

Chemistry 302
Physical Chemistry II
Second Semester 1998-99
SYLLABUS

Instructor

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Office hours: 7:30-7:50 AM M-F or by appointment

Class schedule

Lecture	12:00-12:50 MTThF	(GSC 241)
Lab	2:00-5:50 M	(GSC 259)

Lab Assistant

Dan Denevan

Texts

Peter W. Atkins, "Physical Chemistry," 6th ed., Freeman, 1998. The text includes a CD-ROM. (Lecture: required, cloth).

P. W. Atkins, C. A. Trapp, M. P. Cady, and C. Giunta, "Student's Solutions Manual for Physical Chemistry," 6th ed., Freeman, 1998. (Lecture: required, paper, bundled with text).

David P. Shoemaker, Carl W. Garland, and Joseph W. Nibler, "Experiments in Physical Chemistry," 6th ed., McGraw-Hill, 1996. (Laboratory: required, cloth). Cited as **SGN** in this syllabus.

Supplies

Safety goggles or safety glasses must be worn in the laboratory by all students, even those who wear prescription glasses. Approved safety goggles or safety glasses are available in the Augustana Bookstore. A bound laboratory notebook is needed for lab work. A scientific calculator (not necessarily programmable) is important. Each student should have several floppy disks available for her/his work in this course.

Time expectations

Plan to spend about 8 hours per week efficiently studying text and lecture material and working problems. On the average, another 2-3 hours a week will probably be needed for preparation of lab reports.

Attendance

Attendance is required for exams and laboratories, and is encouraged for lectures. Students absent from lecture are responsible for obtaining lecture notes from a classmate. Principal examples of excused absences: illness, family emergency, or an activity officially excused by Augustana. A student with an excused absence from a unit exam may take the exam the next day, before it is returned to the class. Otherwise a missed unit exam will be covered by the comprehensive final exam (see p. 4).

Nature of the course

This course is the second of a two-semester sequence in physical chemistry. In terms of topics, the course is concerned with quantum chemistry, symmetry, atomic and molecular structure, crystallography and diffraction methods, spectroscopy, statistical thermodynamics, electric and magnetic properties, and macromolecules. Within this framework, the course is distinctly problem-oriented. Facility in calculus is expected, at the level of Math 251, 252. Any additional mathematical background is all to the good. On the other hand, opportunities should arise quite naturally to review or learn some mathematics in the course of studying physical chemistry. We hope that you will grow in intellectual maturity, as you apply mathematical and physical tools to chemical systems.

Disabilities

Any students with disabilities who need reasonable accommodation in this course are encouraged to speak with the instructor as soon as possible.

Class Home Page

Visit our class home page at <http://inst.augie.edu/~viste/302s99/index.html> Please check your e-mail on a daily basis. It provides another avenue for communication in this course.

Problems

Chemistry 302 as a whole is problem-oriented. Problems will be discussed regularly in class.

Working problems from Atkins constitutes an excellent learning opportunity, and provides useful preparation for Chem 302 exams.

Specific **Exercises and Problems** from Atkins are assigned below, and are due at class time on the date indicated. Exercises and Problems are worth 1 point each. Microprojects are worth 5 points each. Any excess over the required 50 points in this Problems category will be treated as Extra Credit. See also p. 4. Timeliness is valued: note the Late Penalty described on p. 4. Please make a serious effort to work exercises and problems before looking over Atkins' version of the solution. Usually there is more than one reasonable approach. Discuss problems freely with classmates and instructor.

Problem Assignments: Atkins

Exercises are (a) unless noted

Date Due	Probs	Chapter	Exercises	Problems	MicroProjects (p. 716)
Feb 12	8	21	12,13b,20,22	1,4,5,15	
18	7	11	13,16,18	2,4,5,12	2.1
25	7	12	1,14	3,8,12,13,14	
Mar 4	7	13	7,10,13,20	2,7,10	2.3*
11	7	14	3b,5,5b,12	9,13,19	2.11
19	8	15	6,9,10b,12,13	8,12,13	
25	7	16	13,18,26,27	8,10,14	2.6
Apr 12	7	17	4,5,6	2,5,7,10	
19	7	18	2,12,17,20	3,6,9	
23	7	19	10,11,12	3,5,6,12	
29	7	20	1,3,9,11,15	8,9	2.20
May 6	8	22	3,5,6,12	5,10,16,18	
13	6	23	2,4,5,10	7,21	

93 problems These suggestions amount to roughly one problem a day during the semester.

