Chemistry 540  PRINCIPLES OF SPECTROSCOPY  Fall 2021

Instructor: Piotr Piotrowiak, LSC 201D, tel. 973-353-3518, e-mail: piotr@newark.rutgers.edu
Class time & place: Monday, 6:00-9:00 PM, Smith Hall 242
Office hours: Thursday 10-12 and by appointment

Textbooks:
The primary reference material for the course will be Quantum Chemistry and Spectroscopy by Thomas Engel, ISBN-13: 978-0321766199; ISBN-10: 0321766199. We will supplement is as needed with excerpts from additional sources.

Objectives:
The course lays down the general theoretical groundwork necessary for the understanding of the interaction between electromagnetic radiation (light) and matter. Practical illustrations will be drawn primarily from electronic and vibrational spectroscopy, however, the main goal is to provide broad conceptual basis applicable to any type of spectroscopy, from routine UV-vis absorption to multidimensional NMR. The course begins with a review of undergraduate-level quantum mechanics and proceeds to introduce the concepts of transition probability, absorption, emission, dispersion, stimulated emission and laser action.

Grading:

1st midterm: October 11 – (a 30 minute in class quiz + a take home component) 15 %
Last date to drop with a grade of W: October 25
2nd midterm: November 22 – (a 30 minute in class quiz + a take home component) 15 %
Graded homework - 15%
Final: Date to be determined – (2 hours in class + an individual take home component) 55 %

Syllabus divided into major conceptual sections of the course:

1. September 8 (Wednesday) and 13 (Monday): Brief review of undergraduate level quantum mechanics including familiar solutions to the particle in the box, rigid rotor and harmonic oscillator. Orthogonality, normalization, eigenvalues, eigenfunctions, expectation values. Approximate methods of QM, i.e. the perturbation theory and the variational theorem.


5a. **October 18**: Intra- and inter-molecular non-radiative relaxation of electronic excited states. Internal conversion (IC), intersystem crossing (IST), vibrational redistribution and relaxation (IVR), conformational change, bond breaking and formation, conical intersections. Energy and electron transfer with examples of key photo-redox processes in living organisms, materials and catalysis.

5b. **October 25 (Last date to drop the course with a grade of W)**: Förster model of energy transfer and Marcus theory of electron transfer with application. Concepts of reorganization energy and electronic coupling (super-exchange).

6. **November 1**: Time-resolved electronic and vibrational spectroscopy (pump-probe, upconversion, photon counting, etc.) including selected practical aspects of the relevant instrumentation and examples.


8. **November 22**: Non-linear optical spectroscopy. Harmonic generation, wave mixing, 2-photon processes, Kerr effect, their spectroscopic and diagnostic applications.


10. **December 12**: Review of the material, distribution of the take-home assignments.

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