

Chem 3310, Fall 2001

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 Winter quarter for Molecular Structure and Energetics II.

Inorganic Chemistry, G. Wulfsberg, University Science Books, 2000. This book is denoted as **W** in the reading assignments. It will also be used Spring quarter for Chemical Systems 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	Reading	Homework due:
Sept. 10	No class – SSE out of town		
12	No class – SSE out of town		
14	No class – SSE out of town		
Sept. 17	Historical Perspective	L: 1-7	
18*	Schrödinger equation	L: 7-19	
19	Exact Solution- particle in a box <u>boxes.mcd</u>	L: 21-28	
21	Free particle, wave packets <u>wavepack.mcd</u>	L: 28-32	L: ch. 1# 3,7,10,14,21 ch. 2# 5,7
24	Operators	L: 35-45	
25*	Eigenfunctions, 3-D box	L: 46-58	
26	Harmonic oscillator <u>harmonic.mcd</u>	L: 62-77	
28	Observables, uncertainties	L: 94-102	L: ch.2 # 21,29 ch3#2,5,12,23,27a,b,32 ch4#15,17
Oct. 1	Angular momentum	L: 102-115	
2*	Ladder operators	L: 115-120	
3	Particle on a ring, <u>ring.mcd</u>	L: 123-127	
5	central force problem, rigid rotor (exact solutions)	L: 127-134	L: ch 5#4,5,21,24,26 30(just operate once), 32
8	Hydrogen atom Schrödinger equation	L: 134-141	
10	H-atom wave functions	L: 142-154	

	Hatomorb.mcd		
12	Variation Method	L: 208-220	L: ch6#5,9,11,16,17,23, 24,34
15	Perturbation Theory	L: 245-256	
17	Variation Treatment of Helium, Effective nuclear charge	L: 256-259	
19	Shapes of orbitals, radial.mcd , www.orbitals.com/orb		L: ch8 #3,5a,12; ch9 #2
22	Electron spin	L: 282-290, 300-302	
24	Exact treatment – H [•] radical	handout	
26	Perturbation treatment – H [•] radical	handout	L: ch10 #6,19,22a-c plus handout
29	MO's for H ₂ ⁺ and H ₂	W: 459-463	
31	MO's for homonuclear diatomic molecules	W: 464-476	
Nov. 2	Heteronuclear diatomics, PC Spartan	W: 476-483	W: ch10# 1,5,11a,b,15, 18, 21 plus handout
5	Symmetry elements and operations	L:347-353, W: 419-425	
7	Point groups, character tables	L:355-363, W:425-430, 438-443	
9	Symmetry applied to chirality, fluxionality	W: 430-438	W: ch10 #10; ch9 # 1a-g, 5,7,8,10,14
12	IR spectra for H ₂ O	W: 443-448	
14	MO's for H ₂ O, PC Spartan		
16	MO's for ML ₆	W: 508-510	
20	comprehensive final exam (moved from Mon. to have it on a different day than Chem3110 final)		

* Three classes are scheduled for Tuesdays to make up for the three days at the beginning of the quarter that SSE will be out of town to attend a scientific conference. The times (9-10 am or 10-11 am) for these meetings will be agreed upon on Mon. Sept. 17th.

Examinations and Homework

A weekly homework assignment will be made on Mondays and due the following Friday. The first assignment will be due on Sept. 21st.

A weekly quiz will be given on Mondays. The first quiz will be given on Sept. 24th

Answers to homework and quizzes will be provided.

Grading

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