

UNIT 5 • COORDINATION COMPOUNDS

Crystal Field Theory

Unlocking d-orbital splitting, magnetic properties,
and the spectrochemical series.

Core Diagnostic Variables

Crystal Field Splitting

The breaking of five-fold d-orbital degeneracy due to asymmetrical ligand fields.

Barycentre

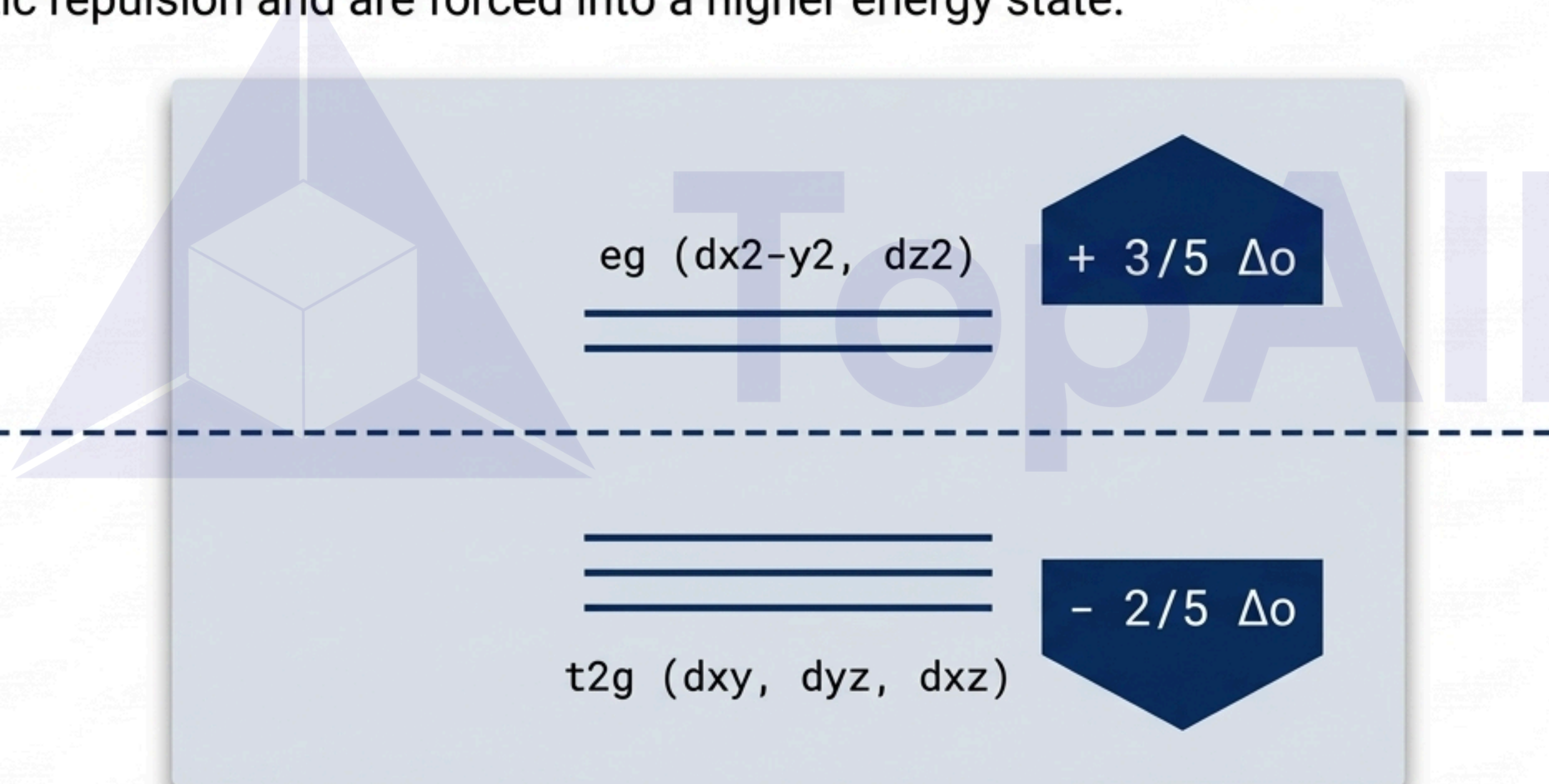
The average energy of d-orbitals in a hypothetical, perfectly spherical crystal field.

$$\Delta_o \quad / \quad \Delta_t$$

The quantifiable energy gap between split orbital levels (Octahedral / Tetrahedral).

Octahedral Splitting (Δ_o)

Ligands approach exactly along the axes. Orbitals ON the axes (eg) experience maximum electrostatic repulsion and are forced into a higher energy state.





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$$E=mc^2$$



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- » Get Clear Explanations, Not Just Marks
- » Track Your Performance Smarter



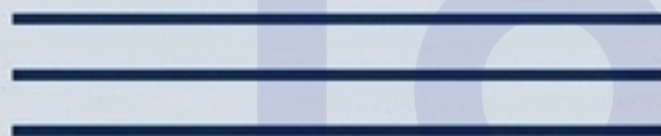
Tetrahedral Splitting (Δ_t)

Ligands approach BETWEEN the axes. The spatial splitting pattern inverts, and the overall energy gap is significantly smaller. Low spin configurations are rarely observed.