* A slight change in language for one sentence in MicroProject 2.3 part (e): Construct the boundary surface plots so that $|\psi|^2$ is constant along the boundary surface.

Answers to Atkins Exercises, Problems, and MicroProjects: p. 955-982 and the Solutions Manual. Tables Index: p. 917-919. Tables of Data: p. 919-950. Subject Index: p. 983-999. Further useful data: inside front and back covers.

Instructional objectives

Some comprehensive objectives may be stated as follows. The student will become able to:

1. rely more on reasoning than on memorization in learning physical chemistry.
2. state definitions and laws on which major results, relationships, and equations in the course are based; i.e. identify the conceptual starting points which form the basis for each subsequent major development.
3. work with and apply each of the concepts and equations specified in learning objectives at the beginning of an assigned chapter of Atkins.
4. work problems similar to those recommended in problem sets, and achieve reasonable success in tackling related types of problems involving similar concepts.
5. become more sure-footed in mathematical modeling and "story problems", in the context of physical chemistry.

Term Paper Due Mon May 3 (100 points): Physical Chemistry of a Small Molecule and a Crystal

Work with the chemical literature is incorporated in courses throughout the Augustana Chemistry curriculum. Study p. 7-12 of the SGN lab manual, a section of the Introduction entitled "Literature Work," together with Appendix F (p. 877-878). Note also that Atkins provides pertinent references in Appendix B, Further Reading (p. B1-B23).

Select one small, reasonably symmetrical molecule, in consultation with the instructor. Coordinate with Lab 2 (Quantum Chemistry, Symmetry, Computer Graphics). Locate a CAS Registry Number for the substance. (There may possibly be more than one CAS Registry Number, particularly if you specify particular isotopic species.) Search the literature and compile a short bibliography with interesting examples of vibrational spectroscopic studies (IR, Raman), electronic spectra (UV/visible), NMR, EPR (esr), some quantum chemistry, and crystal structure determinations (x-ray or neutron diffraction) for this substance. Use Chemical Abstracts in this search. With the help of the instructor, also use Dialog (or CAS ONLINE) to search the recent literature. Your CAS Registry Numbers will be important at this point. For the x-ray crystallography, try using CAN/SND, another online database. Obtain printed copies of a reasonable selection of the papers involved. In cases of articles published in journals not available on campus, submit Interlibrary Loan requests with the aid of the instructor. Allow ample lead time, since Interlibrary Loan requests often take 2-3 weeks to be filled.

Include in your report the following items:

- 1) Bibliography. Include titles, but otherwise follow the format of bibliographic citations in the Journal of Physical Chemistry.
- 2) Printer output from your Dialog (or CAS ONLINE) and CAN/SND searches, and any CD ROM searches.
- 3) Summary and discussion of two of the articles in your bibliography: one spectroscopy paper and one x-ray crystallography paper. Include photocopies of these two articles with your report.
- 4) Some biographical information for one of the authors of one of the articles.
- 5) Pertinent data on the molecule. Include such information as electronic ground state, bond length(s), bond angles, vibrational frequencies (IR/FTIR and/or Raman spectra), normal modes of vibration, electronic transitions (UV-visible spectra), nmr, and esr.
- 6) Include some quantum chemistry results. Coordinate with the Chime Web Page and with Lab 4, as well as with your literature searching.

Chime Web Page Due Mon May 10 (100 pts): Molecular and Crystal Structure, Spartan and HyperChem software, *ab initio* and semiempirical MO calculations

Examine the results of MO calculations on O₂ (Spartan and HyperChem), and on a transition metal complex provided by the instructor (HyperChem), with the help of AV and Dan. Which computational methods were used for these calculations?

Carry out Spartan MO calculations on the small molecule that you have selected as the topic of your term paper. We run the Spartan software on the Xstation in GSC 246A, or a PC Spartan version PC in GSC 261. Carry out the calculations at the *ab initio* 6-31G* level if possible (but consult with the instructor on this point). Include MO surfaces for several MOs which arise from the valence electrons of the constituent atoms. Calculate the normal modes of vibration.

