Physical Chemistry, CH342 **Spring 2017**

Text: T. W. Shattuck, *Physical Chemistry*, *Vol. 2*, 2017

Reserve reading: P.W. Atkins, J. de Paula, *Physical Chemistry 7th ed.*
D. A. McQuarrie, J.D. Simon, *Physical Chemistry: A Molecular Approach*
D. A. McQuarrie, *Quantum Chemistry, 2nd ed.*
M. W. Hanna, *Quantum Mechanics in Chemistry, 3rd. ed.*
M. Karplus, R. N. Porter, *Atoms and Molecules*

Alternate texts: I. N. Levine, *Quantum Chemistry, 4th ed.*
J. P. Lowe, *Quantum Chemistry*

Date	Shattuck	Atkins	McQuarrie	Hanna	Karplus	Topic	Test
1 2/1	23	11	1,2	3	1,2	Foundations of Quantum Mechanics	
2 2/6	23	11, 12	3,4	1-2	2	Foundations of Quantum Mechanics	
3 2/13	24	12	5,6	6.1-.4	3	Quantum: Rotation and Vibration-	
4 2/20	25	13	7,8	6.5-.11	4	Atomic Structure	
5 2/27	26	14	9	7.1-.4	5.6	Molecular Structure	3/3
6 3/6	26	14	10	7.1-.4	6	Molecular Structure	
7 3/13	26,27	14, 15	11-12	7.5-.9	6	Molecular Structure, Spectroscopy	
8 3/27	27	16		4-5	7.1-.10	Rotation & Vibration Spectroscopy	
9 4/3	28	17	15	7.6,8.6	7.7,.11	Electronic Spectroscopy	4/7
10 4/10	29	18	14	9	7.13	Magnetic Resonance Spectroscopy	
11 4/17	12	19	17			Statistical Definition of Entropy	
12 4/24	30	20	18			Statistical Mechanics	
13 5/1	32	27	30			Molecular Reaction Dynamics	

Laboratory.

The laboratory will begin with a series of experiments using NMR. The labs will begin in a structured fashion, but each successive NMR assignment will be less detailed. The series culminates in a project to determine the proton resonance assignments of a terpene or similar compound. Readings for this project will include T. D. W. Claridge, *High-Resolution NMR Techniques in Organic Chemistry*, Pergamon,Oxford, 1999 or equivalently A. E. Derome, *Modern NMR Techniques for Chemistry Research,* Pergamon, Oxford, 1987. In other words, personal initiative will play a pivotal role for these NMR projects.

Next we will spend two weeks on X-ray diffraction. Then three weeks will be devoted to IR and UV/Vis spectroscopy. Theoretical computer projects will also be completed. The problems include molecular mechanics and dynamics of beta-ionone in week 3, molecular orbital calculations for BF_3 and O_3 in week 7, and a classical trajectory calculation for the reaction $H + H\text{-}F \rightarrow F + H_2$ in week 13.

Homework.

A homework assignment, to be handed in on Friday afternoon, will be assigned each Monday. Homework assignments from the text will also be made, but not to turn in. We will discuss homework for the week on Friday afternoon; please come prepared to ask questions on the problems. However, please feel free to ask questions about homework problems, especially back of the chapter homework at any time. The answers will also be on reserve in the library. Please remember that homework gives you the practice that you need to feel confident with the

material. You don't know if you understand the material until you try to use the concepts on your own. Warning: all assignments, late or otherwise, are due before the final examination.
A very approximate point distribution is given below:

Homework	200
Hour tests	200
Final	200
Lab	200
	800

Graded Assignment Policy

Collaboration with your classmates is encouraged, when appropriate. You can learn a lot from listening to each other and from explaining ideas to each other. However, whenever a grade is given for the work, it must represent the accomplishments of the individual, unless explicitly specified as a group project by the instructor. Lab reports, homework to hand in, and tests are to be your own work. Students might make the mistake of assuming that while cheating on tests is dishonorable, collaboration on lab reports or homework to hand in is OK. Please note that lab reports and homework are just as important with regards to academic dishonesty as tests, perhaps even more important. Science advances through the honest and careful reporting of laboratory work. Dishonesty in the lab impedes scientific progress and cannot be allowed. In working with a partner in the lab, your collaboration **ends with the taking of data**. Let's make it clear what is appropriate for individual lab reports and homework to hand in for this course.

