Chemistry 302
Physical Chemistry II
Second Semester 1999-2000
SYLLABUS

Instructor

Arlen Viste
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Office hours: 7:15-7:50 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

John Gilbertson E-mail jdgilber@inst.augie.edu

Texts

Peter W. Atkins, ***Physical Chemistry***, 6th ed., Freeman, 1998. (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**.

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 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.

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.

Active, Cooperative Learning (with less of a paper blizzard)

We hope that you will be actively involved in your own learning in this course. Except for exams, we strongly encourage cooperative work with classmates. Lab work for example will generally be done in groups of three. Let's try hard to set up friendly, compatible groups. We will also try to generate less of a paper blizzard in the course. As part of this, the **302 Portfolio Web Page** provides an opportunity for you to celebrate your accomplishments, creativity, and understanding, without killing a lot of trees in the process. See p. 5.

Instructional objectives

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

1. rely more on reasoning and insight 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 the Checklist of key ideas in each chapter of Atkins.

4. work problems similar to those assigned 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.

Class Home Page

Visit our class home page at http://inst.augie.edu/~viste/302s2000/index.html Please check your e-mail on a daily basis. It provides another avenue for communication in this course.

Old Exams

Exams from Chem 302, Spring 1999 are available online at our web page:
http://inst.augie.edu/~viste/302s2000/exams99.html
Exams this year may or may not be similar.

WWW

We hope that you will frequently use **Netscape** or **Internet Explorer** as a web browser (World Wide Web), in computer labs such as GSC 30 or on the new Chemistry PCs in GSC 261 and 246A. Try these links, for a start.

http://inst.augie.edu/~viste/	Augustana Department of Chemistry
http://inst.augie.edu/~viste/302s2000/	This course, Chem 302 Spring 2000
http://www.whfreeman.com/pchem/index.htm	Web site for our Atkins text
http://www.shef.ac.uk/chemistry/web-elements/	Web Elements
http://jchemed.chem.wisc.edu/Journal/Search/index.html	J Chem Ed Index: Search
http://www-sci.lib.uci.edu/HSG/GradChemistry.html	Martindale's Virtual Chemistry Center

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 301 exams.

Specific **Exercises and Problems** from Atkins are assigned below, 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.

As a required part of your **302 Portfolio Web Page**, post thoughtful solutions to a representative sample (of exercises, problems, and microprojects) that you consider to be the most interesting and significant in our text.

Date	Probs	Chap	Exercises (a) except as noted	Problems	Microprojects
Feb 1 2	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	2.12
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	
May 6	8	22	3,5,6,12	5,10,16,18	
13	6	23	2,4,5,10	7,21	
	93				5 proj

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.

302 Portfolio Web Page

Chem 302 students are to create a home page of their own. The nature and objectives of this web page can be tailored to your own particular interests, through specific agreement with the instructor, but there are several expected components.

The 302 Portfolio Web Page should pull together your activities in this course. In it, document your growing understanding of physical chemistry. The Portfolio as a whole should be more than the sum of its parts.

Overall Theme. A major emphasis in your 302 Portfolio Web Page should deal with **Quantum Chemistry and Spectroscopy** in Chem 302. Your 302 Portfolio Web Page will reside on inst.augie.edu. If you already have a personal home page there, link it to your 302 Portfolio Web Page. AV will create an overall Chem 302 home page for this course, with links to each class member's home page, at URL
http://inst.augie.edu/~viste/302s2000/
Be creative, substantive, and also sensitive to copyright issues.

Term Paper

As part of this web page, please include a term paper as described below (p. 6).

Problems. (See p. 4.) As a required part of your **302 Portfolio Web Page**, post thoughtful solutions to a significant, representative sample (of exercises, problems, and microprojects) that you consider to be the most interesting and significant in our text.

