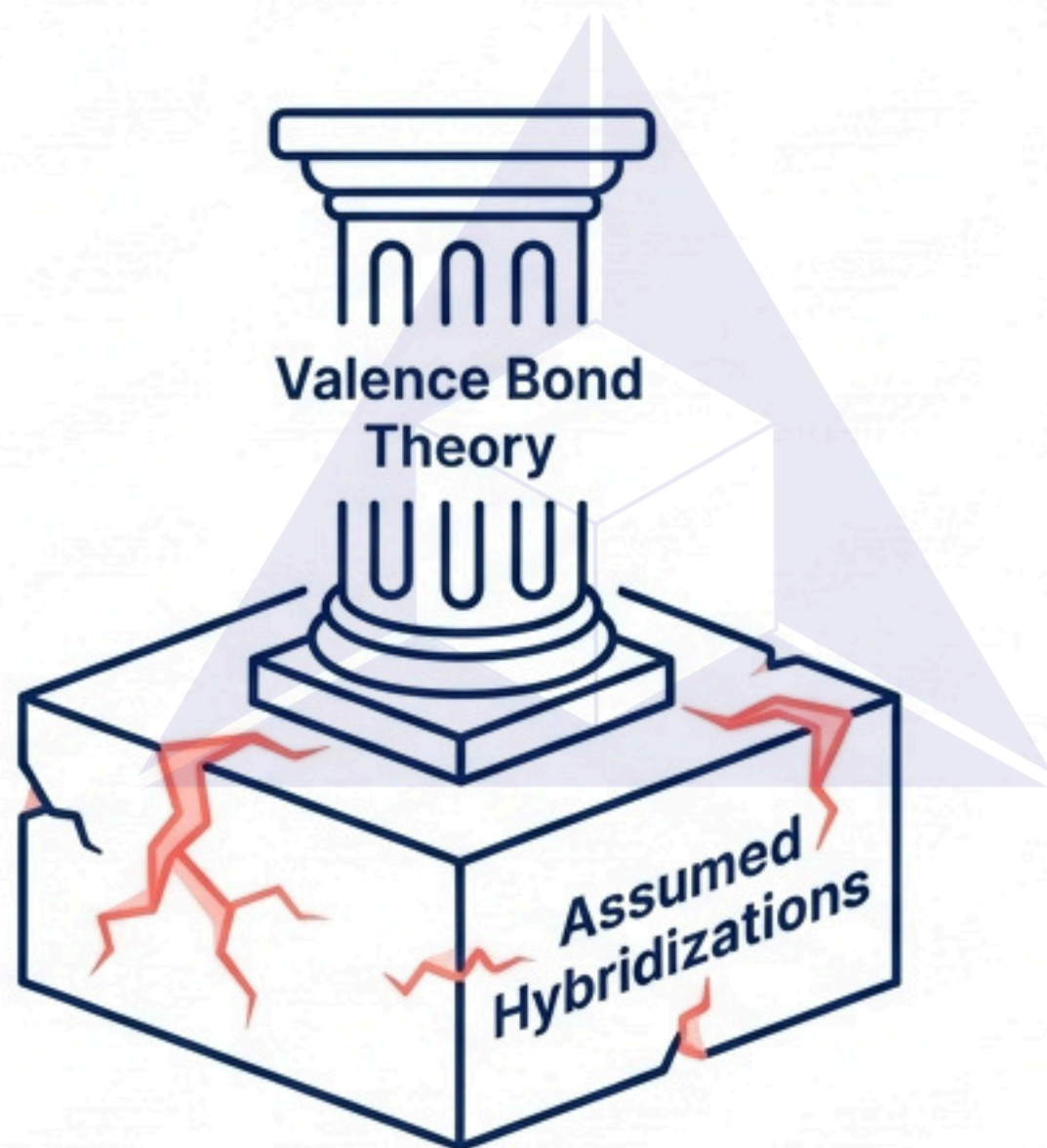


Limitations of Valence Bond Theory

Why Coordination Chemistry Requires a Better Model

THEORETICAL GAP

VBT is Built on a Foundation of Mathematical Assumptions



- While Valence Bond Theory successfully describes basic formation and magnetic states, it lacks a rigorous, first-principles physical basis for coordination compounds.
- **The Diagnostic Flaw:** The theory heavily involves a number of assumptions—treating hybridization as a mathematical manipulation of wave equations rather than explaining the underlying physical or electrostatic realities of the metal-ligand interaction.

