Chemistry 7000
Fall Semester, Session A, 2006

INSTRUCTOR: Dr. Michael D. Morse, Professor of Chemistry
Office: 3428 HEB Telephone: 581-8319
Office Hours: No set office hours. Come by and see me whenever you need to. If I am not in my office when you come by, ask one of my graduate students where I am.
E-mail: morse@chem.utah.edu Please feel free to contact me via e-mail to ask questions about the assigned problems. I check my e-mail frequently.

LECTURES: Lectures: M W F 11:50 am - 12:40 pm in HEB 2006
Discussion section: Tuesdays, 11:50 am - 12:40 pm in JTB110

TEXT: John P. Lowe and Kirk Peterson, *Quantum Chemistry*, 3rd edition.

COURSE DESCRIPTION:
This course is intended to provide chemistry graduate students and senior undergraduates with a strong foundation in quantum mechanics. No previous background in quantum mechanics is required, although a basic familiarity with the concepts covered in a standard physical chemistry course is expected. Mathematical concepts will be developed as needed, but a background in differential and integral calculus, both of a single variable and of several variables is needed. Knowledge of differential equations and linear algebra is also helpful, but these topics will be developed as needed in the course.

The course consists of three lectures per week, plus a discussion section. Attendance at all four class meetings per week is expected. Much of the time, I will use the discussion period to develop the mathematical ideas needed for the course; sometimes I will use this period primarily to answer questions that you may have. I will not follow the textbook exactly, but will instead follow my lecture notes. My notes and other useful materials may be downloaded by going to my webpage: http://www.chem.utah.edu/chemistry/faculty/morse/Morse.htm and clicking on "Courses" in the menu on the left. Next, click on "Chem 7000 - Fall 2006" and you can download whatever I have placed there.

Homework will be given out every week, and students may work together to figure out how to do the problems. Each student should work through the details of the problems individually, however. I view the homework as a means of driving home the concepts, so that you understand the topic better. Nevertheless, completion of the homework is an important exercise, so it will be graded and will account for 30% of the assigned grade in the course. I will also give one midterm exam, which will account for 30% of the grade. The remaining 40% of the grade in the course will be determined by a final exam. The midterm and final exams will be scheduled at times to be arranged, outside of the regular class period.

The University of Utah seeks to provide equal access to its programs, services and activities for people with disabilities. If you will need accommodations in the class, reasonable prior notice needs to be given to the Center for Disability Services, 162 Olpin Union Building, 581-5020 (V/TDD). CDS will work with you and the instructor to make arrangements for accommodations.

All written information in this course can be made available in alternative format with prior notification to the Center for Disability Services.

Chemistry 7000 Schedule of Topics:

(Discussion sections are in italics)

Date	Topic	Reading Assignment
August 23, 25, 28	Introduction; wavefunctions; operators; Postulates of quantum mechanics	Lecture Notes Lowe, Ch. 1 & Ch. 6
August 29	*Theorems regarding linear Hermitian operators*	*Handout sheets* Lowe Ch. 6
August 30	Time-dependent Schrödinger equation; stationary states	Lowe Ch. 6
Sept. 1	The particle in a one-dimensional box	Lecture Notes Lowe Sect. 2-1 to 2-2
Sept. 4	**LABOR DAY HOLIDAY, NO CLASS**	
Sept. 5	*Further theorems of linear Hermitian operators*	*Handout sheets* Lowe Ch. 6
Sept. 6	The particle in a 2- or 3-dimensional box; degeneracy	Lecture Notes Lowe Sect. 2-7
Sept. 8	The harmonic oscillator	Lecture Notes Lowe Ch. 3
Sept. 11	The particle on a ring; angular momentum in two dimensions	Lecture Notes Lowe Sect. 2-6
Sept. 12	*The uncertainty principle*	*Handout sheets*
Sept. 13, 15	Spherically symmetric potentials; orbital angular momentum and spherical harmonics	Lecture Notes Lowe Sect. 4-3 to 4-5
Sept. 18	The hydrogen atom; hydrogenic atomic orbitals	Lecture Notes Lowe Sect. 4-1 to 4-4
Sept. 19	*The Variation Principle*	*Handout sheets* Lowe Sect. 7-1 to 7-3
Sept. 20	The hydrogen atom; hydrogenic atomic orbitals	Lecture Notes Lowe Sect. 4-1 to 4-4
Sept. 22	Nondegenerate Rayleigh-Schrödinger Perturbation Theory	Lecture Notes Lowe Sect. 12-1 to 12-5
MIDTERM EXAM (Date and time to be determined)		
Sept. 25	Nondegenerate Rayleigh-Schrödinger Perturbation Theory (continued)	Lecture Notes Lowe Sect. 12-1 to 12-5
Sept. 26	*The Linear Variation Method*	*Handout Sheets* Lowe Sect. 7-4 & Ch. 9
Sept. 27, 29	The helium atom: Variational approach; The electron correlation problem; the Hartree limit; Hylleraas method; configuration interaction	Lecture Notes Lowe Sect. 7-3
Oct. 2	Spin	Lecture Notes Lowe Sect. 5-3
Oct. 3	*Topic undecided*	
Oct. 4	The generalized Paul principle	Lecture Notes Lowe Sect. 5-4

Oct. 5, 6	**FALL BREAK – NO CLASSES**	
Oct. 9	The ground $1s^2$ and $1s^12s^1$ states of helium	Lecture Notes Lowe Sect. 5-5
Oct. 10	*Addition of angular momenta; atomic terms*	*Handout sheets* Lowe Sect. 5-6 & 5-7
Oct. 11	Slater determinants and the *aufbau* principle	Lecture Notes Lowe Sect. 5-6 & 5-7
Oct. 13, 16	Addition of angular momenta; atomic terms	*Handout sheets* Lowe Sect. 5-6 & 5-7
FINAL EXAMINATION (date and time to be determined)		

ACADEMIC DISHONESTY:
By submitting an assignment, you are representing that it is your own work and that you have followed the rules associated with the assignment. Incidents of academic misconduct (including cheating, plagiarizing, research misconduct, misrepresenting one's work, and/or inappropriately collaborating on an assignment) will be dealt with severely, in accordance with the Student Code (http://www.admin.utah.edu/ppmanual/8/8-10.html). A single instance of academic misconduct may result in a failing grade for the course. Multiple instances of academic misconduct may result in probation, suspension or dismissal from a program, suspension or dismissal from the University, or revocation of a degree or certificate.