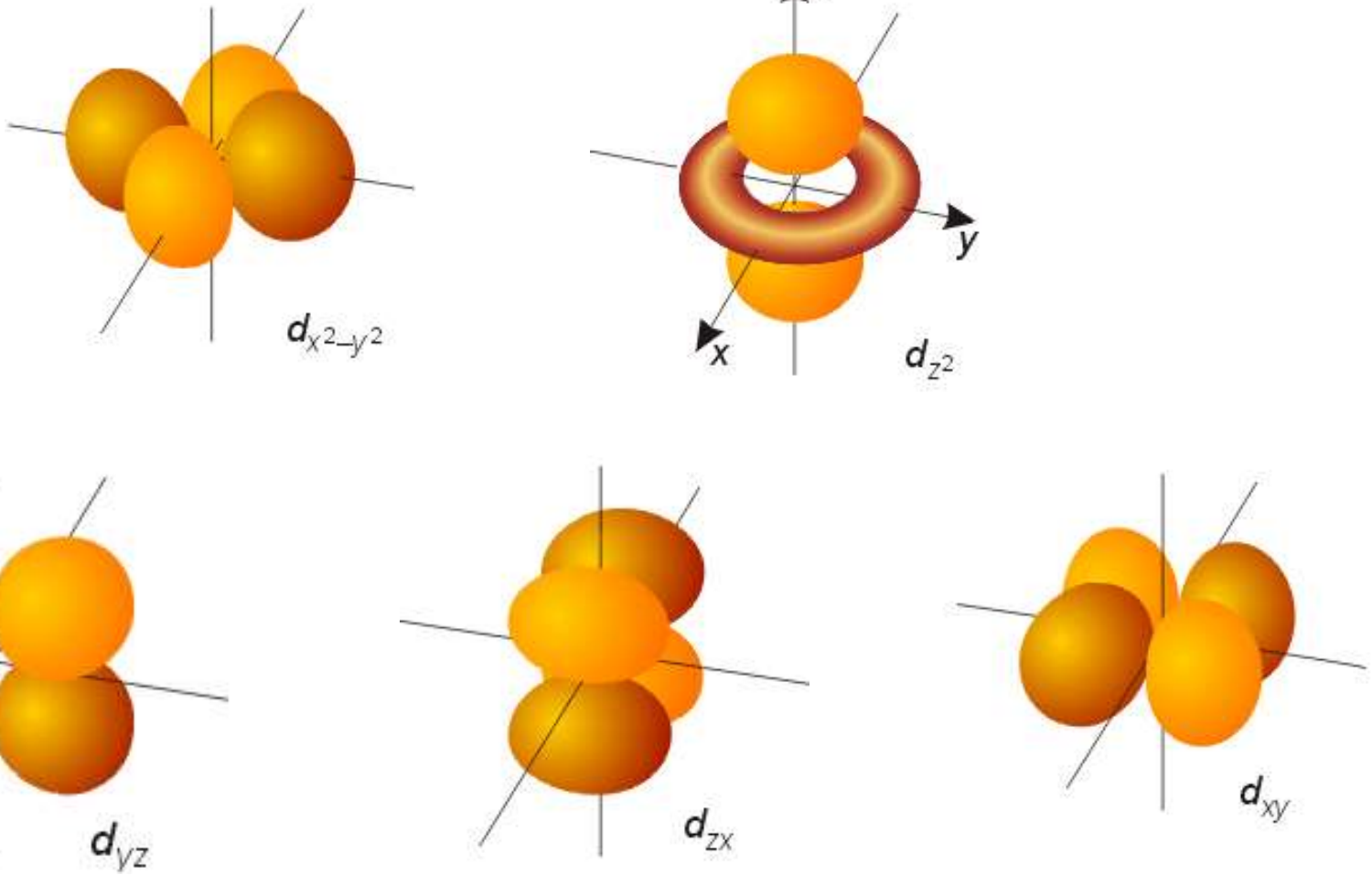


High spin complex

Crystal Field Theory

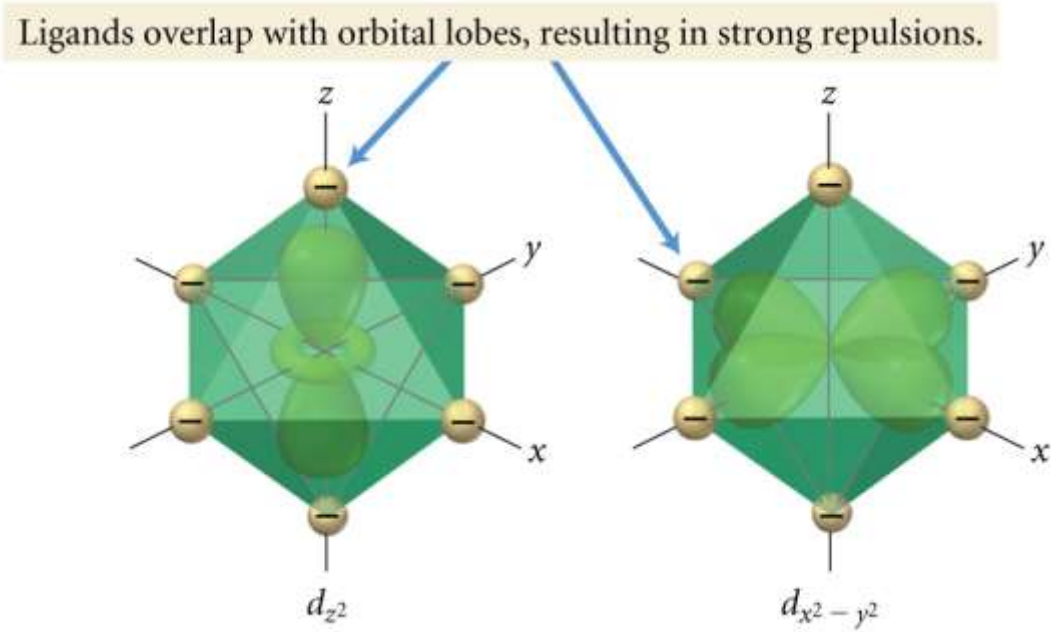
- Crystal Field Theory
  - **Model for bonding in transition metal complexes**
    - **Accounts for observed properties of transition metal complexes**
  - **Focuses on d-orbitals**
  - **Ligands = point negative charges**
  - **Assumes ionic bonding**
    - **electrostatic interactions**

