

Inorganic Chemistry II – 40546

Syllabus

1 Prerequisites

- Inorganic Chemistry I

2 Learning outcomes

At the end of this assignature students should be able to:

- Apply the point group theory to chemistry problems
- Recognize electronic configuration of symmetrical molecules
- Name coordination compounds from the chemical formulas and vice versa
- Apply the ligand field theory to chemistry problems
- Explain in detail the UV-Vis-NIR absorption/emission spectra of transition metal compounds
- Determine molecular spectroscopy terms from electronic configuration

3 Topics

1. Point Group Theory (15h)

1.1. Introduction to group theory ([week 1, 3h](#))

1.1.1. Definitions

1.1.2. Cayley tables

1.1.3. Matrix representation of symmetry operations

1.1.4. Conjugacy classes of a group

1.1.5. Exercises

1.2. Character tables ([week 2, 3h](#))

1.2.1. Irreducible representations and characters

1.2.2. The orthogonality theorem

1.2.3. High symmetry point groups

1.2.4. Exercises

1.3. Projection operators I ([week 3, 3h](#))

- 1.3.1. Definitions
- 1.3.2. Vibrational normal modes
- 1.3.3. Selection rules in Raman and IR spectroscopy
- 1.3.4. Exercises
- 1.4. Projection operators II ([week 4, 3h](#))
 - 1.4.1. Symmetry adapted atomic orbitals
 - 1.4.2. Symmetry adapted molecular orbitals
 - 1.4.3. Electronic configuration of symmetrical molecules
 - 1.4.4. Exercises
- 1.5. Examination ([week 5, 3h](#))
- 2. Introduction to Coordination Chemistry (15h)
 - 2.1. Coordination compounds ([week 6, 3h](#))
 - 2.1.1. The Lewis acids-bases concept: coordination complexes
 - 2.1.2. Nomenclature of coordination compounds
 - 2.1.3. Isomerism in coordination compounds
 - 2.1.4. Exercises
 - 2.2. Ligand field theory I ([week 7, 3h](#))
 - 2.2.1. Multipole expansion of the O_h ligand field
 - 2.2.2. Perturbative treatment of d atomic orbitals in O_h ligand field
 - 2.2.3. Exercises
 - 2.3. Ligand field theory II ([week 8, 3h](#))
 - 2.3.1. The ligand field parameters Dq , Ds and Dt
 - 2.3.2. Splitting of d atomic orbitals in different symmetries
 - 2.3.3. Exercises
 - 2.4. Transition metal complexes ([week 9, 3h](#))
 - 2.4.1. The stabilization energy
 - 2.4.2. The spectrochemical series
 - 2.4.3. Magnetic properties of transition metal complexes
 - 2.4.4. Exercises
 - 2.5. Examination ([week 10, 3h](#))
- 3. UV-Vis-NIR Spectroscopy of Coordination Compounds (18 h)
 - 3.1. Atomic term symbols of transition metals ([week 11, 3h](#))
 - 3.1.1. The Russell-Saunders coupling scheme
 - 3.1.2. The Racah parameters B and C
 - 3.1.3. Exercises
 - 3.2. Molecular term symbols of coordination compounds ([week 12, 3h](#))
 - 3.2.1. Permutation group theory
 - 3.2.2. Irreducible representations and characters of permutation groups

- 3.2.3. The Young tableaux
- 3.2.4. The $t_{2g}^n e_g^m$ electronic configurations
- 3.2.5. Exercises
- 3.3. Determination of the ligand field (Dq) and Racah (B, C) parameters ([week 13, 3h](#))
 - 3.3.1. The Tanabe-Sugano and Auxiliary Tanabe-Sugano diagrams
 - 3.3.2. The nephelauxetic series
 - 3.3.3. The Ruby laser
 - 3.3.4. Exercises
- 3.4. Molecular orbital theory of transition metal complexes ([week 14, 3h](#))
 - 3.4.1. Symmetry adapted ligand molecular orbitals
 - 3.4.2. Hückel description of acetylacetonato based transition metal complexes
 - 3.4.3. Exercises
- 3.5. Ligand-metal and metal-ligand charge transfer ([week 15, 3h](#))
 - 3.5.1. UV-Vis absorption spectrum of the permanganate molecular ion
 - 3.5.2. Photochemical processes initiated by charge transfers
 - 3.5.3. Exercises
- 3.6. Examination ([week 16, 3h](#))

4 Grading

- 3 exams (25%, 25%, 25%)
- Self-study work (25%)