Inorganic Chemistry II – 40546 Syllabus

Prof. Jhon Fredy Pérez Torres

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 simmetries
 - 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%)