On individual work for a grade, any assistance that you give or receive from another student must be limited to correcting errors in the data as recorded in the laboratory. It is wrong to show your work to another student as a means of helping. Recording another person's answer is also plagiarism whether it is given verbally or in writing. Sharing spreadsheets or parts of spreadsheets is also not allowable. You must also maintain access privileges on your fileserver folders to ensure that other students do not have access to your work. You may, however, honestly consult the instructor as a way of checking if you are on the right track.

On the other hand, working in a group on suggested problems that are not to be turned in for a grade is an excellent idea. In other words, the suggested homework provides ample opportunity to share ideas and provide help to others. Regular meetings of such help groups are a useful way to keep up with course work.

As in all your academic work, any ideas or information that you obtain from the literature should be properly cited. Citing literature sources is necessary even if you do not give a direct quote. Formal lab reports should use ACS format for references. References to text tables, the CRC, or Lange's Handbook can be simply given in-line, including the edition. For example:

The literature value for the enthalpy of formation is –134.23 kJ/mol (CRC 48th Ed.)

These guidelines are consistent with the College's policy on academic honesty as discussed in the College Student Handbook and the Catalog. If you have any problems on any assignment, you are strongly encouraged to come in to my office for help.

Resources

The **Answers** for the problems in Shattuck, Atkins, and McQuarrie and Simon are on reserve in the science library. Previous year's tests are on reserve also, in addition to copies on the course Web page.

Process Skills and Learning Goals

The focus of any chemistry course is the in-depth understanding of chemical reactivity using structure-function relationships. Thermodynamics, chemical kinetics, quantum mechanics, and statistical mechanics provides a coherent, unified, and powerful set of ideas and a point of view that enables chemists to be effective at solving important challenges in human health, energy technology, environmental stewardship, and improving the general quality of life. These theoretical ideas also satisfy the liberal arts desire to understand our world as completely as possible. We also show the interrelationships among the sub-disciplines of chemistry, among the sciences, and between the sciences and the goals of society. Gaining facility with abstraction is the primary goal. Building mathematical models, working through the implications of those models, and assessing the validity and inherent errors in the ability of the models to predict and explain physical phenomena is the central core of the curriculum.

Laboratory.

Date		Laboratory
2	2/6	NMR-T1 determination, *Web Lab Manual*, Claridge 2.1-2.5.2, Breit 3.3.2
3	2/13	NMR- DEPT, COSY, HMQC of β-Ionone, Claridge 5.1-5.4, 5.7, 6.1-6.3, (Wüthrich Ch. 2) Molecular Orbital Calculations-Intro, Spartan; MOE help.
4	2/20	NMR-Nuclear Overhauser Effect of β-Ionone, *Web Lab Manual*, Claridge 8.1-8.7, (Wüthrich 6.1-6.3)
5	2/27	Independent project, 2D-NMR, Claridge 5, 6, 8.8, (Wüthrich 6.1-6.3, 7)
6	3/6	Independent project, 2D-NMR, Claridge 5, 6, 8.8, (Wüthrich 6.1-6.3, 7)
7	3/13	O_3 and BF_3 Molecular Orbital Calculations, *Web Lab Manual*.
8	3/27	X-ray diffraction, Powder diffraction. Sime 37 (Library on-line reserve)
9	4/3	X-ray diffraction, Single Crystal. Sime 38, 40 (Library on-line reserve)
10	4/10	Spectroscopy, see attached list, *Web Lab Manual*
11	4/17	Spectroscopy, see attached list, *Web Lab Manual*
12	4/24	Spectroscopy, see attached list, *Web Lab Manual*
13	5/1	Classical Trajectory Calculation, *Web Lab Manual*

Laboratory Reports.

