Chemistry 474B   2006-07
Advanced Quantum Chemistry and Spectroscopy

Instructor: Professor Rob Lipson
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Prerequisites: Chemistry 374a

Internet: http://instruct.uwo.ca/chemistry/474b/

Lectures: Tuesdays, Thursdays 11:30 am -12:30 pm in CB115.
Wednesday 10:30 am -11:30 am in CB115

Textbook: None required. All suggested books below will be on short term (3-day) loan in the library
- A popular choice is Atoms and Molecules: An Introduction for Students of Physical Chemistry, M. Karplus and R. N. Porter, W. A. Benjamin, Inc. 1970 (QD461.K33).

Other useful books include:
- Molecular Spectroscopy, I. N. Levine, Wiley Interscience, 1975 (QC454.M6L48)
- Quantum Chemistry 5th Edition, I. N. Levine, Allyn and Bacon, Inc., 2000 (QD462.L47 2000)
- Molecular Quantum Mechanics, P. W. Atkins, Oxford University Press, 1983 (QD462.A84 1983)

Evaluation:
One term test of 2 hour duration. Date to be announced: 35%
Final exam: 50%
Problem Sets (~7 in total) 15 %.

Course Outline: Details, emphasis and ordering of the material may change as the course proceeds. Specific mathematical notation and tools will be introduced as they are needed. Some of the material is an extension of that encountered in Chem. 374a/b. It is worthwhile to review those notes in the early part of the course. Some of this material will be reviewed in class as needed.

Possible topics to be covered include:
Time-independent non-degenerate perturbation theory, matrix algebra, time-independent degenerate perturbation theory, time-dependent perturbation theory, selection rules, angular momentum: the basics, coupled and uncoupled representations, application to spin-orbit coupling in H-atoms, many electron atoms: quantum numbers, terms, Slater determinants, energies including Coulomb and Exchange contributions, Variational theory, Hartree-Fock calculations, the periodic table and periodicity trends, Born-Oppenheimer approximation, molecular orbitals

versus the valence bond method, etc.

Legal Notice

Unless you have either the requisites for this course or written special permission from your Dean to enroll in it, you will be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from the course for failing to have the necessary prerequisites.