CHEM 750 Quantum Chemistry & Spectroscopy

Fall 2010 (3 credits)

Lectures: TR 9:30 – 10:45 AM, 1003 Malott

Instructor: Krzysztof Kuczera, 5090 Malott, 864-5060, kkuczera@ku.edu

Office Hours: We can meet and discuss material as needed

Text: *Molecular Quantum Mechanics*, 4th edition by P. Atkins and R. Friedman, Oxford University Press, Oxford, New York, 2005,

Grading:

Midterm exam	35%
Final exam	35%
Homework	30%

Homework:

Regular work on problem solving is crucial for understanding any area of chemistry. To help you grasp the material, regular homework sets will be assigned on an approximately weekly basis. It is a good idea to form groups to work through the more difficult questions. There will also be a weekly time to meet with the instructor to dicuss the homework. Please remember that all finally submitted work should be your own.

Office hours and discussion time:
Please do not hesitate to ask questions before, during and after class. We will schedule one or two times a week when we can meet and discuss class material and homework problems outside of the lecture. For unscheduled questions - drop in my office.

Alternative texts:
To expand your information and explore alternative views of quantum chemistry, consider looking into these texts:

D.A. McQuarrie, *Quantum Chemistry*.
I.N. Levine, *Quantum Chemistry*.
C.E. Dykstra, *Quantum Chemistry and Molecular Spectroscopy*.

Approximate schedule of lectures

Dates	Chapter
Aug 19	**0**. Introduction
Aug 24-26	**1**. Foundations of quantum mechanics
Aug 31 – Sep 7	**2**. Linear motion and the harmonic oscillator
Sep 9 - 16	**3**. Rotational motion and the hydrogen atom
Sep 21 - 23	**4**. Angular momentum
Sep 28 – Oct 5	**5**. Group theory
Oct 7	**MIDTERM** (in class)
Oct 12 - 21	**6**. Techniques of Approximation
Oct 26 - 28	**7.** Atomic spectra
Nov 2 - 9	**8.** Introduction to molecular structure
Nov 11 - 18	**9.** Electronic structure calculations
Nov 23 - 30	**10.** Molecular rotation and translation
Dec 2 - 7	**11.** Molecular electronic transitions
Dec 9	**12.** Electric properties of molecules
Dec 17	**FINAL EXAM** (7:30 am, 1003 Malott)