Laboratory

Lab notebook data, computer work, lab reports should be presented thoroughly and creatively. Experiments available for lab are listed on p. 9. Variation with respect to content and schedule is possible. During the semester, reports are required for each item of lab work, both experimental work and computer work. These are part of the **302 Portfolio Web Page**. Please read SGN p. 1-89, and especially p. 10-24, concerning the nature of the report and methods of data analysis. Appropriate use of the computer in data analysis is encouraged as well. **Work posted by members of a lab group should be distributed among the web pages of the group members - not primarily on one member's web site.**

You may also want to incorporate some of your career or avocational interests, particularly as they intersect the concerns this course. Certainly the web page should reflect your own personality. It should be obvious that this needs to be your own work, in consultation with AV as necessary. Using a "hired gun" to create a flashy web page for you would be worth zero points. Thus the web page should include a statement of authorship, and a virtual signature of some sort. We will link each student web page to the one for this course, at URL http://inst.augie.edu/~viste/302s2000/

Be sensitive to issues of plagiarism, copyright, and Augustana guidelines.
http://www.benedict.com/
http://www.augie.edu/info/guidelines.html
Include interesting graphics, your own writing, and a rich sampling of links to relevant

Internet sites across the world. And be aware that your work will be publicly accessible across the world.

To begin to get oriented to some of the Chemistry material on the Internet, begin to browse the Web, starting from our Augustana Chemistry Department home page,
http://inst.augie.edu/~viste/
and continuing from there to a wide variety of sites for which links are provided there. In addition it will be pertinent to utilize search engines, such as
http://www.alltheweb.com/
http://www.altavista.digital.com/
http://www.dogpile.com/
http://alabanza.com/kabacoff/Inter-Links/science.html
http://www.infoseek.com/

Suggestions for starting on a web page (prepared by AV) are available at
http://inst.augie.edu/~viste/webstart.html

Please do not use frames in your web page. Do not use unnecessarily elaborate black-box software (such as Microsoft Front Page) to produce your web page. The organization and structure of your web page are your own responsibility. We recommend using Netscape to create and edit your web page directly. Occasionally you will probably need to edit the html code itself. You are welcome to interact and consult with classmates and AV as needed.

Term Paper (100 pts, May 10): Physical Chemistry of a Small Molecule and of 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, also use compilations of structures (see the instructor). 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) Summary of your Dialog (or CAS ONLINE) search, 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. Provide photocopies of these two articles to the instructor.

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.

7) 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.

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

9) 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 in GSC 261.

10) Post this work on your **302 Portfolio Web 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. Display the crystal structure on the web, using Chime or similar tool. For examples of the use of Chime, see the Links on our class home page,
http://inst.augie.edu/~viste/302s2000/

Lab reports

Post your lab reports directly on your **302 Portfolio Web Page** (p. 5). These should include comparison of your results with data from the literature, documented through appropriate literature references. Consult the sample lab report shown in p. 15-26 of the SGN lab manual. At the end of each experiment, the SGN manual provides some lead references. However note the **caveat** in the last paragraph of SGN p. 7: locating comparative literature data will generally require some digging.

Point distribution

Take-home unit exams (3 @ 150)	450
Homework problems on 302 Portfolio Web Page	75
Lab Reports on 302 Portfolio Web Page	225
Term Paper on 302 Portfolio Web Page	100
Final exam: ACS standardized exam (Quantum Chem)	150
Total	1000

Grade lines

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

+ and - grades normally extend ±3% from each grade line. Thus 87-89.9% for B+, 90-92.9% for A-.

However there is room for some flexibility, particularly if the 302 Portfolio Web Page is sensational or the ACS exam is unusually fine.

What grade do you think you have earned in this course? Take into account the scope and quality of your overall work. Submit this statement to the instructor individually, either at the end of the 302 Portfolio Web Page, or privately. As the instructor assigns final grades for the course, such a statement of your own realistic self-assessment will provide important input in the process.

