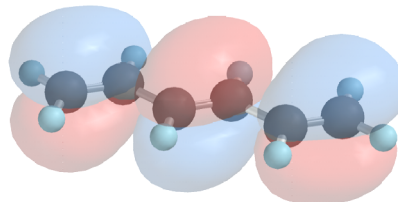


Physical Chemistry II 3150:314
July 14 – Aug. 15, 2008

INSTRUCTOR: Prof. David S. Perry
Office: KNCL 302
Phone: 375-6825
E-mail: DPerry@UAkron.edu
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OFFICE HOURS: To be arranged

PREREQUISITES: Physical Chemistry I (3150:313) or Organic Chemistry II (3150:264)
Physics - 3650:292 (Elementary Classical Physics I&II)
Mathematics - 3450:235 (through Differential Equations)

If you do not have credit in one or more of the above prerequisites, or if you are unsure of your background, then please discuss your situation with me. If you do not have all of the prerequisites you need my permission before starting the course.

OVERVIEW: The objective of this course is for each of you to gain a working knowledge of the basic concepts of quantum theory, atomic structure, chemical bonding, and molecular spectroscopy. Course activities include lectures, reading, working problems, and a computational project.

TEXT and SOFTWARE:

“*Quantum Chemistry and Spectroscopy*”, by T. Engel and P. Reid (The valuepack that includes the Spartan software is recommended. The valuepack costs about \$20 more than the text without the software.) Alternatively, the larger text “*Physical Chemistry*” by the same authors also contains the same material.

Spartan Student Physical Chemistry Edition, available for Mac or Windows. (Optional; this software is available for your use without charge in KNCL 314) (\$100. from www.wavefun.com).

You will also need a **USB Flash Drive** and you will need to access your **UA ZipSpace** and your **UA Email**.

LECTURES: MTWRF 2:15 - 3:45 p.m. KNCL 321

ASSIGNMENTS: Regular problem assignments will be an important part of the course. The examinations and quizzes will include many questions similar to the assigned problems.

QUIZZES: Ten minute quizzes will be given twice weekly. Each quiz will contain one problem or a few short answer questions. Your average score on the quizzes will be constructed by first dropping the 2 lowest scores and then averaging the remainder. If you are absent for a particular quiz, then that quiz will be one of the 2 dropped from your average. Please bring a calculator and a ruler to each quiz.

QUANTUM CHEMISTRY PROJECT:

Pairs of students may undertake a quantum chemistry project in which they use the Spartan software to calculate molecular properties. The Spartan software is installed on front two rows of computers in KNCL 314. Software manuals, tutorials, and TA's are there to help you. If decide not to do a quantum chemistry project, you still need to complete the Spartan assignments A and B.

Today, quantum chemistry methods are extremely powerful and are used routinely by chemists in all subdisciplines of chemistry. You will see how the principles that you learn in this class are used to solve real chemical problems. You will also see beautiful three dimensional graphics of the molecular orbitals responsible for chemical bonding. This project will give you the opportunity to have fun with chemistry at the same time as you learn a great deal.

The projects are due on *Friday Aug 15* at the beginning of the final exam. I will grant an automatic extension until Monday Aug. 18 at 5:00 pm to hand in your report. Note that the computer lab in KNCL 314 will be closed by the end of the final exam and will not be open on the weekend or on Monday Aug 18. Therefore, your calculations need to be done before the final exam.

EXAMINATIONS: Two exams will be given, each of which will be comprehensive. Please bring a calculator and a ruler to each exam. A schedule for the exams is given below. Any changes will be announced at least one week in advance.

