The Hebrew University of Jerusalem

Syllabus

INTRODUCTION TO SPECTROSCOPY - 69922

Last update 05-11-2015

HU Credits: 4

Degree/Cycle: 1st degree (Bachelor)

Responsible Department: chemistry

Academic year: 0

Semester: 1st Semester

Teaching Languages: Hebrew

Campus: E. Safra

Course/Module Coordinator: Prof. Sandy Ruhman

Coordinator Email: sandy@mail.huji.ac.il

Coordinator Office Hours: By appointment

Teaching Staff:

Prof Sanford Ruhman
Ms. Maayan Bonjack

<u>Course/Module description:</u>
This is an introductory course to spectroscopy and to light-matter interactions, which combines qualitative and quantitative descriptions of different absorption and scattering molecular spectroscopies.

Main Subjects:

Interaction of light and matter, the electronic oscillator model vs the transition dipole, Rotational, vibrational and ro-vibrational spectra of diatomics including Raman scattering. Vibrational spectroscopy of polyatomic molecules and normal modes. Symmetry analysis of vibrational activity of polyatomic molecules. Electronic spectroscopy and Franck Condon factors, vibronically allowed transitions. Photoelectron spectroscopy and orbital energies.

<u>Course/Module aims:</u>
See Learning Outcomes.

<u>Learning outcomes - On successful completion of this module, students should be able to:</u>
Describe basic light-matter interactions in molecules.

Know basic equipment which is used in spectroscopic studies.

Quantitatively analyze absorption and scattering spectra of simple molecules, and extract the relevant molecular parameters.

Use symmetry consideration in analysis and prediction of molecular spectra.

Solve questions from different fields of spectroscopy.

<u>Attendance requirements(%):</u>
None

Teaching arrangement and method of instruction: Lecture and Exercise.
80% of homework assignments must be handed in.

<u>Course/Module Content:</u>

Intro - spectroscopy, light and EM radiation, classical description of irradiation field, light-matter interaction.

Basics of spectrophotometry - absorption spectrum, Beer-Lambert Law.

Classical model for absorption (Lorentz model)

Optical transition: a quantum description - Einstein model for absorption in a TLS, Einstein coefficients, transition dipole - definition, importance, relation to absorption cross section and extinction coefficient,

Born-Oppenheimer approximation, transition dipole and nuclear motions in a di-atom: rotation and vibration.

Rotational spectrum: rigid rotor - energetics and selection rules, transitions, examples (CO) and astrochemical applications.

Vibrational absorption spectrum: harmonic oscillator, selection rules.

Rotational-vibrational absorption spectrum: selection rules, examples, anharmonicity (Birge-Sponer interpolation), selection rules for anharmonic oscillator, vibration-rotation coupling.

Raman spectrum: light scattering, microscopic description of scattering and the polarizability tensor, spectrum of scattered light, classical and quantum descriptions of Raman scattering, intensities and selection rules, transitions.

Vibrations in polyatomics: normal modes, examples (CCl4), Raman vs. IR, functional groups.

Molecular symmetry: intro to symmetry, symmetry considerations in prediction of selection rules in a polyatomic, symmetry groups, the trace, algebra of trace vectors, symmetry considerations in the quantum description.

Electronic spectrum: energy state in a diatomic, MO model, electronic terms of diatomics and selection rules, Vibronic structure and Franck-Condon principle, extension to polyatomics, Benzene as an example.

Photo-electron spectroscopy and orbital energies: description and examples.

Introduction to photochemistry: Jablonski diagram, examples: photochemistry of oxygen and ozone, photochemistry of small molecules in space.

Required Reading:
For most of the course:

M. Hollas, Modern spectroscopy (QC 451 H64)

Additional Reading Material:

For advanced reading:

J. Mchale, Molecular spectroscopy

Course/Module evaluation:

End of year written/oral examination 100 %
Presentation 0 %
Participation in Tutorials 0 %
Project work 0 %
Assignments 0 %
Reports 0 %
Research project 0 %
Quizzes 0 %
Other 0 %

Additional information:

Prerequisite knowledge:

1. *Perturbation theory.*
2. *Linear Algebra.*
3. *Quantum treatment of Harmonic Oscillator, a particle in a box and rigid rotor.*