d Orbitals

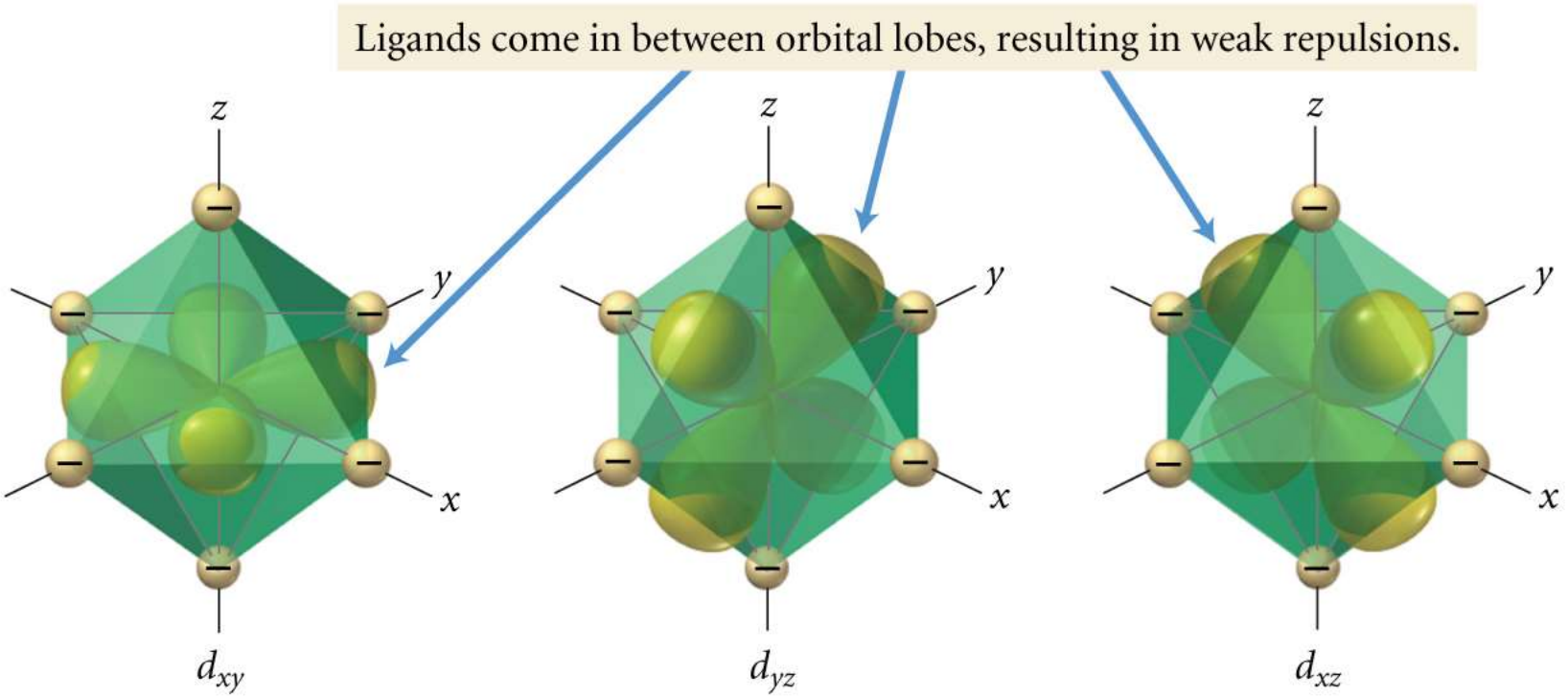


Crystal Field Theory

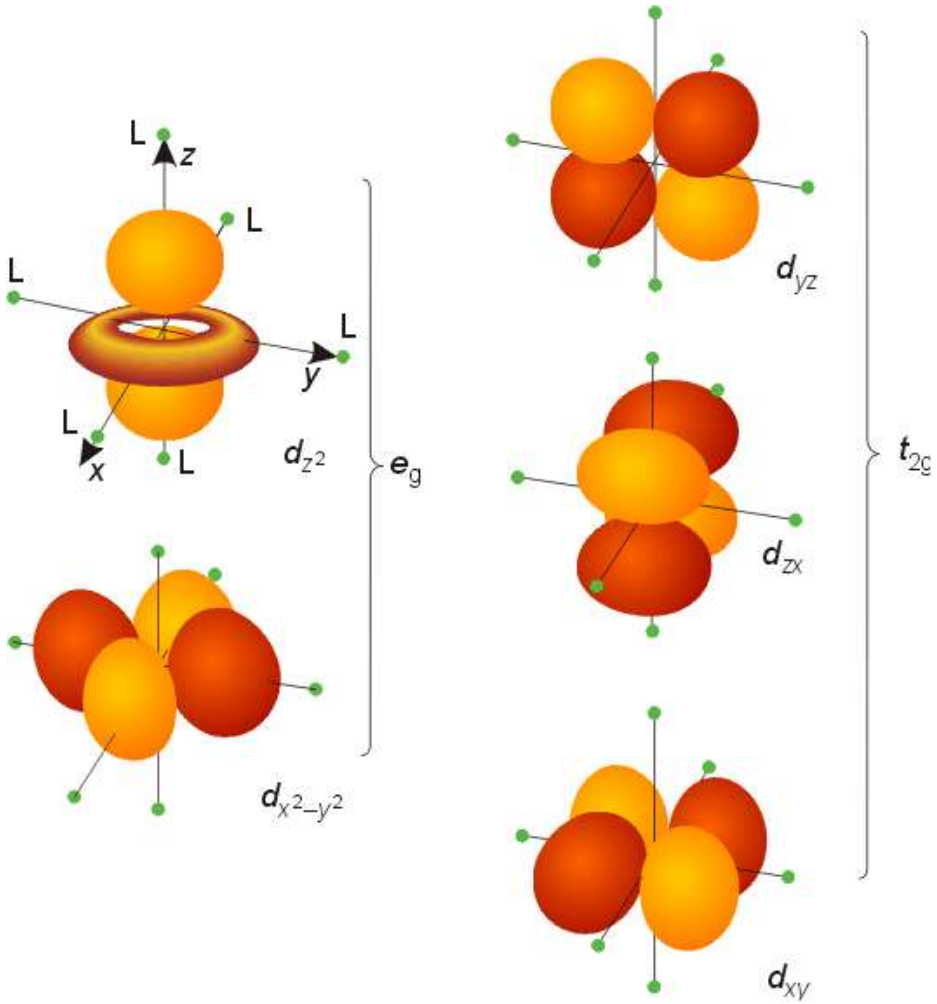
LIGANDS, VIEWED AS POINT CHARGES, AT THE CORNERS OF AN OCTAHEDRON AFFECT THE VARIOUS *D* ORBITALS DIFFERENTLY.



