

Chem 3310, Fall 2006

Molecular Structure and Energetics I

Updated 9/13/06

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. It will also be used Winter quarter for Molecular Structure and Energetics II.

Updated versions of the syllabus, including homework assignments, will be posted on the Blackboard page for this class.

Note that there will be three Tuesday meetings of the class (Sept. 19, Oct. 17, and Oct. 24) at 10 am in the chemistry conference room (Olin 204), to compensate for no class meetings on Sept. 11, Oct. 18 and Oct. 20.

Tentative Course Outline

Date	Topic	Reading	Homework assignments:
Sept. 13	Historical Perspective	p. 1-7	
15	Schrödinger equation	p. 7-19	
18	Exact Solution- particle in a box	p. 21-28	
19*	Free particle, box with sloping bottom	p. 28-32	
20	Operators, Eigenfunctions	p. 35-45	
22	Expectation values, 3-D box	p. 46-58	Ch. 1 #3, 7, 10, 14, 21 Ch. 2 #5, 7, 29 Ch. 3 #2, 5, 12
25	Harmonic oscillator	p. 62-77	
27	Observables, uncertainties	p. 94-102	
29	Angular momentum	p. 102-115	
Oct. 2	Ladder operators	p. 115-120	
4	Particle on a ring	p. 123-127	
6	Central force problem, rigid rotor (exact solutions)	p. 127-134	
9	Hydrogen atom Schrödinger equation	p. 134-141	
11	H-atom wave functions	p. 142-154	
13	Variation Method	p. 208-220	
16	Perturbation Theory	p. 245-256	
17*	Variation treatment of helium, Effective nuclear charge	p. 256-259	

23	Shapes of orbitals, www.orbitals.com/orb		
24*	Electron spin	p. 282-290, 300-302	
25	Exact treatment – H [·] radical	handout	
27	Perturbation treatment – H [·] radical	handout	
30	MO's for H ₂ ⁺ and H ₂	handout	
Nov. 1	MO's for homonuclear diatomic molecules	handout	
3	Heteronuclear diatomics, Spartan	handout	
6	Symmetry elements and operations	p. 347-351	
8	Point groups, character tables	p. 355-363	
10	Symmetry applied to molecular properties	p. 351-353	
13	IR spectra for H ₂ O	handout	
15	MO's for H ₂ O, Spartan	handout	
17	MO's for ML ₆	handout	
20	comprehensive final exam		

*Tuesday class: 10 am in Chemistry Conference Room, Olin 204.

Examinations and Homework

A weekly homework assignment will be due on Fridays, starting Sept. 22nd.

A weekly quiz will be given on Mondays, starting Sept. 25.

Answers to homework and quizzes will be provided on Blackboard.

Grading

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