

The Physical Description of Chemical Systems
CH21b: Spectroscopy (1-2 MWF, 151 Crellin)

Texts: *Molecular Quantum Mechanics*, Atkins & Friedman; *Statistical Thermodynamics*, A. Maczek

Grades will be based equally on weekly problem sets, a mid-term take-home exam (the middle, slightly extended, problem set) and a final exam.

- Problem Set #1: Handed out 1/11/08; due 1/18/08.
- Problem Set #2: Handed out 1/18/08; due 1/19/08.
- Problem Set #3: Handed out 1/25/08; due 1/26/08.
- Problem Set #4: Handed out 2/01/08; due 2/02/08.
- Problem Set #5: Handed out 2/08/08; due 2/09/08. (Mid-term)
- Problem Set #6: Handed out 2/15/08; due 2/16/08.
- Problem Set #7: Handed out 2/22/08; due 2/23/08.
- Problem Set #8: Handed out 2/29/08; due 3/02/08.
- Problem Set #9: Handed out 3/07/08; due 3/12/08.
- Final Exams: 3/17-19/08 (classes end 3/12/08).

Course Outline (Reading in parenthesis):

- I. Perturbation Theory (Mostly class notes and Ch. 6 Atkins)
 - I.1. Time-independent, non-degenerate & degenerate perturbation theory
 - I.2. Time-dependent perturbation theory
 - I.3. The interaction Hamiltonian of light with matter
- II. Rotational Spectra of Molecules (10.1-10.7 Atkins)
 - II.1. Diatomic rotational spectra, eigenstates and intensities
 - II.2. Linear molecular rotational spectra
 - II.3. Symmetric top rotational spectra
 - II.4. Asymmetric top rotational spectra
- III. Rovibrational Spectra of Molecules (10.8-10.18 and Ch. 5 [group theory] Atkins)
 - III.1. Diatomic rovibrational spectra, eigenstates and intensities
 - III.2. Linear molecular rovibrational spectra
 - III.3. Symmetric top rovibrational spectra
 - III.4. Asymmetric top rovibrational spectra
 - III.5. Vibrational spectroscopy of liquids and solids
- IV. Electronic Spectra of Molecules (Ch. 11 Atkins, review Ch. 7 & 8 as nec.)
 - IV.1. Diatomic electronic spectra, eigenstates and intensities
 - IV.2. Linear molecular electronic spectra
 - IV.3. Symmetric top electronic spectra
 - IV.4. Asymmetric top electronic spectra
 - IV.5. Photodissociation (types of, and resulting spectral lineshapes), Photoionization
 - IV.6. Energy transfer processes
- V. NMR/ESR Spectroscopies (Ch. 13 Atkins & class notes)
 - V.1. Quantum mechanical origin of chemical shifts, NMR spectra
 - V.2. Spin relaxation times
 - V.3. Magnetic resonance imaging, biopolymer structure determination
- VI. Statistical Thermodynamics (an Introduction leading to Ch21c, Maczek)
 - VI.1. The Boltzmann Law and Partition Functions
 - VI.2. Thermodynamic Functions and Ideal Gas Laws
 - VI.3. Equilibrium Constants