Crystal Field Theory

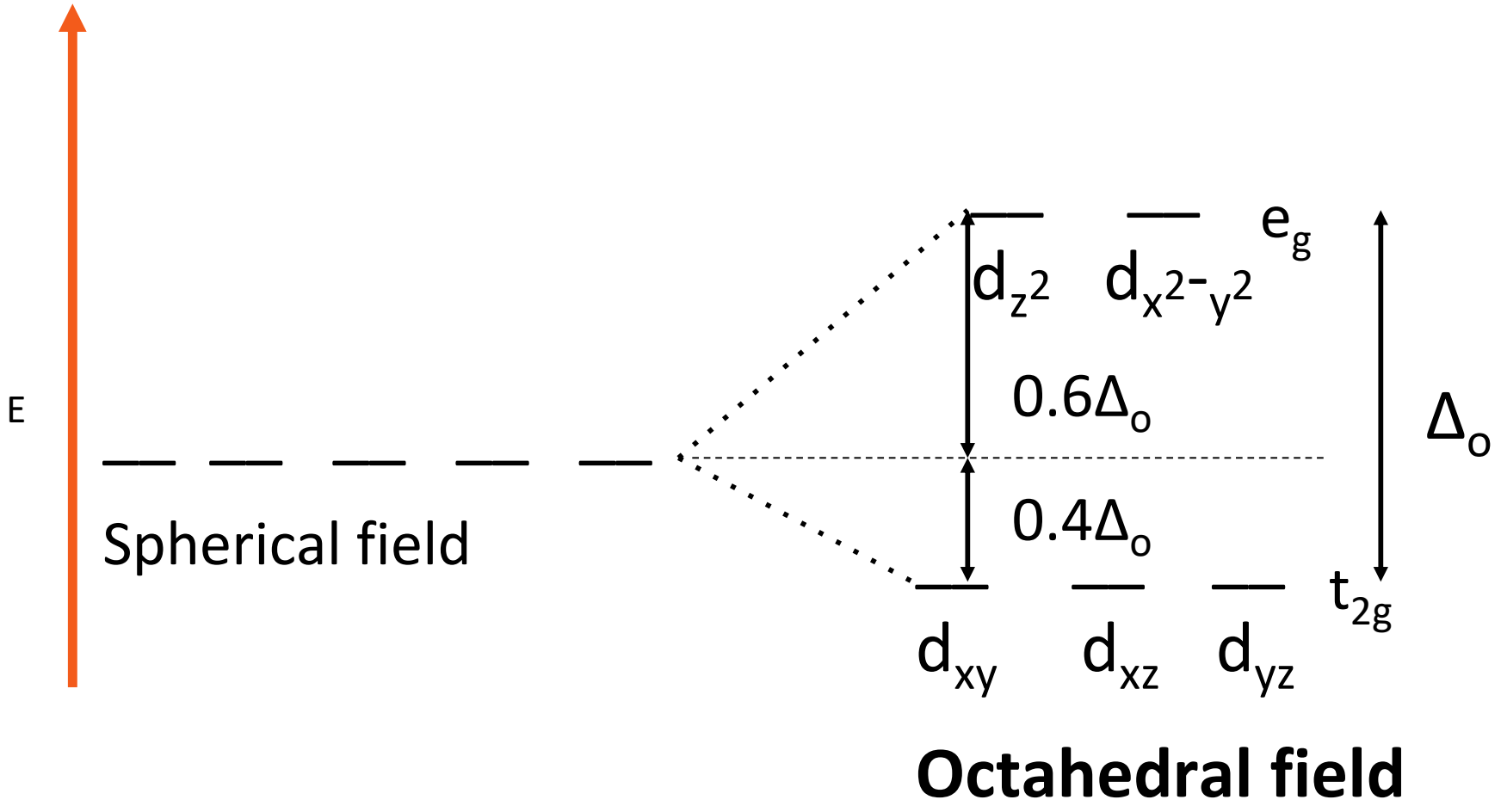


Crystal Field Theory



The repulsion between ligand lone pairs and the d orbitals on the metal results in a splitting of the energy of the d orbitals.

d ORBITAL SPLITTING