Measure bond lengths and bond angles in Spartan. Record calculated vibrational frequencies and sketch the normal modes of vibration. Capture the MOs as images in consultation with the instructor.

Repeat using HyperChem 5 on your molecule, carrying out AM1 and an *ab initio* calculation (selected in consultation with AV). If time allows, calculate the UV-visible spectrum as well. HyperChem 5.1 is on a PC in GSC 261.

By the due date, post this work on the Web, linked to your home page. Include graphics, such as MOs, structures, and normal modes. Use Chime to display several interesting molecular structures, in relation to their point group symmetry. For examples of the use of Chime, see the Links on our class home page, <http://inst.augie.edu/~viste/302s99/>
<http://inst.augie.edu/~viste/302s99/links.html>

Point distribution

Hour exams (4 @ 100)	400
Problems *	50
Small Molecule term paper	100
Chime Web page	100
Final exam	100
Laboratory	<u>250</u>
Total	1000

* The first 50 points earned for exercises and problems count toward this 50 point item. Additional points in this category, including any MicroProjects, will be treated as extra credit.

Late Penalty

Due dates are stated in the syllabus for problems (exercises, problems, and microprojects), lab reports, Term Paper, and Web page. Points will be deducted for late work, as follows: 4% of the possible points, per day late (MTWThF). All written work for which students want to receive any credit must be turned in by the last day of class: May 14, 1999.

Possible exceptions will be considered in cases of documented illness, family emergencies, and activities officially excused by Augustana.

Final Exam as an Opportunity

The final exam counts 10% of the semester grade, equal to one hour exam. It represents a further opportunity as well. If the final exam % score is higher than the % score of one or more of the four previous hour exams, then the final exam % score will replace the lower % score on the hour exam(s). Thus it is important to perform at the peak of your ability on the final exam. Study diligently for it.

Approximate Grade lines

A/B	90 %
B/C	80
C/D	60
D/F	50

+ and - grades extend $\pm 3\%$ from each grade line. Thus 87-89.99% for B+, 90-92.99% for A-.

Laboratory

Experiments available for lab are listed on p. 6. Concerning computer work, please read SGN Chapter III: Use of Computer Software (p. 71-89). It is important that you complete your lab work and lab reports at a steady pace, so that you are not confronted with a large amount of work at the end of the semester. Your lab report may be submitted jointly with your partners, provided that each person participates fairly in the preparation of the report. Lab work in groups of 3-4 is permitted. The title page of your report should list the names of all partners in the lab work. It should separately list the names of all partners submitting the report (perhaps only a subset of the first list). Each reporting partner needs to sign the cover page as well, to certify her/his fair sharing both in preparing the report and in the original lab work. For a joint experimental report, the lab notebooks of all reporting partners need to be handed in along with the report. Late reports will risk a grade penalty.

Lab reports

Formal reports are required for each lab. Each report will be graded and returned. Lab reports should include comparison of your results with data from the literature, documented through appropriate literature references. Consult the sample lab report shown in p. 12-26 of the SGN lab manual. Study p. 9-10 of the SGN lab manual, a section of the Introduction entitled "Literature Work," together with Appendix D & E (p. 746-754). Note also that Atkins provides pertinent references at the end of each chapter. At the end of each experiment, the SGN manual provides some lead references. However locating comparative literature data will generally require some digging. Please read SGN p. 1-89, and especially p. 10-24, concerning the nature of the report and methods of data analysis. You are encouraged to use word processing to prepare all or part of your report. Appropriate use of the computer in data analysis is encouraged as well.

Record your original observations in your lab notebook rather than on random scraps of paper. Provide a title page and an up-to-date Table of Contents at the beginning of your lab notebook, as in other courses such as Chem 201. Turn in your lab notebook along with the lab report. The SGN lab manual contains an excellent discussion of the use of various types of apparatus and procedures (p. 529-732), and several useful Appendices (p. 733-764). Your report should indicate an understanding of the experiment based not only on the experiment itself, but also on relevant portions of SGN p. 529-764 and of Atkins (both of which should be cited as references in your report as appropriate).

