

Chem 3310, Fall 2004

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. 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 two Tuesday meetings of the class (Oct. 5 and 19), to compensate for no class meetings on Oct. 25 and 27.

Tentative Course Outline

Date	Topic	Reading	Homework assignments:
Sept. 13	Historical Perspective	p. 1-7	
15	Schrödinger equation	p. 7-19	
17	Exact Solution- particle in a box	p. 21-28	Ch. 1 #3, 7, 10, 14, 21
20	Free particle, wave packets	p. 28-32	
22	Operators	p. 35-45	
24	Eigenfunctions, 3-D box	p. 46-58	
27	Harmonic oscillator	p. 62-77	
29	Observables, uncertainties	p. 94-102	
Oct. 1	Angular momentum	p. 102-115	
4	Ladder operators	p. 115-120	
5*	Particle on a ring	p. 123-127	
6	Central force problem, rigid rotor (exact solutions)	p. 127-134	
8	Hydrogen atom Schrödinger equation	p. 134-141	
11	H-atom wave functions	p. 142-154	
13	Variation Method	p. 208-220	
15	Perturbation Theory	p. 245-256	
18	Variation treatment of helium, Effective nuclear charge	p. 256-259	
19*	Shapes of orbitals, www.orbitals.com/orb		
20	Electron spin	p. 282-290, 300-302	