d ORBITAL SPLITTING

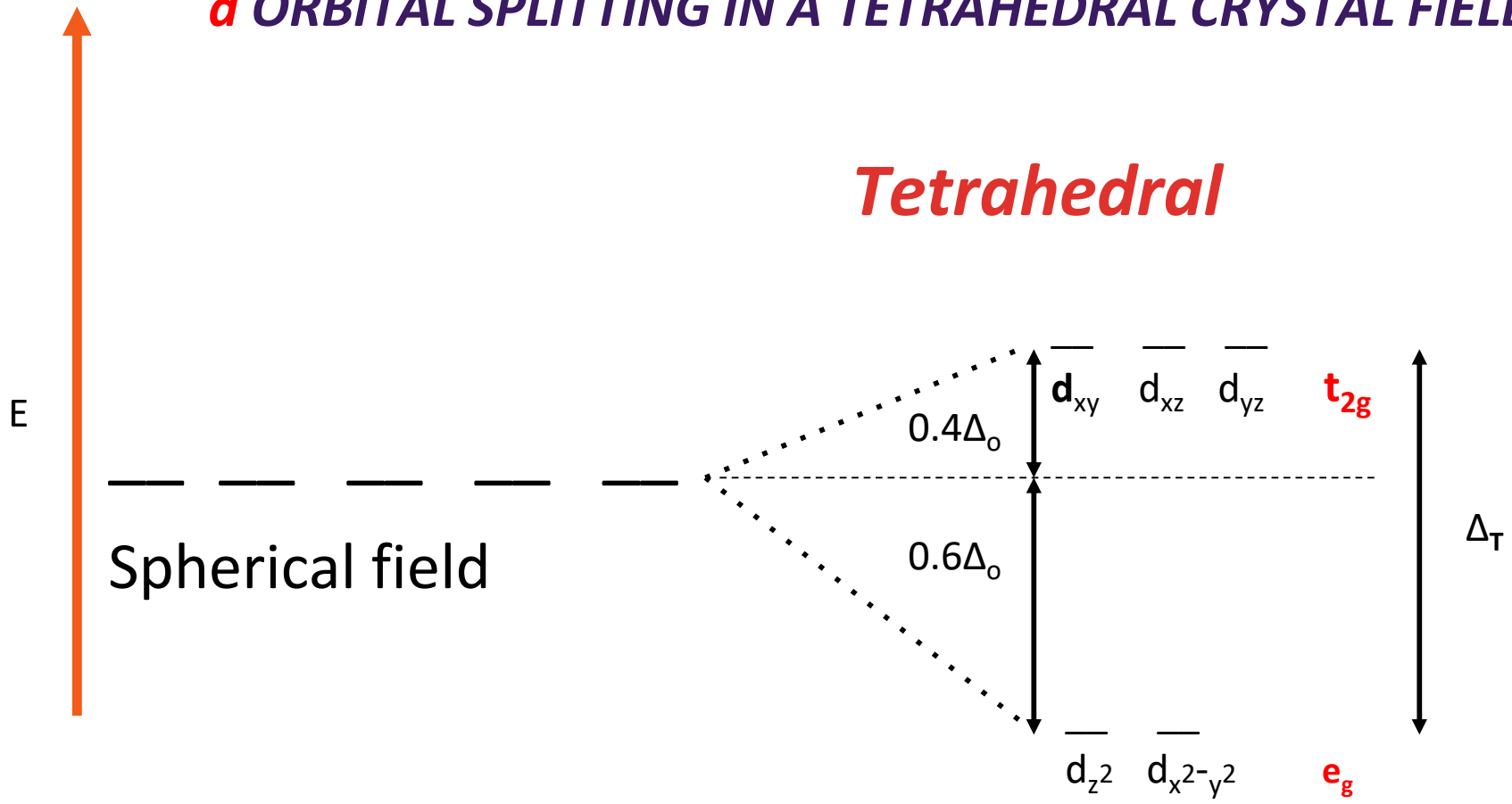
In some texts and articles, the gap in the d orbitals is assigned a value of 10Dq. The upper (e_g) set goes up by 6Dq, and the lower set (t_{2g}) goes down by 4Dq.

