UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Physical Chemistry III and Laboratory

2021-3-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.

Knowledge and understanding

At the end of the course the student knows:

- the relationships between spectroscopy and quantum mechanics

- the main quantum mechanical models for interpreting vibrational and rotational spectra

- a classic method of describing the working principle of Raman spectroscopy which allows a correct interpretation of Raman spectra

- the principles of operation of the various components of a spectrophotometer (sources, wavelength separators and detectors)

Applied knowledge and understanding

At the end of the course the student is able to:

- analyze, critically a vibrational and rotational spectrum and a Raman spectrum

- obtain information from it on chemical and physical properties and not only the analytical ones

- use several spectrometers in a conscious way and correctly

Autonomy of judgmenet

At the end of the course the student is able to:

- choose the most appropriate spectroscopic method for the study of the system of interest;

- correctly and critically analyze a spectrum also in relation to the collection method and the technical characteristics of the instrument in question

Communication skills

Knowing how to describe in a technical report in a clear and concise way and orally present the objectives, the procedure and the results of the processing carried out with language properties.

Ability to learn

Being able to apply the acquired knowledge to different contexts 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

During the COVID-19 emergency, lectures will be registered or doing in streaming and available online on the elearning platform .

The laboratory will be carried out with a reduced number of students for safety reason.

Textbook and teaching resource

C. N. Banwell "Fundamentals of Molecular spectroscopy" 3rd Edition McGraw Hill Book Company

Lecture notes "Guida alle esperienze di spettroscopia" S. Binetti- C. Greco (provided by the professor)

Semester

Third year, first (fall) semester

Assessment method

The exam consists of an oral exam preceded by the delivery of a written report on laboratory experiences. For the preparation of the report, guidelines will be provided to be followed. The report can be one per work group or single and must be delivered in paper form at least one week before the date of the oral exam. The report will be evaluated in thirtieths and will weight for one third of the final mark.

A written partial exam (with open questions) is scheduled at the end of the lectures, it will regard only the topics covered during the classroom lectures. Al the students that pass this partial test with a grade > 22/30 will be subsequently probed at the oral exam only with questions on the part of the course related to the laboratory experiences and on the principles of operation of the spectrophotometers. Also in this case, the evaluation of the laboratory report will weight for one third of the final mark.

For Erasmus student the oral exam can be given in Englsh

The evaluation of the tests (written or oral) takes into account the completeness and accuracy of the answers, as well as the clarity in the presentation

During the Covid-19 emergency period, oral exams and the class presentation will only be online. They will be carried out using the WebEx platform and on the e-learning page of the course there will be a public link for access to the examination of possible virtual spectators

Office hours

All days from Monday to Friday upon e-mail request