CHE 325 PHYSICAL CHEMISTRY
Fall 2007
Marian College
3200 Cold Spring Road, Indianapolis IN 46222

Instructor:	Dr. Roderick M. Macrae
Phone:	955-6064 (home: 255 9139)
E-mail:	rmacrae@marian.edu

Office Hours:	MWF 10.00-10.50 am R 2.00-4.00 pm
Lecture:	3 semester hours 11.00-11.50 am MWF Room 355
Laboratory:	1 semester hour – time TBD

Course Description: Study of the fundamental concepts of quantum mechanics, atomic and molecular structure, chemical bonding, symmetry and group theory, and molecular spectroscopy including rotational, vibrational, and electronic spectroscopy as well as magnetic resonance methods.

Textbooks:	Physical Chemistry: A Molecular Approach, Donald McQuarrie and John Simon, University Science Books, 1997.
	Problems and Solutions to accompany Physical Chemistry: A Molecular Approach, Heather Cox, University Science Books, 1997. (optional)
Other needs:	Scientific calculator (preferably TI-89 or better) Mathcad software (optional but recommended)

Course Summary: CHE 325 is a required course for chemistry majors and a recommended course for mathematics majors. Physical chemistry is the study of the mathematical and physical principles which underlie all branches of chemistry. Hence, the course revisits some of the topics of CHE 151 and CHE 152, such as the electronic structure of atoms or the nature of chemical bonding, but goes into considerably more detail towards a quantitative and predictive understanding of chemical concepts. The primary goal is to acquaint students with experimental and computational methods in chemistry and the mathematical models which shape them. Mastery of the course is associated with the ability to identify and use appropriate mathematical methods for the solution of chemical problems. The textbook we will use accompanies new mathematical techniques with "MathChapters" which explain them.

Successful attainment of the Course Objectives of CHE 325 (below) contributes to attainment of General Education objectives in the areas of Scientific and Quantitative Understanding and of Effective Communication. Particular areas include:

1. Scientific (empirical) method of problem-solving and inquiry.
2. Fundamental laws of nature and their significance.
3. Mathematical reasoning, techniques of understanding numerical data, computer literacy.
4. Critical, analytical, and creative thinking skills in written and oral communications.

Assessment of the Course Objectives is through (1) several take-home problem sets, a midterm examination, and a comprehensive two-part final examination (one part in-class, one part take-home), (2) quizzes based on reading of textbook material (3) a term paper related to applications of physical chemistry, and (4) laboratory worksheets, written laboratory reports, and an investigative research project.

Course Objectives: The main goals of this course are to cultivate skills based on mathematical inquiry and their application to chemical problems, including:

1. demonstrated ability to translate a word problem into a mathematical problem, and solve it;
2. ability to apply the methods of calculus appropriately to the constructions of models of the physical world;
3. the ability to manipulate symbolic (algebraic) expressions;
4. the ability to carry out calculations (using the factor label method introduced in CHE 151) and produce quantitative results,
5. correct use of scientific units and significant figures in the presentation of results;
6. the use of relevant computer software (primarily Mathcad) to facilitate analysis of problems;
7. demonstrated understanding of the historical development, terminology, and methods of physical chemistry;
8. demonstrated understanding of the relationship between mathematical models and experimental data.

Laboratory objectives: The main goals of this course component are to cultivate skills in mathematical and computational methods of molecular electronic structure determination and spectroscopic data analysis , including:

1. the ability to use mathematical models of molecular electronic structure and the chemical bond to obtain useful data,
2. the ability to relate the laws of quantum mechanics to the features observed in atomic and molecular spectra,
3. the ability to carry out detailed mathematical analysis on spectroscopic data and produce quantitative results,
4. the ability to keep a clear and accurate laboratory notebook, and
5. the ability to design, carry out, and report the results of an independent project in either experimental or theoretical physical chemistry,
6. the ability to manipulate symbolic expressions (algebraic and chemical equations),
7. the correct use of sign, significant figures, and unit labels, and
8. skill in the use of relevant computer software to facilitate algebraic formula manipulation, electronic structure computation and spectroscopic data analysis.