The actual size of the gap varies with the metal and the ligands.

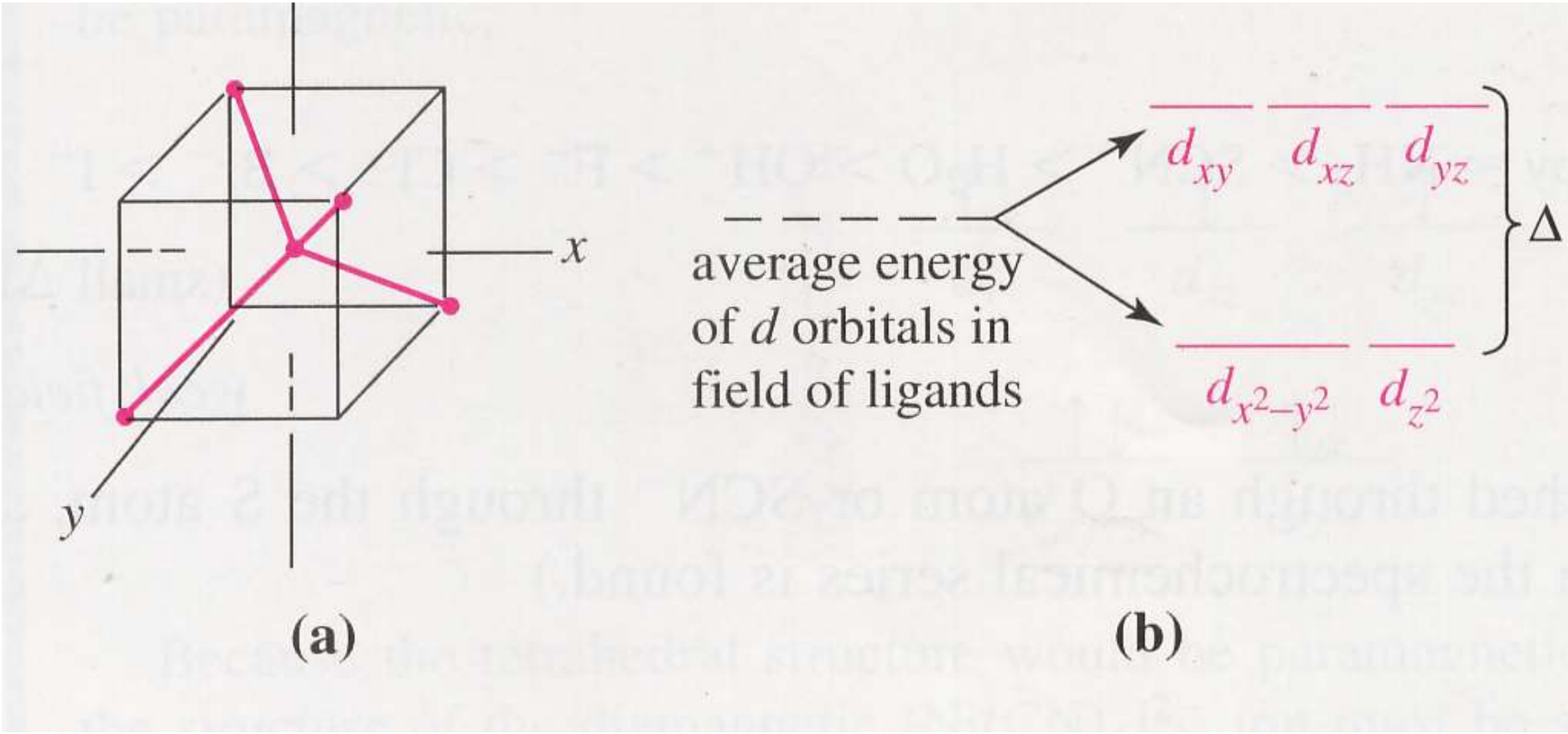
Crystal Field Theory

- Can be used to account for
  - Colors of transition metal complexes
    - A complex must have partially filled d subshell on metal to exhibit color