Lab safety

Read SGN p. 6-7 and Appendix C (p. 739-745), and act accordingly with respect to lab safety. Wear safety glasses in the laboratory at all times, and use proper caution in handling chemicals. Never pipet by mouth, and never bring food into the laboratory.

Scheduling lab work

We wish to honor your choices of experiment and lab partners, within constraints of equipment and preferences of other students in the class. Work in three lab groups of 3-4 each is encouraged. Lab partners may change or regroup during the semester. We will try to have necessary equipment and supplies ready for your use. However solution preparation will be part of your lab work in the experiment. We expect you to attend lab regularly: for 4 hours each week. If you complete your lab work early in a particular unit, plan to spend the rest of your lab period in the Chemistry seminar room, doing literature work and working on your lab report.

The nominal order is indicated on the next page for the lab units and experiments.

However **rotation of groups** through lab units 3 and 4 is recommended, with at least one group reversing the indicated order.

Chem 302 Laboratory
Second Semester 1998-99

Unit	Date Work	Date Due	Pts	Topic	SGN Expt	Atkins Ch. (6e)
1: Expt/ Computer Crystals	2/8 -2/22	3/1	65	X-ray powder patterns or Buerger precession photos, and NRCVAX: X-ray crystal structure determination	45,46*	21
2: Computer	3/1 -3/22	4/12	65	Quantum Chemistry, symmetry, computer graphics [Spring Break: Mar 29-Apr 5]	*	11-15,21
3: Expt/ Computer	4/12 -4/19	4/26	60	Vibration-rotation spectra: HCl, CO, NO, CO ₂ , HCN, C ₂ H ₂	37,38	14-16
4: Expt/ Computer	4/26 -5/3	5/10	60	Magnetic susceptibility and Multinuclear NMR	*32 *	13-22

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Rotation of groups through units 3 and 4 is recommended, with at least one group reversing the order.

* Instructions for each computer lab (1 and 2, partially 3 and 4) will be given in lab.
Formal reports are required for each lab.

C Course

Chemistry 302, like Chemistry 301, is a "C" course. This designation means that it satisfies Area 2.4, Computer Interaction, within the Augustana General Education requirements. Computers and software are increasingly pervasive in Chemistry, reflecting a significant trend which has been in progress since at least the early 1960s. In Chemistry 302, several assignments involve significant computer interaction. Examples include the following. In each case the instructor provides introductory instruction, assistance, and encouragement as needed. The lab assistant is also available for help and encouragement.

1. X-ray crystallography calculations, using NRCVAX software.
2. Choice of computer controlled instrumentation, such as FTIR and FT-NMR.
3. Basic quantum chemistry, using Hückel MO calculations on a PC, atomic structure calculations using SCF Xa software, and harmonic oscillator calculations through Mathcad.
4. Significant use of contemporary quantum chemistry software, including Spartan and HyperChem, including graphical presentation and visualization of results.
5. The Small Molecule term paper, which includes online searching of the highly important *Chemical Abstracts* database through Dialog or CAS Online.
6. The Chime Web Page, which includes presenting material on a Web page, and uses the contemporary Chemistry software tool called Chime.
7. Effective use of word processing and spreadsheet software is also expected routinely.

Chem 302 Class Schedule
Lecture-discussion and Problems
Second Semester 1998-99

Date	Topic	Read Atkins Ch
Feb 8,9,11,12 15,16,18	Diffraction techniques Quantum theory: introduction & principles	21 11
Feb 19 (F)	Exam 1	
22,23,25 26, Mar 1,2,4	Quantum theory: techniques & applications Atomic structure and atomic spectra	12 13
Mar 5,8,9,11	Molecular structure	14
Mar 12 (F)	Exam 2	
15,16,18,19 Mar 22,23,25	Symmetry: its description and consequences Rotational and vibrational spectra	15 16
Mar 26 (F)	Exam 3	
[Spring Break: Mar 29-Apr 5]		
Apr 6,8,9,12 13,15,16,19 20,22,23 26,27,29 30, May 3,4,6	Electronic transitions Magnetic Resonance Statistical thermodynamics: concepts Statistical thermodynamics: machinery Electric and magnetic properties	17 18 19 20 22
May 7 (F)	Exam 4	
May 10,11,13 14	Macromolecules and colloids Review	23
May 17 (Mon, 1:00-3:00)	Final Exam	