Course Requirements and Assessment Method:

1. Work should be legible and in ink and written assignments should be word processed (and spellchecked).
2. There will be approximately six take-home problem sets, a midterm, and a comprehensive final exam. The final exam will be in two parts: an open-book short question exam will be held on Wednesday, December 12, from 1.00 to 2.45, and an open-book exam with longer problem-type questions will be assigned approximately one week beforehand and be due on the day of the exam. All in-class exams must be taken on the scheduled days unless there is a valid reason not to take the exam at that time. If you miss an exam for a valid reason, the exam must be taken as soon as possible after the scheduled day.
3. We will cover material from chapters 1-15 of the textbook. It will not be possible to cover all of this material comprehensively, so we will exercise selectivity.
4. Other requirements include quizzes based on chapter material from the textbook, and the writing of a "technical" paper on the application of physical chemical methods in some area of contemporary science.
5. You are encouraged to participate actively in class by reading the relevant material beforehand, asking questions, and taking notes. Ideally, the class should form a fertile environment for mastery of chemical ideas. You are encouraged to form study groups and meet regularly and review the material.
6. Mathcad will be used to carry out some calculations. For others, a programmable calculator with scientific functions and notation will be adequate.
7. The MathChapters which review various aspects of the mathematics required for the course will be covered as necessary; to encourage review of mathematical concepts, homework will be assigned from these chapters as well as from the main body of the text.

Course Requirements and Assessment Method (laboratory):

1. The laboratory course includes *exercises* (graded via worksheets to be handed in on completion), *laboratory experiments* (for which data should be taken in laboratory notebooks, and which should be written up in formal laboratory reports), and an *independent research project* (which should be treated in the same way as a laboratory experiment).
2. Laboratory notebooks should be kept, containing dated entries made in ink, and laboratory reports should be word processed (and spellchecked).
3. Laboratory reports and worksheets should be turned within one week of completing experiments. All work for the semester will be due the day before Reading Day (Thursday 7 December).
4. Mathcad, Gaussian 03, and other software will be used to carry out calculations and analysis.

You are expected to understand and adhere to the College's policy on academic honesty as outlined in the Marian College *Code of Student Rights*. (http://www.marian.edu/forms/studentcodebook.pdf).

Attendance:
Regular attendance in both lecture and laboratory is important for your learning and for maximizing your interaction with the instructor and with others in the class. This will be reflected in a grade penalty of approximately one partial grade per three absences.

Grading Criteria:

The overall grade is calculated as follows:

Problem sets and assignments:	40%
Midterm exam:	10%
Laboratory grade:	30%
Final exam:	20%

The laboratory component of the grade is calculated according to:

Lab notebook:	50 points
Exercise worksheets	20 pts each
Lab reports	20 pts each
Independent project:	100 points

The letter grading scale follows common standards, with >90% corresponding to A, 80-89% corresponding to B, 70-79% corresponding to C, 60-69% corresponding to D, and <60% corresponding to F. The marks may be curved if needed.

Schedule of Laboratories: (tentative)

1. Introduction to Mathcad. (E)
2. Blackbody radiation – Mathcad exercise.(E)
3. Waves – Mathcad exercise.(E)
4. Absorption spectra of conjugated dye molecules.(L)
5. Atomic orbitals – Mathcad exercise.
6. Introduction to computational chemistry with Gaussian 03.(E)
7. Wavefunctions of diatomic molecules.(E)
8. Polyatomic molecules - the Hückel molecular orbital method.(E)
9. Diatomic vibrations - the Morse potential.(E)
10. High-resolution UV spectrum of I_2.(L)
11. Infrared spectral analysis – HCl and DCl.(L)
12. Infrared study of hydrogen bonding.(L)
13. IR and Raman spectroscopy – vibrations and group theory.(E)
14. Fluorescence spectra. (L)

(E) – Exercise
(L) – Laboratory experiment

Research projects will be assigned approximately midterm.

Supplementary texts:

These may be useful at various stages in the course, and can either already be found in Marian College library (in which case their catalog number is shown) or have been placed on order there.

Atkins, P. W. *Molecular Quantum Mechanics*, QD462.A77 (newer edition on order)
Barrante, James R., *Applied Mathematics for Physical Chemistry*, QD455.3.M3B2
Brandt, S., Dahmen, H. D. *Quantum mechanics on the Macintosh,* QC174.17.D2B7
Herzberg, G. *Atomic Spectra and Atomic Structure*, QC451.M28
Herzberg, G. *Molecular Spectra and Molecular Structure*, QC451.H3
Pauling, L., Wilson, E. B. *Introduction to quantum mechanics, with applications to chemistry*, QC174.1 .P24
Simon, J., Nichols, J. *Quantum Mechanics in Chemistry*, QD42.345
Slater, J. C. *Quantum Theory of Atomic Structure*, QC174.1.S5
Eddington, Arthur S. *The Nature of the Physical World*
Noggle, Joseph H. *Physical Chemistry using Mathcad*
G. A. D. Ritchie and D. S. Sivia, *Foundations of Physics for Chemists*
Green, N. J. B., *Quantum Mechanics 1: Foundations*
Green, N. J. B., *Quantum Mechanics 2: The Toolkit*
R. J. Silbey, R. A. Alberty, *Physical Chemistry*