Amherst College

DEPARTMENT OF CHEMISTRY

Chem-351 Quantum Chemistry and Spectroscopy

Fall 2011

This course presents an introduction to quantum mechanics. We will examine the historical development of the subject, its applications to simple systems, particles and waves, wave mechanics, and atomic structure and the Periodic Table. In addition we discuss applications to spectroscopy, chemical bonding, molecular orbital theory, and molecular structure and photochemistry

Instructor: Professor E. R. Young, Office: Merrill 521, x 5480, eyoung@amherst.edu
Office hours: Wednesday 10:30-11:30am and Thursday 10-11:30.

Lectures: Monday, Wednesday, Friday 9:00–9:50 AM in Merrill 401

Laboratory: Wednesday and Thursday 2:00–6:00 PM in Merrill 419

You will be given a lab manual that contains all of the experiments and write-ups for each experiment. Bring your lag manual to every lab session along with a laboratory notebook and a calculator.

The lab reports are due one week after the completion of the experiment. Lab reports turned in late will not be graded. **You must complete all experiments and lab reports in order to receive a passing grade for the course.**

Laboratory Assistants: Mable Lam – mlam12@amherst.edu
Cynthia Chio – tchio12@amherst.edu

Textbook: D. A. McQuarrie, Quantum Chemistry, 2ed, University Science 2007.

Books on Reserve: D. A McQuarrie, Mathematical Methods for Scientist and Engineers, University Science Books, 2003.

C. E. Dykstra, Quantum Chemistry & Molecular Spectroscopy, Prentice-Hall 1992

P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, 3 Ed, Oxford, 1997.

G. Herzberg, Molecular Spectra and Molecular Structure I. Spectra of Diatomic Molecules, 2 Ed., Van Nostrand Reinhold, 1989.

R. W. B. Pearse and A. G. Gaydon, The Identification of Molecular Spectra, 4ed, Wiley, 1976.

C. K. Cheung, G. E. Keough, R. H. Gross and C. Landraitis, Getting Started With Mathematica, 2ed, Wiley, 2005.

Homework: Problems will be assigned every Friday in lecture and will be due by 3:00 PM on the following Friday at Merrill 521 (in the folder labeled for homework collection). Late problem sets are not accepted. Homework will be graded and the solutions will be posted on the course website.

Examinations: There will be ***three*** take-home mid-term exams and a final examination. An information sheet summarizing details of the examinations will be distributed prior to each examination. Mid-term exam dates are listed in the syllabus and the final exam will be distributed during finals week.

Grades: A total of 600 points is possible in the course as follows: each of the hour exams counts 100 points, the homework counts 100 points, and the final counts 200 points. The final grade will be determined from these scores.

Academic Intellectual Responsibility: The Statement of Intellectual responsibility for Amherst College can be found at https://www.amherst.edu/academiclife/dean_faculty/fph/policies/sir. The statement should be reviewed and carefully considered by each student. The code states:

"Every person's education is the product of his or her own intellectual effort and participation in a process of critical exchange. Amherst cannot educate those who are unwilling to submit their own work and ideas to critical assessment. Nor can it tolerate those who interfere with the participation of others in the critical process. Therefore, the College considers it a violation of the requirements of intellectual responsibility to submit work that is not one's own or otherwise to subvert the conditions under which academic work is performed by oneself or by others."

Students enrolled in Chem 351 are bound to operate under the Statement for Intellectual Responsibility put forth by the College. Violation of the principles espoused by this Statement will result in offending party's removal from the course and assignment of a failing grade.

Specific implications for the application of Intellectual Responsibility to this course are:

1. ***Exams***: Discussion and collaboration on problems assigned for examinations is strictly not allowed. The exams are to be worked completely on one's own; any comments given or received that in any way assist in the understanding or solving exam problems is a violation of the Statement for Intellectual Responsibility.

2. ***Homework***: Homework problems may be discussed among students in this course or those who have previously taken the course. Discussion can be a helpful way to more fully engage the material. However, each student must be able work the problems on their own and any problem turned in should be a result of the students understanding of the material.

3. ***Laboratory***: In Chemistry 351, laboratory work will be complete in pairs, and students are encouraged to discuss experimental design and concepts covered in the lab. The answers to all problems must be in the students own words and represent their own understanding of the experiment. All data presented and analyzed must have been taken by the student. Any collaboration in obtaining data and solving problems must be acknowledged in the laboratory report.

