

Chemistry 529

Physical Methods in Inorganic Chemistry

The basic goal of this course is provide students with a fundamental understanding of spectroscopic methods and their applications in inorganic chemistry. The course is divided into three main sections: (i) foundations of physical inorganic chemistry; (ii) ground state spectroscopic methods; and (iii) excited state spectroscopic methods (including valence and core excitation methods). A more detailed outline of the material is given below. The fundamental concepts that govern each of the reviewed techniques are investigated through literature examples and in-depth discussion of the information derived from different physical methods. *Emphasis is generally mostly placed on transition metal (d-block) systems, although examples from main group and lanthanide chemistry are also used.*

Administrative Details

- Instructor** Pierre Kennepohl (Chemistry D314, pierre@chem.ubc.ca, 2-3817)
- Office Hours** by appointment
- Prerequisites** There are no official course prerequisites. However, students are expected to have a good grasp of basic atomic theory (hydrogenic atomic orbitals, many-electron atomic states) and bonding models in inorganic chemistry (crystal/ligand field theory, molecular orbital theory) at the level of a 3rd year undergraduate inorganic chemistry course.
- Textbook** There is no official textbook other than reading materials made available in the course. Students will be expected to search the literature and read a selection of recent (and not so recent) articles available electronically through the UBC library.
- Reference Texts** Additional reference texts are available in the library. Some useful reference information may be obtained from the following:
- Ballhausen, C. J. & Gray, H. B. *Molecular Orbital Theory* (1964)
 - Cotton, F. A. *Chemical Applications of Group Theory* (1990)
 - Solomon, E. I. & Lever, A. B. P. *Inorganic Electronic Structure and Spectroscopy I/II* (1999)
- Grading** Students will be tested on the material based on their performance on problem sets (20%) and a take-home final exam (40%). A portion of the final grade is also given for participation during class time as this is an integral part of this course (40%).
- Problem Sets** Students are encouraged to discuss the material amongst each other and assist each other wherever possible. However, problem set questions should be answered *individually*; every student must submit their own unique solutions to the questions.
- Participation** The course structure is designed to encourage discussion of current literature and extend students beyond the specifics of the material itself. For this reason, it is important for students to participate during in-class discussion and contribute significantly. This model also requires students to prepare for class ahead of time and not simply assume that others can fill in the blanks for them. In addition, students will be required to participate in the creation of a course wiki - as described in the first lecture (participation in this activity is mandatory!).
- Final Exam** The final examination is an open book take-home exam that focuses on the application of the techniques and concepts developed during the course. Students cannot discuss the exam with anybody other than the instructor – additional details will be provided when appropriate.

General Outline of Course Content (subject to change without prior notice)

1. Group Theory, Molecular Structure, and Spectroscopy

- 1.1 Symmetry & Group Theory
- 1.2 Basics of Molecular Electronic Structure
- 1.3 Fundamentals of Molecular Spectroscopy

2. Ground State Spectroscopic Methods

- 2.1 Angular Momentum States & the Zeeman Effect
- 2.2 Nuclear Magnetic Resonance (NMR)
- 2.3 Electron Paramagnetic Resonance (EPR)
- 2.4 Mossbauer Spectroscopy

3. Excited State Spectroscopic Methods

- 3.1 Electronic Transitions and Electronic Excited States
- 3.2 Photoelectron and Ionization Methods
- 3.3 X-ray Absorption and Emission Methods