Lab reports are due on Wednesday of the week following the completion of each lab. Late lab reports will not be accepted more than two weeks late, except that all assignments, late or otherwise, are due before the final examination. All lab reports, including calculations, are independent.

All lab reports follow the "short form" style from CH341:

1. In the Introduction, describe the experiment in one or two sentences.

2. For the Theory and Procedure sections just reference the lab write-up and briefly mention any changes in procedure from the lab write-up. In other words, the Theory and Procedure sections are just references (e.g.: please see CH342 Lab Manual for the theory and procedure) and usually nothing else.

3. For the Results section, provide the data in a tabular format, including **all information necessary to repeat your calculations**. Attach all your graphs. Graphs should fill at least a third of a page and include clearly labeled axes including units. (Axes labels and units, etc. can be hand written.) Include uncertainties for all derived values (see the error analysis handout for instructions for representing uncertainties). For example, slopes and intercepts from curve fitting should always be given with uncertainties.

4. In the Discussion section, discuss the chemical significance of the results. In other words, state why these results are useful and important. Are the results for this system unusual or do they fall within the normal range for other systems? Answer any questions in the calculations and discussion section of the lab write-up. Also comment on the uncertainty of the final results: what is the predominate experimental error; are the errors larger than the technique is capable of? Compare your final results to literature values, if easily available. (Easily available means one of the referenced papers in the lab write-up, or in Lange's Handbook, the CRC, or NIST WebBook. Ask the instructor if you are unsure, before spending lots of time on this.)

Computational Labs.

For the three computational labs you just hand in the answers to the questions in the exercise write-up. You answer these questions independently. In other words, the computational labs are just like homework.

List of Experiments for Weeks 10-12.

Spectroscopy and Kinetics.

1. Rate constant for Fluorescence Quenching. *Web Lab Manual.* Perkin Elmer 650-10S Spectrofluorometer, and Power Point or .pdf Instrument Instructions on the Lab Web Page, which you must view before coming to the lab..

2. NMR Determination of the Rotational Barrier in N,N-dimethylacetamide. *Web Lab Manual.* Varian-VNMR 500. Read the 1-D *Instrument Instructions* on the Lab Web page.

3. Laser Flash Photolysis. *Web Lab Manual*. Luzchem LFP.

Spectroscopy and Molecular Structure.

4. Rotation-Vibration Spectrum of HCl-DCl. *Web Lab Manual*. Bruker Tensor 27 FT-IR.

5. Dissociation Energy of Halogen Gases (I_2 and Br_2). *Web Lab Manual*. Perkin Elmer UV/Vis 200.

6. Dye Lasers. *Web Lab Manual*. Nitrogen Pumped dye laser, Perkin Elmer 650-10S Spectrofluorometer. and Power Point or .pdf Instrument Instructions on the Lab Web Page, which you must view before coming to the lab. Also Agilent 8453 UV/Vis, read the *Instrument Instructions* on the Web.

7. Raman Spectroscopy: Vibrational Spectrum of CCl_4. *SGS 37.* Oriel CCD Raman and Bruker IFS66vs.

References.

Breit: E. Breitmaier, W. Voelter, *Carbon 13 NMR Spectroscopy*, 3rd. ed., VCH, New York, N. Y., 1987.

Claridge: T. D. W. Claridge, *High-Resolution NMR Techniques in Organic Chemistry*, Pergamon,Oxford, 1999.

SGS: D. P. Shoemaker, C. W. Garland, J. W. Nibler, *Experiments in Physical Chemistry*, 5th. ed., McGraw Hill, New York, N. Y., 1989.

Sime: R. J. Sime, *Physical Chemistry*, Saunders, Philadelphia, PA, 1990.