5.61 Lecture Schedule
Fall 2008

Lecture	Date	McQuarrie	Topic
1	09/07	Chapter 1.1-1.9	Historical development
2	09/09	Chapter 5.1-5.3	Failures of Classical Mechanics
3	09/12	(Math Chapt A)	Pre-lab lecture: Organic Solar Cells
4	09/14		The Atom of Niels Bohr
5	09/16	Chapter 1.10-1.14	Wave nature, de Broglie, Uncertainty principle
6	09/19	Chapter 2	Classical wave equation
7	09/21	Chapter 3	Stationary waves, Schrödinger equation,
8	09/23	(Math Chapt B)	Probabilities and Normalization
9	09/26	Chapter 3	Particle in a box
10	09/28	Chapter 4.1-4.3	More on Particles and Vectors in QM
11	09/30		Expectation values, operators
12	10/3	Chapter 4.4-4.7	Postulates of quantum mechanics I
13	10/5		Postulates of quantum mechanics II
14	10/7		Operators and Commutators
			FIRST EXAM – hand out 10/7; due 10/12
	10/10		**No Class**
15	10/12	Chapter 5	Classical harmonic oscillator
16	10/14		Quantum harmonic oscillator
17	10/17	Chapter 5	Quantum H.O. and Energy Levels
18	10/19		Anharmonicity, Vibrational Spectra
19	10/21		Hermite Polynomials
20	10/24	Chapter 6	Rigid Rotor
21	10/26	(Math Capt E)	Rotation and Ro-Vibrational Transitions
			SECOND EXAM – hand out 10/26; due 10/28
22	10/28		Spherical harmonics, Angular Momentum
23	10/31	Chapter 7.1-7.3	Hydrogen atom I
24	11/02	(Math Chapt F)	Hydrogen atom II
25	11/04	Chapter 8.1-8.2	Variation principle
26	11/07	Chapter 8.4-8.6	Perturbation theory
27	11/09	Chapter 9.1-4	Helium atom
28	11/11		Hartree-Fock, SCF
29	11/14	Chapter 7.5	Electron spin
30	11/16		Pauli principle
			THIRD EXAM – hand out 11/16; due 10/18
31	11/18	Ch 10.1-5	Born-Oppenheimer approximation
	11/21-25		**No Classes**
32	11/28		Molecular orbital theory, H_2^+
33	11/30		LCAO-MO Theory
34	12/02	Chapter 11	LCAO-MO Theory
35	12/05	Chapter 11	Qualitative Molecular Orbital Theory
36	12/07		Huckel MO Theory, polyatomic
37	12/09		Electronic Transitions
30	12/12		Electronic Spectroscopy
31	12/14		Electron Transfer Theory

Laboratory Schedule

The laboratory experiments taking place each week will vary so that each group may rotate through each experiment.

Please take careful note of which group you are a part of and which experiment you will be performing during each week of laboratory (on your lab day, Wednesday or Thursday). You must be prepared (with pre-lab questions answered and experimental procedure read and understood) for your scheduled experiment.

Date	α Group	β Group	γ Group	ε Group
9/14, 9/15	SciFinder	SciFinder	SciFinder	SciFinder
9/21, 9/22	Mathematica	Mathematica	Mathematica	Mathematica
9/28, 9/29	EULER	EULER	EULER	EULER
10/5, 10/6	N2 week 1	-	Far IR	-
10/12, 10/13	N2 week 2	N2 week 1	-	Far IR
10/19, 10/20	Far IR	N2 week 2	N2 week 1	-
10/26, 10/27	-	Far IR	N2 week 2	N2 week 1
11/2, 11/3	FL	IR week 1	-	N2 week 2
11/9, 11/10	FL (2)	IR week 2	FL	IR week 1
11/16, 11/17	IR week 1	FL	FL (2)	IR week 2
11/30, 12/1	IR week 2	FL (2)	IR week 1,2	FL, FL (2)
12/7, 12/8	MO	MO	MO	MO

Lit Search	Searching the Literature for Information on Organic Solar Cells
EULER	Numerical Solution of the Schrödinger Equation
N_2	N_2 Emission Spectrum: A Real Quantum Oscillator
Far-IR	The Pure Rotational Spectrum of HCl
IR	Gas Phase Infrared Spectroscopy
FL	The Photochemistry of Ruthenium Bipyridyl, $[Ru(bpy)_3]^{2+}$
MO	Molecular Orbital Calculations with HyperChem