Chem 3310, Fall 2000
Molecular Structure and Energetics I

Class Times: MWF 10:00 – 10:50 am, Olin 103
Instructor: Sandra S. Eaton
Office: Seeley G. Mudd Rm. 178
Office Hours: MWF 8:00 am – 9:00 am, or by appointment

Texts:
Quantum Chemistry, I. N. Levine, 5th ed., Prentice Hall, 2000. This book is denoted as **L** in the reading assignments. It will also be used during Winter quarter for Molecular Structure and Energetics II.
Inorganic Chemistry, D. Shriver and P. Atkins, 3rd ed., Freeman, 1999. This book is denoted as **S** in the reading assignments. It will also be used during Spring quarter for Chemical Systems II.
Homework assignments will be added weekly to the version of the outline that is posted on the web page for the class (www.du.edu/~seaton/chem3310.htm).

Tentative Course Outline

Date	Topic	Reading	Homework due:
Sept. 11	Historical Perspective	**L**: 1-7	
13	Schrödinger equation	**L**: 7-19	
15	Exact Solution- particle in a box boxes.mcd	**L**: 21-28	**L:** ch. 1 #4,8,12,22,29
18	Free particle, wave packets wavepack.mcd	**L**: 28-32	
20	Operators	**L**: 35-45	
22	Eigenfunctions, 3-D box	**L**: 46-58	**L:** ch. 2 #7,17,25,29; Ch. 3 #1a-d,2, 5a,b
25	Harmonic oscillator harmonic.mcd	**L**: 62-77	
27	Observables, uncertainties	**L**: 94-102	
29	Angular momentum	**L**: 102-115	**L:** ch. 3 #26, 31a, 37; ch. 4 #6a-d, 16, 17; ch. 5 #3, 5
Oct. 2	Ladder operators	**L**: 115-120	
4	Particle on a ring, central force problem	**L**: 123-127	
6	Rigid rotor (exact solutions), ring.mcd	**L**: 127-134	**L:** ch. 5 #19a, 21,22,26, 31 (first set of "show that's"), ch. 6 # 4
9	Hydrogen atom Schrödinger equation	**L**: 134-141	
11	H-atom wave functions Hatomorb.mcd	**L**: 142-154	
13	Variation Method	**L**: 208-220	**L:** ch 6 #6,8,9,12,17,23, 37, compare answers from 17, 23, and 37

16	Perturbation Theory	**L**: 245-256	
18	Variation Treatment of Helium, Effective nuclear charge, radial.mcd	**L**: 256-259	
20	Shapes of orbitals, Atomic orbitals program		**L:** ch. 8 #5a,9; ch. 9 #2.
23	Electron spin	**L**:282-290, 300-302	
25	Exact treatment – $H^{\cdot}$ radical	handout	
27	Perturbation treatment – $H^{\cdot}$ radical	handout	**L:** 7, 18a-c, 19, 22a-c + handout
30	MO's for H_2^+ and H_2	**S**: 81-84	
Nov. 1	MO's for homonuclear diatomic molecules	**S**: 84-89	
3	Heteronuclear diatomics, PC Spartan	**S**: 89-94	
6	Term Symbols	**L**:323-334	
8	Symmetry elements and operations	**L:**347-355, **S**: 117-120	
10	Character tables, point groups	**L:**355-363, **S**: 120-129	
13	Reducible Representations, IR spectra for H_2O	**S**: 132-140	
15	Reducible Representations, MO's for H_2O	**S**: 130-132	
17	MO's for ML_6	**S**: 236-239	
20	comprehensive final exam		

Examinations and Homework

A weekly homework assignment will be due on Fridays.
A weekly quiz will be given on Mondays.
Answers to homework and quizzes will be provided.

Grading

Homework:	20%
Quizzes:	40%
Final exam:	40%