<i>Midterm Exam</i>	<i>Friday Aug. 1</i>	KNCL 321	<i>2:15 pm – 3:45 pm</i>
<i>Final Exam</i>	<i>Friday, Aug 15</i>	KNCL 321	<i>2:15 pm – 3:45 pm</i>

GRADING: The final scores will be computed by one of the following schemes (whichever yields the higher score):

Exam #1	30%	20%
Average Quiz Score	25%	25%
Spartan Assignments A & B	5%	
Spartan Project		25%
Final Exam	<u>40%</u>	<u>30%</u>
TOTAL	100%	100%

Please to not miss either exam. The summer session is short and intense and there is no structured opportunity for make-ups. If you miss one exam for a compelling reason, such as hospitalization, I will give you an individual oral exam. Unacceptable reasons include vacation plans, sporting commitments, and family issues other than serious illness.

I have no fixed grading scale for assigning final letter grades (A, B, etc.) for the course. The break points between the different letter grades will depend on the difficulty of the exams, the level of the class performance, and the location of natural breaks in the distribution of numerical grades. When exam #1 is returned, I will post an approximate scale for that exam to let you know how you stand in the course.

CHM 314 Sign-Up
Summer 2008

Name UA Student ID Number

Major Phone Email

() I have completed all of the prerequisites for this course.

() I have not completed the following prerequisite courses:

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.....
.....

Chemistry 314 Syllabus
Summer 2008

	Chapter
I. The Quantum Theory	
A. Motivation	1.1
B. Classical Theory	2.2 – 2.3
C. The Failures of Classical Physics	1.2 – 1.7
D. The Concepts of the Quantum Theory	2.4 – 2.7; 3; 6.3
E. Particle-in-a-box	4
F. Tunnelling	5
G. Vibrational Motion	7.1
H. Rotational Motion	7.2 – 7.8
II. Atomic Structure and the Periodic Table	
A. The Hydrogen Atom	9
B. Intrinsic Spin	6.2
C. Multielectron Atoms	10, 11.1
III. Chemical Bonding	
A. The Born-Oppenheimer Approximation	12.2
B. The H_2^+ Molecule and the Origin of Bonding	12.2- 12.5
C. The Molecular Orbital and Valence-Bond Approaches	12.6-.7; 13.3-.5
D. Approximation Methods	10.4-.5; 13.2; 14.7; 16
IV. Molecular Spectroscopy	
A. Microwave Spectroscopy	8.6
B. Infrared Spectroscopy	8.1 – 8.5, 8.7
C. Raman Spectroscopy	8.8
D. Electronic Spectroscopy	15.1 -15.7
E. Magnetic Resonance	18

Reserve Reading List
for CHM 314 (3150:314)

Books at about the level of this course:

Physical Chemistry, A Molecular Approach,
D.A. McQuarrie and J. D. Simon
University Science Books, 1997
QD463.2 .M394 1997

Quantum chemistry, Donald A. McQuarrie
University Science Books, 1983
QD462 .M4 1983

Physical Chemistry, P.W. Atkins
Freeman 1978, 1982, 1986, 1990, 1994
QD453.2 .A88 1990

Atoms and Molecules, M. Karplus and R.N. Porter
Benjamin Cummings 1970
QD461 K33

Physical chemistry, Farrington Daniels and Robert A. Alberty
Wiley 1975
QD453 .D322 1975

Books at a higher level than this course:

Physical Chemistry, R.S. Berry, S.A. Rice, and J. Ross
Wiley 1980
QD453.2 B48 1980b

Quantum Chemistry, I.N. Levine
4th Ed., Allyn & Bacon 1991
QD462 L48 1991 (Earlier editions are also available in the library. The 5th edition was published in 200 but is not in the library.)

Modern quantum chemistry : Introduction to advanced electronic structure theory,
Attila Szabo, Neil S. Ostlund
McGraw-Hill, 1989
QD462 .S95 1989

A Guide to Molecular Mechanics and Quantum Chemical Calculations
Warren H. Hehre
Wavefunction, Inc., 2003
QD 462.6 D38 H447 2003

Ab initio molecular orbital theory, W. J. Hehre, L Radom, P. Schleyer, and J. A. Pople
Wiley, 1986
QD461 .A185 1986