

## Chem 3310, Fall 2002

### 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

**Text:** *Quantum Chemistry*, I. N. Levine, 5<sup>th</sup> ed., Prentice Hall, 2000. This book also will be used Winter quarter for Molecular Structure and Energetics II.

Homework assignments will be added weekly to the version of the outline that is posted on the Blackboard page for this class.

#### Tentative Course Outline

Date	Topic	Readings from text	Homework
Sept. 9	Historical Perspective	p. 1-7	
11	Schrödinger equation	p. 7-19	
13	Exact Solution- particle in a box <a href="#">boxes.mcd</a>	p. 21-28	Ch.1 # 4, 8, 12, 22, 29
16	Free particle, wave packets <a href="#">wavepack.mcd</a>	p. 28-32	
18	Operators	p. 35-45	
20	Eigenfunctions, 3-D box	p. 46-58	
23	Harmonic oscillator <a href="#">harmonic.mcd</a>	p. 62-77	
25	Observables, uncertainties	p. 94-102	
27	Angular momentum	p. 102-115	
30	Ladder operators	p. 115-120	
Oct. 2	Particle on a ring, <a href="#">ring.mcd</a>	p. 123-127	
4	central force problem, rigid rotor (exact solutions)	p. 127-134	
7	Hydrogen atom Schrödinger equation	p. 134-141	
9	H-atom wave functions <a href="#">Hatomorb.mcd</a>	p.142-154	
11	Variation Method	p. 208-220	
14	Perturbation Theory	p. 245-256	
16	Variation Treatment of Helium, Effective nuclear charge	p. 256-259	
18	Shapes of orbitals, <a href="#">radial.mcd</a> , <a href="http://www.orbitals.com/orb">www.orbitals.com/orb</a>		
21	Electron spin	p. 282-290, 300-302	

23	Exact treatment – H <sup>•</sup> radical	handout	
25	Perturbation treatment – H <sup>•</sup> radical	handout	
28	MO's for H <sub>2</sub> <sup>+</sup> and H <sub>2</sub>	handout	
30	MO's for homonuclear diatomic molecules	handout	
Nov. 1	Heteronuclear diatomics, PC Spartan	handout	
4	Symmetry elements and operations	p. 347-351	
6	Point groups, character tables	p. 355-363, handout	
8	Symmetry applied to molecular properties	p. 351-353, handout	
11	IR spectra for H <sub>2</sub> O	handout	
13	MO's for H <sub>2</sub> O, PC Spartan	handout	
15	MO's for ML <sub>6</sub>	handout	
18	comprehensive final exam		

### Homework and Quizzes

A weekly homework assignment will be made on Mondays and due the following Friday.

A weekly quiz will be given on Mondays.

Answers to homework and quizzes will be provided.

### Grading

Homework: 20%

Quizzes: 40%

Final exam: 40%