CHEM 122 - QUANTUM MECHANICS AND SPECTROSCOPY (3 UNITS)

(Taken from the UC Berkeley Course Guide (http://guide.berkeley.edu))

COURSE OVERVIEW

SUMMARY

Postulates and methods of quantum mechanics and group theory applied to molecular structure and spectra.

PREREQUISITES

CHEM 120A (chem120a.html)

TOPICS COVERED

- Introduction to spectroscopy: Light and electromagnetic radiation, classical description of radiation field, light-matter interaction.
- Optical transitions: Einstein model for absorption in a two-level system, Einstein coefficients, time-dependent perturbation theory, transition dipoles, relation to absorption cross section and extinction coefficient.
- Born-Oppenheimer approximation: Electronic and nuclear Schrödinger equations, translations, rotations, vibrations, and electronic levels. Separation of energy scales.
- Rotational absorption spectrum: The rigid rotor for linear molecules, wavefunctions and eigenenergies. Selection rules, populations, and transitions. Isotope effects.

Coupling of molecular rotations and nuclear spin. Bose-Einstein and Fermi-Dirac statistics. The non-rigid rotor. Symmetric and asymmetric tops, selection rules.

- Vibrational absorption spectrum: The harmonic oscillator, lowering and raising operators, selection rules and overtones. Anharmonic corrections. Dissociation energy. Isotope effects.
- Vibrational-rotational absorption spectrum: Rotation-vibration coupling and selection rules. R, P and Q branches. Zero gap. Role of temperature. Anharmonic and non-rigid corrections. Band head.
- Vibrations of polyatomic molecules and molecular symmetry: Normal modes. Molecular symmetry and symmetry groups, representation of normal coordinates. Symmetry considerations in prediction of selection rules.
- 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.
- Electronic spectrum: Molecular orbital model, electronic terms and selection rules, vibronic structure and the Franck-Condon principle. Birge-Sponer extrapolation to determine the dissociation energy.

WORKLOAD

COURSEWORK

- List of stuff required from students

TIME COMMITMENT

3 hours of lecture per week.

CHOOSING THE COURSE

WHEN TO TAKE

This course is primarily for upper division students/graduate students. Ideally, you should take this course after Chem 120A, as the material in this course delves into the practical aspects of quantum mechanics. This course can also be taken in conjunction with CHEM 125 (chem125.html).

WHAT NEXT?

- CHEM 125 - Physical Chemistry Laboratory (chem125.html)
- Graduate level physical chemistry

- Physical Chemistry research

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