



UNIVERSITÀ  
DEGLI STUDI DI MILANO-BICOCCA

## SYLLABUS DEL CORSO

### Teoria e Metodi per le Spettroscopie

2425-1-F5401Q075

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#### 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 spettroscopy. Practical exercise I (Analysis of the vibrational spettroscopy of  $\text{Mn}(\text{CO})_5\text{Br}$ ). Part III: Quantum mechanical methods (Density Functional Theory). Part IV: UV-vis spettroscopy. Practical exercise II (Analysis of the UV-vis spettroscopy of  $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ ). Part V: EPR spettroscopy. Practical exercise III (Analysis of the EPR spettroscopy of  $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ ).

#### 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 spettroscopy. Transition dipole moment. Symmetry selection rules. Normal modes of vibration. Practical exercise I (Analysis of the vibrational spettroscopy of  $\text{Mn}(\text{CO})_5\text{Br}$ ). Part III: Quantum mechanical methods. Basis sets. Review of Hartree-Fock theory. Fundamentals of density functional theory. Kohn-Sham formalism. Types of exchange and correlation functionals. Part IV: UV-vis spettroscopy. 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 spettroscopy of  $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ ). Part V: EPR spettroscopy.

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  $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ ).

## Prerequisites

Knowledge of quantum mechanics.

## Teaching form

16 two-hour lectures in person, Delivered didactically  
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.

## Office hours

The professor receives appointment.

## **Sustainable Development Goals**

AFFORDABLE AND CLEAN ENERGY

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