    - A complex with 0 or 10 d e$^-$s is colorless
  - Magnetic properties of transition metal complexes
    - Many are paramagnetic
    - of unpaired electrons depends on the ligand

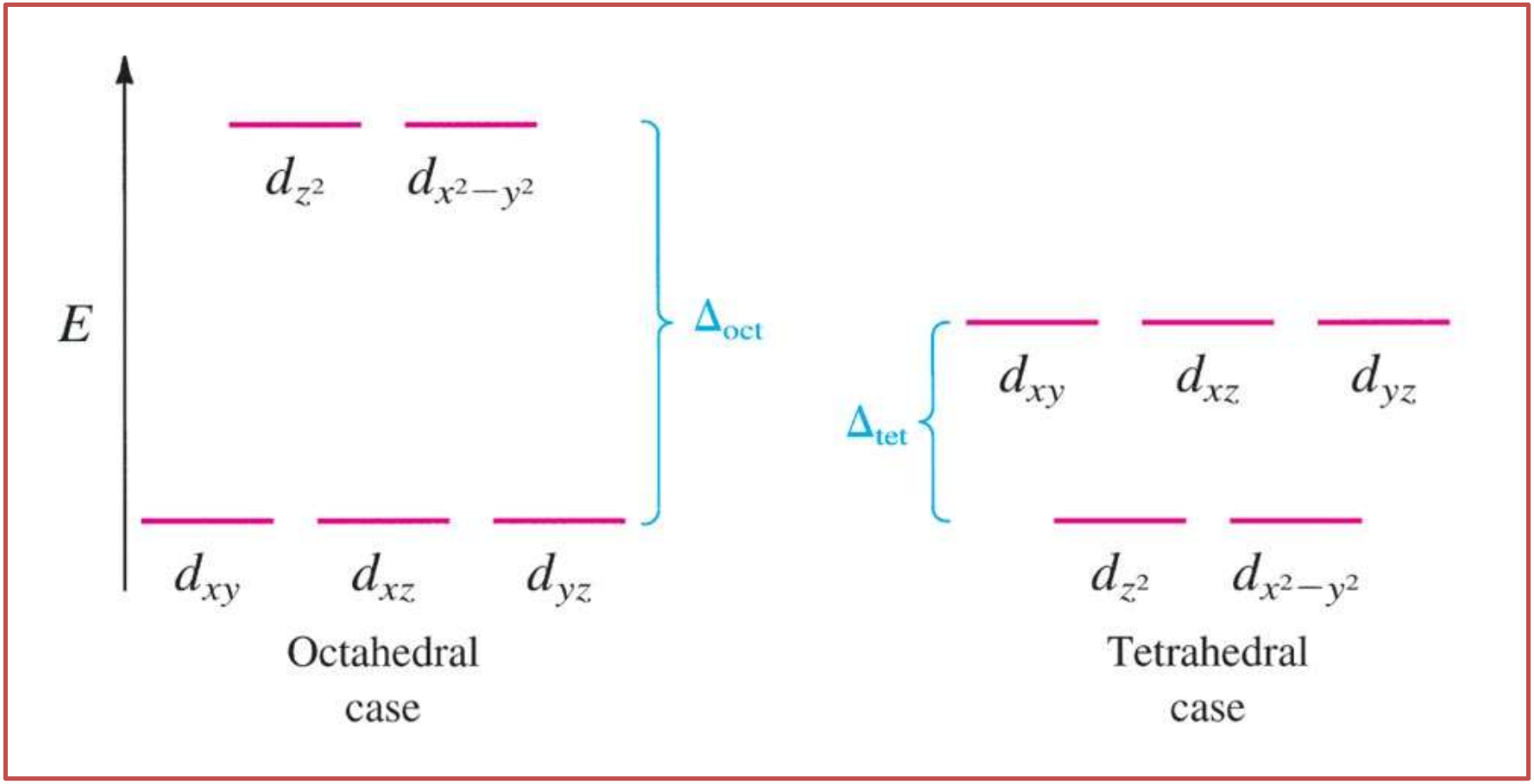
d ORBITAL SPLITTING IN A TETRAHEDRAL CRYSTAL FIELD



