1.1 Metal-Ligand Bonding

- Interactions between metals and ligands
- Valence-bond theory
- Molecular orbital theory
- Crystal field theory

- Theory should help explain
  - Stability of metal complexes
  - Magnetic and electronic properties
  - Spectroscopic properties (color)

1.2 Metal-Ligand Bonding

- Lewis acid-base theory

1.3 Metal-Ligand Bonding

- Valence bond description

1.4 Metal-Ligand Bonding

- Valence bond description
1.5 Metal-Ligand Bonding

- VB theory accounts for general structures and geometries but does not explain stability, magnetic properties or spectroscopic properties (colors)

- Molecular orbital theory
  - Electrons as standing waves
  - Wavefunctions are molecular orbitals
  - Molecular orbitals describe regions of space where electrons are likely to be found
  - Energy levels of molecular orbitals can explain electronic properties of transition metal compounds
  - Mathematically complex and somewhat obscure

1.6 Metal-Ligand Bonding

- Crystal field theory
  - Interaction between the metal and ligand (often an anion or anion-like) is purely electrostatic
  - Considers the electrostatic effect of a field of ligand electrons on the metal’s d orbitals (valence orbitals). How do the orbital energies shift?
  - Assumes the metal d orbitals contain electrons
  - Conceptually simple...just need to understand
  - Coulomb’s Law (+ and – charges)
  - Shapes of d orbitals

1.7 Orbital Shapes

1.8 Orbitals

- Why are the orbitals arranged in this way (s lower than p lower than d)?

- Degeneracy

- Why does d_{z^2} look special?
Chapter 4

1.9 d-Orbital Shapes

2.1 Crystal field theory

- CFT examines the effect of ligand field (ligand electrons) on the d orbitals
- Octahedral ligand fields and energy level diagrams

2.2 Crystal field theory

- Stage I
- Stage II

2.3 Crystal field theory

- Stage III
- Stage IV
2.3 Crystal field theory
- Stage III

2.4 Crystal field theory
- Octahedral ligand field splitting of the d orbitals (e_g and t_2g orbitals)
  - Barycenter and other quantitative aspects

2.5 Crystal field theory
- Tetragonal distorted octahedral ligand field

2.6 Crystal field theory
- Square planar ligand field

Potential energy
- \( d_{xz} \)
- \( d_{yz} \)
- \( d_{xy} \)
- \( d_{z^2} \)
Chapter 4

2.7 Crystal field theory

- Tetrahedral ligand field

![Diagram of tetrahedral ligand field]

Chapter 4

2.8 Crystal field theory

- Five-coordinate ligand fields

Chapter 4

2.9 Crystal field theory

- $d_{x^2-y^2}$
- $d_{z^2}$
- $d_{xy}$
- $d_{xz}$
- $d_{yz}$

![Diagram of d-orbitals]

Chapter 4

3.1 Energetics

- Crystal field splitting energy
- Pairing energy
3.2 Energetics
- High spin, low spin states

3.3 Energetics
- Crystal field stabilization energy (CFSE)
- CFSE always compared relative to unsplit state

3.4 Factors Affecting $\Delta$
- Ion charge
- Size of metal

3.5 Factors Affecting $\Delta$
- Ligand spectrochemical series
- Ligand size
3.6 Factors Affecting $\Delta$

- $\sigma$-bonding
- $\pi$-bonding

3.7 Factors Affecting $\Delta$

- back-bonding effects
  (filled metal d orbital $\rightarrow$ unfilled ligand orbital)
- $\pi$-bonding effects
  (filled ligand orbital $\rightarrow$ unfilled metal d orbital)

4.1 Magnetism

- Magnetic susceptibility
- Guoy balance
- Diamagnetism
- Paramagnetism

4.2 Magnetism

- Magnetic moment
- Relationship to unpaired spins
**Chapter 4**

### 4.3 Magnetism

- Examples

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### 5.1 Absorption Spectroscopy

- Absorption versus transmission

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### 5.2 Absorption Spectroscopy

- Light/energy calculations

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### 5.3 Absorption Spectroscopy

- Speed of light: $2.998 \times 10^8$ m/s$^{-1} = c = \lambda \cdot \nu$
  - Blue light has shorter wavelength than red light
  - Blue light has higher frequency than red light
  - Blue light is more energetic than red light
Chapter 4

5.4 Absorption Spectroscopy

- Rationalizing colors

Chapter 4

5.5 Absorption Spectroscopy

- Rationalizing colors