UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Chimica Fisica III e Laboratorio

2425-3-E2702Q097

Aims

Provide students with an introduction to the chemical-physical principles of molecular spectroscopy and describe the operating principles and technical components of the main spectrophotometers.

D1 Knowledge and Understanding
At the end of the course, the student should be able to demonstrate knowledge of:

The relationships between spectroscopy and quantum mechanics.
The main quantum mechanical models to interpret vibrational and rotational spectra.
A classical method to describe the operating principle of Raman spectroscopy that allows for the correct interpretation of Raman spectra.
The operating principles of the various components of a spectrophotometer (sources, wavelength separators, and detectors).

D2 Ability to Apply Knowledge and Understanding
At the end of the course, the student should be able to:
Critically analyze vibrational, rotational, and Raman spectra.
Extract information from them about the chemical-physical properties of molecules, not just analytical information.
Interface with the main spectroscopy instruments and use them in a conscious and correct manner.

D3 Judgement Autonomy
At the end of the course, the student should be able to:
Choose the most appropriate spectroscopic method for studying the system of interest.
Correctly and critically analyze a spectrum, considering the data collection method and the technical characteristics of the instrument used.****

D4 Communication Skills
Be able to describe clearly and concisely in writing (a technical report) and orally, with appropriate language, the objectives, procedure, and results of the analyses and experiments conducted.**

D5 Learning Skills
Expected outcomes: being able to apply the knowledge acquired to contexts different from those presented during the course, and to distinguish between an analytical use and a chemical-physical use of spectroscopy.

Contents

Interpretation of Rotational spectra, vibrational spectra and Raman spectra by quantum mechanics concepts. Collection of spectra during the laboratory activities.

Detailed program

Rotational spectra. Vibrational spectra. Roto-vibrational spectra: roto-vibrational states in the Born-Oppenheimer approximation. Quantitative computation of structural parameters. Raman spectra. Electronic molecular spectra. Selection rules and transition probability. Different spectroscopic experiments and data elaborations will be carried out with a particular attention to technical aspects of instruments used. The arguments of the experiments are the following: determination of bond length of molecules by rotovibrational spectrum analysis collected by infrared (IR) spectroscopy; analysis of absorption spectra in UV-VIS region to determine electronic transitions of molecules; use of Raman spectroscopy to study vibrational signatures of molecules.

Prerequisites

Physical Chemistry II (in particular The theory of quantum mechanics: principles and applications, Schroedinger equation). Physics II (in particular electromagnetic waves and their interaction)

Teaching form

The course includes 4 CFU of lectures and 2 CFU exercises in the laboratory. In the laboratory students are assigned, divided into small groups, the task of collecting and processing spectra with different spectrophotometers using the methodologies presented in the theoretical lessons. Methods are also proposed to produce a clear and accurate elaborate in the process. Hours of exercises are also dedicated to writing reports with the support of teachers

14 lessons of two-hour in person, Delivered Didactics
6 laboratory activities of 4 hourin person, Interactive Teaching

Textbook and teaching resource

C. N. Banwell “Fundamentals of Molecular spectroscopy" 3?? Edition McGraw Hill Book Company available in the elearning page

Lecture notes “Guida alle esperienze di spettroscopia” S. Binetti- (provided by the professor and available in the elearning page)

Semester

Third year, first (fall) semester

Assessment method

The assessment of learning outcomes related to descriptors D1-D5 is conducted through an oral examination and the evaluation of a written report on the laboratory experiences. Guidelines and a format for drafting the report correctly are provided on the e-learning page. The report can be either group-based or individual and must be submitted one week before the scheduled exam date to the laboratory instructors, following the procedures outlined on the e-learning page.