d ORBITAL ENERGY DIAGRAM IN TETRAHEDRAL COMPLEX

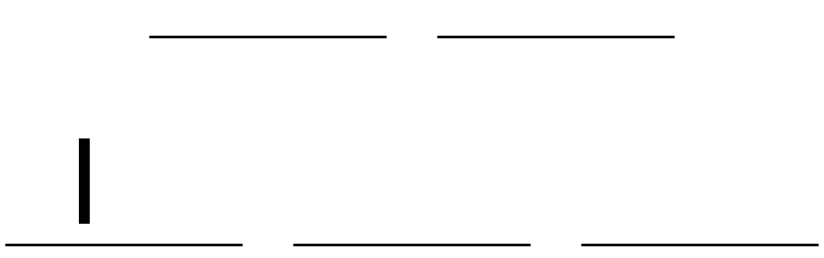


The Crystal Field Diagrams for Octahedral and Tetrahedral Complexes



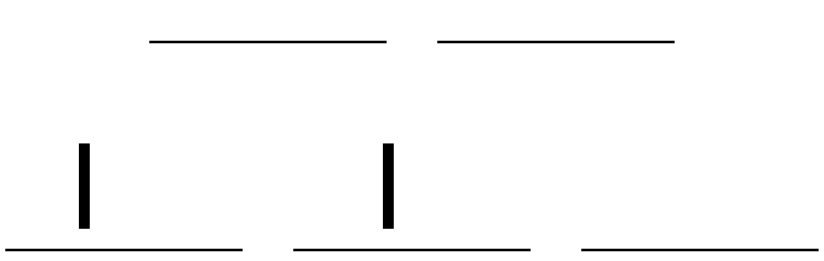
d-orbital energy level diagrams octahedral complex

d^1



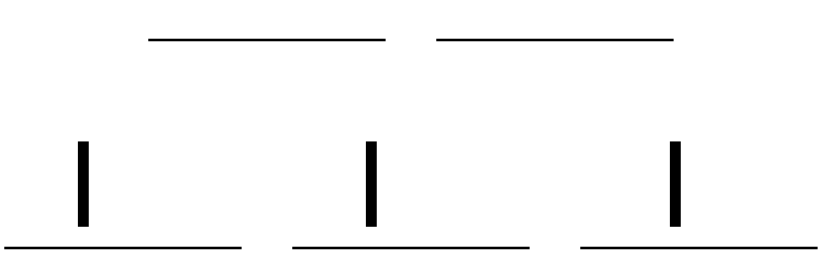
d-orbital energy level diagrams octahedral complex

d^2



d-orbital energy level diagrams octahedral complex

d^3



d-orbital energy level diagrams
octahedral complex

d^4

high spin

$\Delta < P$

low spin

$\Delta > P$

d-orbital energy level diagrams
octahedral complex

d^5

high spin

$\Delta < P$

low spin

$\Delta > P$

d-orbital energy level diagrams octahedral complex

d^6

high spin

$\Delta < P$

low spin

$\Delta > P$

d-orbital energy level diagrams octahedral complex

d^7

high spin

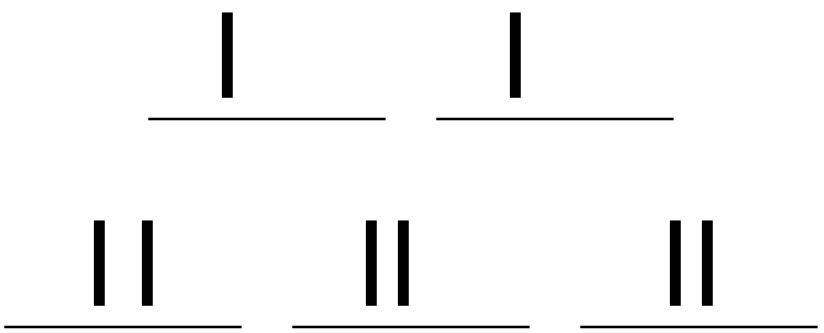
Δ < P

low spin

Δ > P

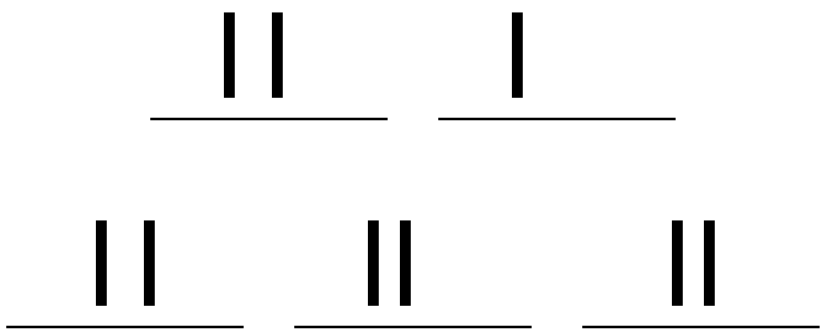
d-orbital energy level diagrams octahedral complex