The Model Fails to Provide Quantitative Interpretations

Magnetic Susceptibility

VBT can label a complex as paramagnetic or diamagnetic based on unpaired electrons, but it does not give a quantitative interpretation of magnetic data.



Thermodynamic & Kinetic Stability

VBT explains bonding geometry but does not give a quantitative interpretation of the thermodynamic or kinetic stabilities of coordination compounds.





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Key Highlights

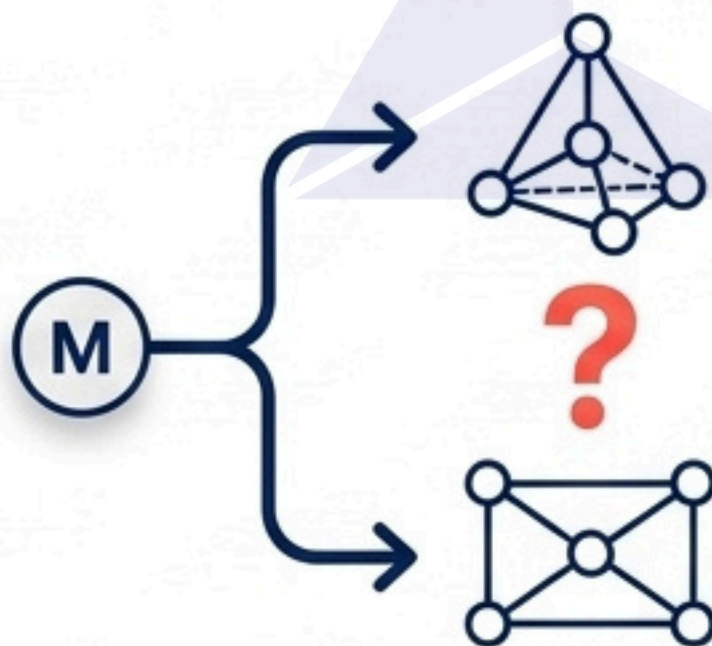
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VBT Breaks Down Against Observable Phenomena

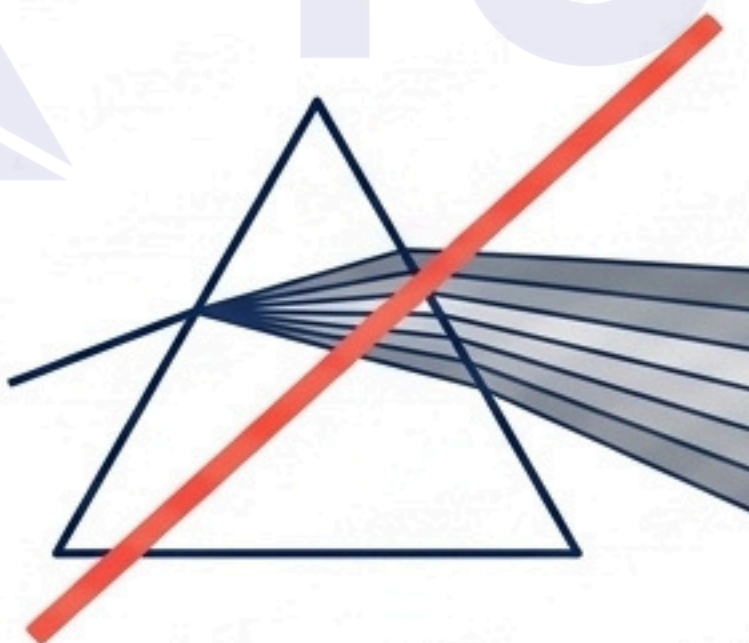
4-Coordinate Ambiguity

It does not make exact predictions regarding the tetrahedral and square planar structures of 4-coordinate complexes.