Pace yourself

The last day of class (**Friday May 12**) is the ultimate and final deadline for all work for credit in this course (other than the final exam). However we strongly recommend that you pace yourself, and complete the assigned work steadily throughout the course. Aim at completing lab reports and problems within a week of the date scheduled for the work.

If you would like your work to be graded as discrete items during the semester, then live with this deadline, and let the instructor know when your work is posted on the web and ready for grading. Otherwise the Chem 302 Portfolio Web Page will be graded as a whole at the final deadline, May 12, at the end of the semester.

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.

Laboratory Work

Please maintain a lab notebook, as in other Chemistry courses. See SGN p. 7.

Unit	Pts	Topic	SGN Expt	Atkins Ch
L1	100	Library instruction with Ann Smith Dialog search, term paper		
E1	20	X-ray powder patterns	45	21
C1	35	Crystal structure determination using NRCVAX or ShelX software package	✱	21
E2	35	Atomic emission spectra (Grotrian diagrams) Absorption spectrum of a conjugated dye	40 (5ed) 34	13 14,17
C2	35	Quantum chemistry, symmetry, computer graphics	✱	12-16
E3	20	FTIR spectra: Vibration-rotation HCl, CO, NO, CO_2, HCN, C_2H_2 etc	37,38	16
E4	25	Raman spectra	✱ 36	16
C3	35	Vibrations in quantum chemistry and Chime	✱	16
E5	20	Magnetic susceptibility and Multinuclear NMR	✱32	18.22
	225			

✱ Instructions and guidance for this lab and computer work will be provided by the instructor.

Lab Work Schedule by Lab Group

	Group 1	Group 2	Group 3	Group 4	Group 5	Group 6
Feb 7	E1	E1	E1	E1	E1	E1
Feb 14	C1	C1	C1	E2	E2	E2
21 (3:00)	L1	L1	L1	L1	L1	L1
21	C1	C1	C1	E2	E2	E2
28	E2	E2	E2	C1	C1	C1
Mar 6	E2	E2	E2	C1	C1	C1
13	C2	C2	C2	E3	E3	E3
27	C2	C2	C2	E4	E4	E4
Apr 3	E3	E3	E3	C2	C2	C2
10	E4	E4	E4	C2	C2	C2
17	E5	E5	E5	C3	C3	C3
May 1	C3	C3	C3	E5	E5	E5
8	C3	C3	C3	C3	C3	C3

Reports and other work posted by members of a lab group should be distributed among the web pages of the group members - not primarily on one member's web site.

See page 8 for comments about deadlines and grading.

Chem 302 Class Schedule
Lecture-discussion and Problems
Second Semester 1999-2000

Date	Topic	Read Atkins Ch
Feb 7,8,10	Diffraction techniques	21
11,14,15	Quantum theory: introduction & principles	11
17,18,21	Quantum theory: techniques & applications	12
22,24,25	Atomic structure and atomic spectra	13
28,29, Mar2,3	Molecular structure	14
Mar 3 (F)	Receive **Take-home Exam 1** (Due Fri Mar 10)	
6,7,9,10	Symmetry: its description and consequences	15
13,14,16	Rotational and vibrational spectra	16
	[Spring Break: Mar 20-24]	
17,27,28,30	Electronic transitions	17
31, Apr 3,4,6	Magnetic Resonance	18
Apr 6 (Th)	Receive **Take-home Exam 2** (Due Fri Apr 14)	
7,10,11	Statistical thermodynamics: concepts	
13,14,17	Statistical thermodynamics: machinery	20
	[Easter Break: Apr 21-24]	
18,25,27	Electric and magnetic properties	22
28, May 1,2	Macromolecules and colloids	23
May 2 (Tu)	Receive **Take-home Exam 3** (Due Tues May 9)	
May 4,5,8,9,11,12	Review, and complete your 301 Portfolio Web Page [Reading Day: Tuesday May 16]	
May 18 (Thurs, 8:00-10:00)	Final Exam	