d^8



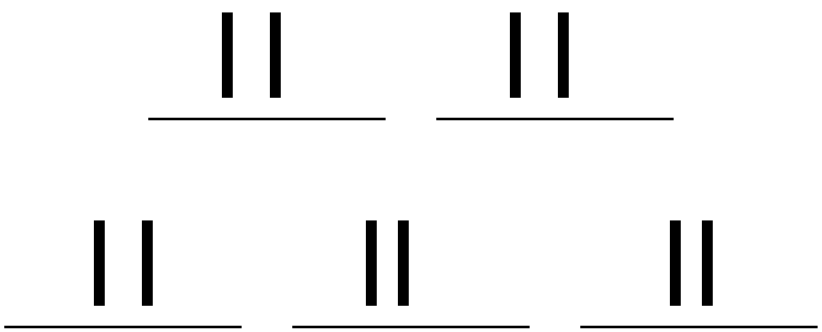
d-orbital energy level diagrams octahedral complex

d^9



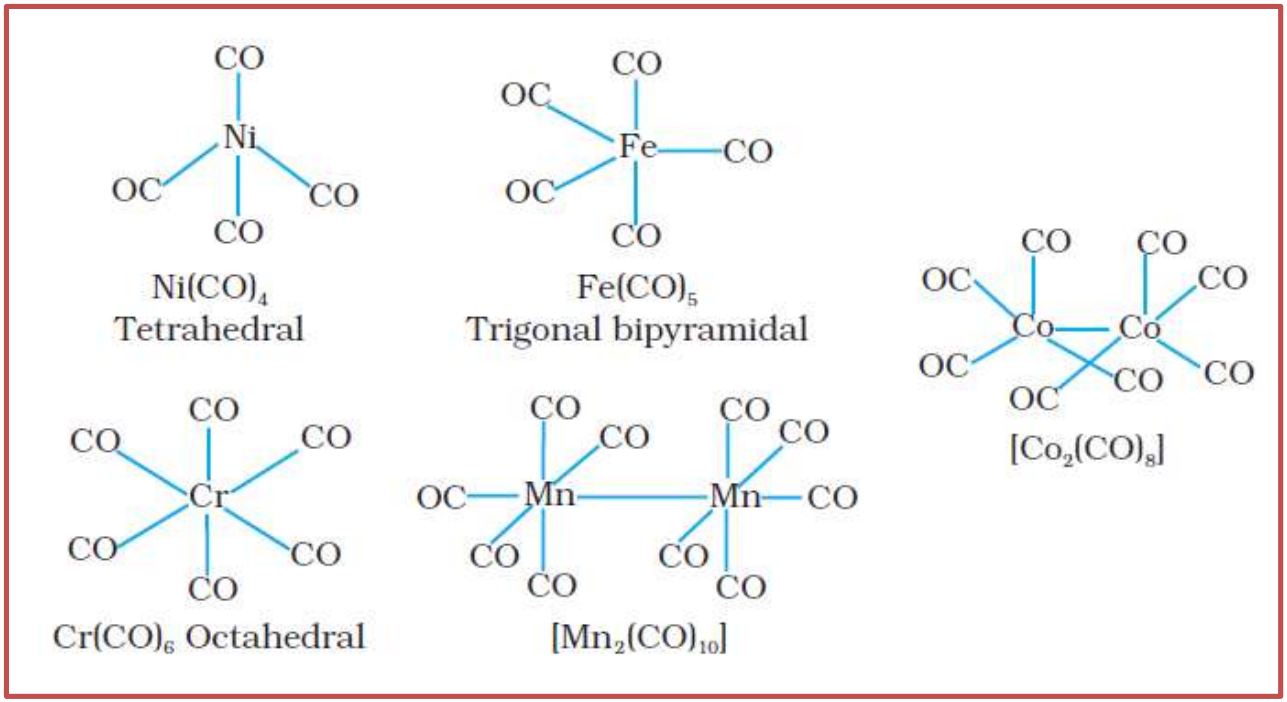
d-orbital energy level diagrams octahedral complex

d^{10}



Bonding in Metal Carbonyls

- ❖The homoleptic carbonyls (compounds containing carbonyl ligands only) are formed by most of the transition metals.
- ❖These carbonyls have simple, well defined structures.
- ❖Tetracarbonylnickel(0) is tetrahedral
- ❖Pentacarbonyliron(0) is trigonalbipyramidal
- ❖ Hexacarbonyl chromium(0) is octahedral




THANK YOU