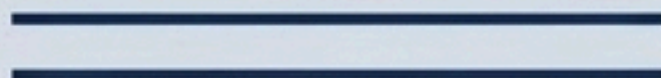
$$\Delta_t = (4/9)\Delta_o$$

(No 'g' subscript due to lack of symmetry center)

t₂



e

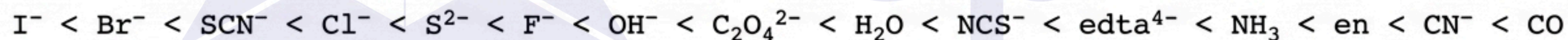


The Spectrochemical Series Map

Experimentally determined via light absorption. The ligand's position position dictates the magnitude of the crystal field splitting (Δ_o).

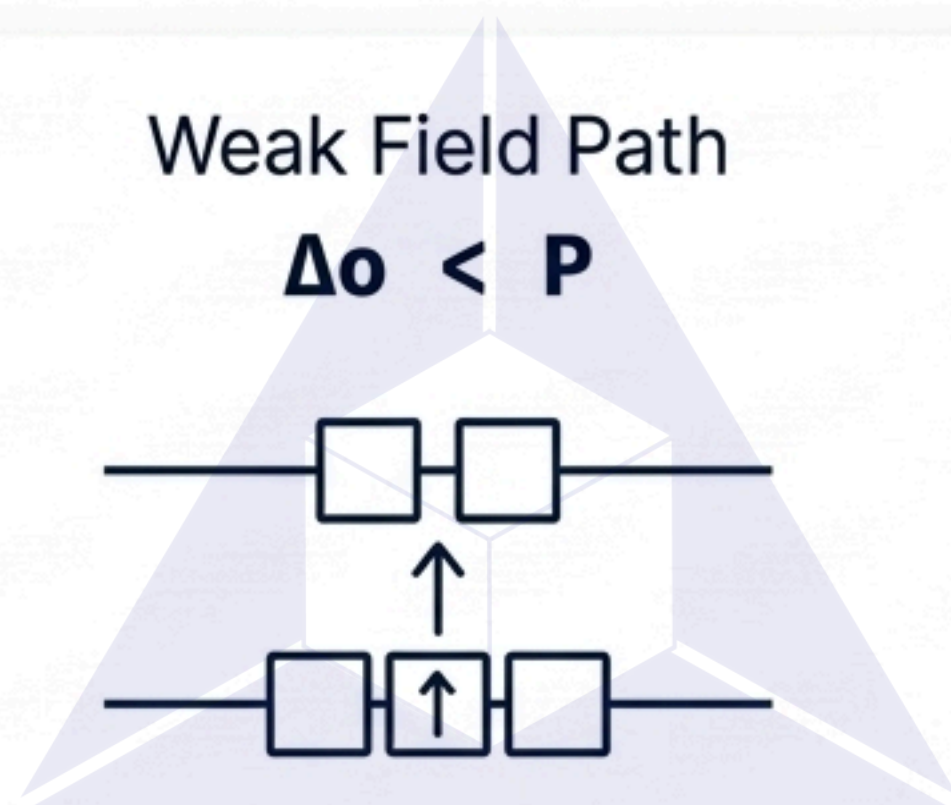
Weak Field / High Spin

Strong Field / Low Spin



The `d4` Electron Dilemma

When the 4th electron arrives, it takes the path of least energetic resistance.



High Spin Complex
 $t_{2g}^3 e_g^1$

The gap is smaller than the pairing energy (P), so the electron jumps up.

Strong Field Path
 $\Delta_o > P$



Low Spin Complex
 $t_{2g}^4 e_g^0$

The gap is too large to jump; the electron pays the energy penalty (P) to pair up below.

Spatial Mapping Pro-Tip

Advanced MCQs frequently test your ability to map specific d-orbitals to their energy states in octahedral splitting. Do not confuse which orbitals go UP (eg) and which go DOWN (t_{2g}). The mnemonic **tinny orbin** it.

Axial Orbitals = UP

dx^2-y^2 , dz^2

Think: Squares go up.



Planar Orbitals = DOWN

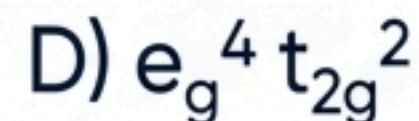
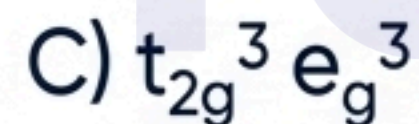
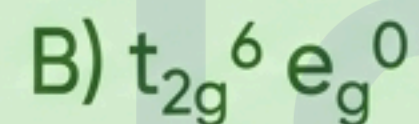
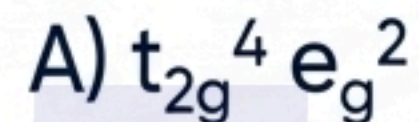
dxy , dyz , dxz

Think: No squares go down.



Knowledge Check

For a d^6 metal ion in a strong octahedral field (where $\Delta_o > P$), what is the correct electronic configuration?



Strong field = large splitting ($\Delta_o > P$). Electrons prefer to pair in the lower t_{2g} level rather than jump the massive gap to e_g . All 6 electrons pair up safely at the bottom: t_{2g}^6 .

Summary: Crystal Field Theory

- **Geometry determines splitting:** Octahedral fields push axial orbitals (eg) higher, while tetrahedral fields invert this pattern, yielding a much smaller energy gap ($\Delta_t = (4/9)\Delta_o$).
- **Ligand strength drives spin:** The spectrochemical series dictates if a complex is High Spin ($\Delta_o < P$, weak field) or Low Spin ($\Delta_o > P$, strong field).



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