UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Spettroscopia di Composti Inorganici

2122-1-F5401Q064

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.

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 $[Ti(H_2O)_6]^{3+}$) and Practical exercise IV (Analysis of the EPR spectrum of N_2^- in ionic solids: KCl e MgO).

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 $[Ti(H_2O)_6]^{3+}$). Practical exercise IV (Analysis of the EPR spectrum of N_2^- in ionic solids: KCl e MgO).

Prerequisites

Knowledge of quantum mechanics.

Teaching form

Lectures in the class with PowerPoint presentations and practical exercises in the computational lab.

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 must be delivered at least one week before the date of the exam session.

The reports on the exercises and practicals, both the computational ones carried out in the computer lab, and the experimental ones carried out in the chemical laboratory are evaluated with a score in thirtieths. This assessment must be equal to or higher than 18/30 to be admitted to the oral exam.

The oral exam consists of a first part of discussion on possible errors or lacks present in the reports. Subsequently, some questions are asked of both a general nature or more detailed on the topics developed in the classroom during the lectures or on the contents of the lab exercises.

Office hours

The professor receives appointment.