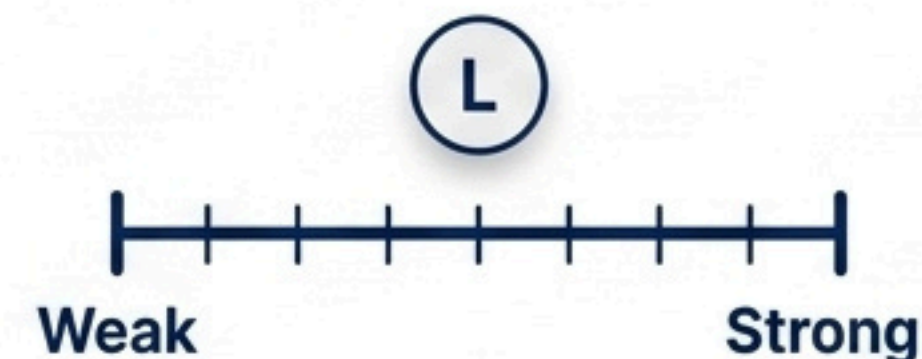
The Color Deficit

It completely fails to explain the vibrant colors exhibited by coordination compounds (e.g., the d-d transitions seen in ruby or emerald).



Ligand Blindness

It treats ligands equally and does not distinguish between weak and strong ligands, entirely ignoring the spectrochemical series.



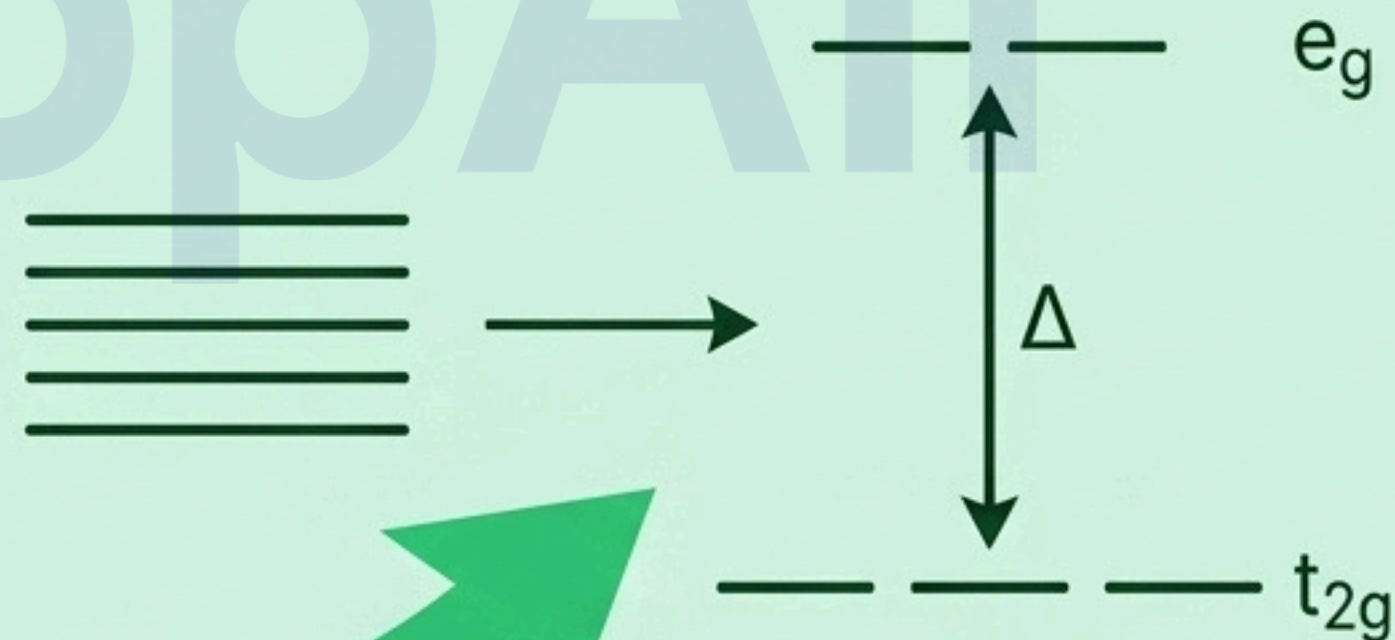
Diagnostic Summary and the Path Forward

SYSTEM FAILURES LOGGED

- ✗ 1. Relies on mathematical assumptions.
- ✗ 2. Lacks quantitative magnetic data.
- ✗ 3. Cannot explain complex colors.
- ✗ 4. Lacks quantitative stability metrics.
- ✗ 5. Cannot predict 4-coordinate geometries perfectly.
- ✗ 6. Cannot distinguish weak vs. strong ligands.

SOLUTION DESIGN // CRYSTAL FIELD THEORY

To resolve these gaps, coordination chemistry requires an electrostatic model. **Crystal Field Theory (CFT)** lifts d-orbital degeneracy to explain color, predict stability, and quantify magnetic behavior.





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