UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Theory and Methods of Spectroscopies

2526-1-F5402Q009

Aims

The course aims at introducing the student to vibrational, electronic and magnetic spectroscopy making extensive use of group theory and quantum mechanics as essential tools to the modern practice of spectroscopy for transition metal complexes.

- Knowledge and understanding
  The student must demonstrate the knowledge and methodological tools necessary to interpret the phenomena underlying the interaction of electromagnetic radiation with matter. The student must be able to identify independently which factors determine the likelihood of light absorption by the investigated molecular system. The student must be able to define the selection rules for the different spectroscopes. The student must become familiar with the terms of the discipline, and explain to experienced people the notions about light/matter interactions, their relationship with spectroscopy and their application to simple systems in coordination chemistry.
- Applied knowledge and comprehension skills
  The student must demonstrate that he is able to solve molecular quantum chemistry calculations with the Gaussian code to obtain the vibration frequencies, the energies of the molecular orbitals, the excitation energies and electron resonance spectroscopy parameters for simple coordination compound systems.
- Autonomy of judgment
  The student has the ability to collect and interpret data deemed useful in determining the answer to a given quantitative or qualitative problem, related to spectroscopic properties of a molecular system. The student has the ability to integrate knowledge and manage complexity, as well as formulate conclusions based on partial information collected.
- Communication skills
  The student, thanks to the writing of a report of the lab experiments in quantum chemistry, can communicate information clearly and unambiguously, ideas, problems and solutions relating to the spectroscopic properties of molecular systems to specialist and non-specialist interlocutors.
- Ability to learn
  The student develops those learning skills that are necessary to undertake further study and research activities mostly in a self-directed or autonomous way.

Contents

Part I: Group theory and molecular orbitals theory. Part II: Introduction to spettroscopy. Vibrational spectroscopy. Practical exercise I (Analysis of the vibrational spectrum of $Mn(CO)_5Br$). Part III: Quantum mechanical methods (Density Functional Theory). Part IV: UV-vis spectroscopy. Practical exercise II (Analysis of the UV-vis spectrum of $[Ti(H_2O)_6]^{3+}$). Part V: EPR spectroscopy. Practical exercise III (Analysis of the EPR spectrum of $[Ti(H_2O)_6]^{3+}$).

Detailed program

Parte I: Group theory. Point groups. Symmetry. Character tables. Reducible and irreducible representations. Decomposition formula. Molecular orbitals theory. LCAO. Perturbation theory. Projection operators. Part II: Introduction to spettroscopy. Vibrational spectroscopy. Transition dipole moment. Symmetry selection rules. Normal modes of vibration. Practical exercise I (Analysis of the vibrational spectrum of $Mn(CO)_5Br$). Part III: Quantum mechanical methods. Basis sets. Review of Hartree-Fock theory. Fundaments of density functional theory. Kohn-Sham formalism. Types of exchange and correlation functionals. Part IV: UV-vis spectroscopy. Electronic transitions. Franck-Condon principle. Strength of the transition dipole moment. Spin and symmetry selection rules. Oscillator strength. Term symbols. Crystal field. Jahn-Teller effect. d-d transitions. Vibronic coupling. Orgel and Tanabe-Sugano diagrams. Spectrochemical Series. Excitation energy calculation with time-dependent DFT (TD-DFT). Practical exercise II (Analysis of the UV-vis spectrum of $[Ti(H_2O)_6]^{3+}$). Part V: EPR spectroscopy. Magnetism. Zeeman effect. Hyperfine interaction. Spin-orbit coupling. g tensor. A hyperfine tensor. Isotropy and anisotropy. Practical exercise III (Analysis of the EPR spectrum of $[Ti(H_2O)_6]^{3+}$).

Prerequisites

Knowledge of quantum mechanics.

Teaching form

16 two-hour lectures, in person, Delivered Didactics
6 four-hour lab activities, in person, Interactive Teaching

Textbook and teaching resource

Teaching resources in terms of slides and notes.

Textbooks: Symmetry and spectroscopy by D. C. Harris and M. D. Bertolucci (Dover).

Physical methods in chemistry by R. S. Drago (Saunders).

Semester

Second semester.

Assessment method

The reports on the computational laboratory part, which are expected to be delivered at least one week before the date of the exam session, are evaluated.
The oral exam consists of a first part of discussion on the report. Then some questions are asked both of a general nature and more in detail on the topics covered during the lectures and on the contents of the exercises carried out in the laboratory.

The positive evaluation (18-30L) is established according to the following criteria:
18-19: preparation on a small number of topics in the course program, with limited discussion and analysis skills that, in the case of the oral exam, emerge only following the teacher's help and questions; expository skills and vocabulary that are not always correct, with limited critical processing skills;
20-23: preparation on a part of the topics in the course program, independent analysis skills only on purely practical and executive issues, use of correct vocabulary even if not entirely accurate and clear and an expository skill that is at times uncertain;
24-27: preparation on a large number of topics in the course program, ability to independently carry out argumentation and critical analysis, ability to apply knowledge to contexts and connect themes to concrete cases, use of correct vocabulary and competence in the use of disciplinary language;
28 – 30/30L: complete and exhaustive preparation on the topics in the exam program, personal ability to deal independently and critically analyze the topics, ability to reflect and self-reflect and to connect the topics to concrete cases and different contexts, excellent ability to think critically and autonomously, full mastery of the disciplinary vocabulary and a rigorous and articulated ability to present, ability to argue, reflect and self-reflect, ability to make connections to other disciplines.

Office hours

The professor receives appointment.

Sustainable Development Goals

AFFORDABLE AND CLEAN ENERGY