The oral examination, in addition to verifying the acquisition of disciplinary knowledge and skills, will assess the student's ability for critical analysis, independent judgment, and clarity of presentation. The final grade for the oral exam alone is assigned according to the following criteria:

18-20: Preparation covering only a limited number of topics from the course syllabus, with limited ability to discuss and analyze, emerging only with the help of the instructor’s questions; inconsistent accuracy in exposition and vocabulary, with minimal critical thinking skills.
21-23: Preparation covering some of the course topics, autonomous analytical ability only for purely practical and procedural matters, correct but not entirely precise and clear vocabulary, and somewhat uncertain presentation skills.
24-27: Preparation covering a broad range of topics from the syllabus, ability to conduct independent argumentation and critical analysis, ability to apply knowledge to different contexts and relate topics to real-world cases, correct vocabulary, and proficiency in disciplinary language.
28-30: Complete preparation on the exam topics, independent ability to discuss and critically analyze issues, ability to reflect and connect topics to real-world cases and different contexts, critical and independent thinking, mastery of disciplinary vocabulary, rigorous and well-structured exposition, argumentation, and interdisciplinary connections.
30L: Comprehensive and exhaustive preparation on the exam topics, independent ability to discuss and critically analyze issues, deep reflection and self-reflection, connections between topics and real-world cases, excellent critical and independent thinking, full mastery of disciplinary vocabulary, rigorous and structured exposition, argumentation, and interdisciplinary connections.
The written report is also graded on a scale of thirty and assessed according to the following criteria:

8-20: The report covers only a limited part of the laboratory experiences, with a superficial and poorly detailed description; presence of methodological and interpretative inaccuracies; unclear exposition with inconsistent use of technical language; minimal or absent analytical and critical reflection; graphs and figures either irrelevant or poorly understandable; absence or inadequate use of bibliographic sources.
21-23: The report covers some laboratory experiences with a generally correct but superficial description; limited application of the scientific method and difficulties in data interpretation; comprehensible exposition with some terminological inaccuracies; restricted autonomous analysis to practical and procedural aspects; graphs and figures present but not always well-executed or sufficiently discussed; limited bibliography, not always relevant or correctly cited.
24-27: The report comprehensively addresses laboratory experiences, with a well-structured and correct exposition; adequate application of the scientific method and conscious data interpretation; ability to connect

theoretical concepts from the course; appropriate use of technical language and good clarity in exposition; well-executed graphs and figures effectively supporting the analysis; bibliography present, though sometimes not correctly formatted.
28-30: A well-structured and in-depth report, rigorously covering laboratory experiences and critically interpreting data; ability to relate experimental results to theoretical concepts and other disciplines; precise and well-articulated scientific language; clear, logical, and coherent exposition; accurate, well-labeled, and correctly interpreted graphs and figures; bibliography present, relevant, and correctly cited.
30L: An excellent, comprehensive, and exhaustive report, with an autonomous and critical approach to laboratory experiences; in-depth analysis and original reflection on experimental data; outstanding use of scientific language; clear, rigorous, and well-structured exposition; high-quality graphs and figures effectively integrated into the analysis and accompanied by a thorough discussion; bibliography present, relevant, and correctly cited.
The overall grade will be a weighted average of the grades from the oral examination and the written report, based on the credit distribution between the lecture-based and laboratory components.

There is an optional mid-term exam at the end of the lecture period during the November academic break. This exam covers the topics discussed in lectures, except for those related to the principles of operation of the spectrophotometers available in the laboratory, their components, and the description and execution of experiments. The mid-term exam is written and consists of four open-ended questions, each with a specified maximum score out of thirty. The evaluation of each response considers the completeness and accuracy of the answers as well as clarity in written expression.

If students pass the mid-term exam, they may choose to take the oral examination only on the topics not covered in the mid-term (i.e., the principles of operation and components of laboratory spectrophotometers and the execution of experiments). However, students may decide at the time of the oral exam whether to retain their mid-term grade or take the oral examination on the entire course syllabus.

Erasmus students may request to take the mid-term exam, oral examination, and write the report in English.
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Office hours

All days from Monday to Friday upon e-mail request

Sustainable Development Goals

QUALITY EDUCATION | GENDER EQUALITY