Class Web Site: http://www.uwosh.edu/facstaff/gutow/physical-chemistry-2 contains some publicly available class content (syllabus) and useful links. Most class content will be in D2L: http://www.uwosh.edu/d2lfaq/d2l-login/.

Course Overview: This course concentrates on learning to use 20th and 21st century developments in chemical theory to model and understand reactivity and structure. We will begin at the microscopic level using quantum mechanics to describe molecular structure. The theoretical results will be compared to evidence from measurements of molecular spectroscopy and physical properties. We will finish by considering kinetics at both the macroscopic and microscopic levels. The experiments in lab will follow this same pattern.

You should be able to use these models to predict the behavior of matter. This means both estimating the range in which a measurement will fall and solving mathematical story problems, using approximations where valid. A summary list of the models and the types of systems to which you should be able to apply them is at the end of this syllabus.

A secondary, but very important goal of the course, is to help you develop effective communication skills. You will work on communication skills primarily in lab where you will produce written and web-based reports on your work.

Required Texts: Cooksy, *Physical Chemistry* (2 volume set, *Thermodynamics* and *Quantum Mechanics*), with modified Mastering Chemistry code for online homework.
Barrante, *Applied Mathematics for Physical Chemistry,* 3rd edition.

Required Equipment: bound duplicating laboratory notebook, pen (for writing in lab notebook), scientific calculator and goggles.

Prerequisites: Physical Chemistry I (Chem 370), calculus III and calculus-based physics II.

Class times: *Lectures*: MWF 10:20-11:20 (HS 457); *Lab* (HS 428): M 1:50-5:10 (sec 1) or T 1:20 - 4:30 (sec 2).

Instructors:

Name (Office)	E-mail	Class Sections	Office Hours
Dr. Gutow (HS 412)	gutow@uwosh.edu	Lecture & Lab 1	M 11:30-12, WF 11:30-12:30 , TTh 10:30-11:30 *or by appointment*.
Dr. Foley (HS 440)	foleym@uwosh.edu	Lab 2	TBA

Reading Assignments and Homework will cover a week or two and will have parts due at the beginning of each class meeting. Assignments will not be accepted late, but some of your lowest scores will be dropped.

Reading Assignments will come primarily from the textbook. Other sources will be used as necessary.

Homework will be due for each class and usually have an online and written component. Online parts will be due at 8 A, written parts at the beginning of lecture. You will see three different types of questions. The first two types will focus on material we will be discussing during the class meeting for which the assignment is completed.

Critical Thinking Exercises/Discussion Questions: The questions are designed to help you learn how to use the textbook and other reference sources to prepare for class. For example, you might be asked to find definitions, compare two models and explain when it is appropriate to use each or work through some 'what if' calculations.

Practice Exercises: These will be primarily online and similar to the end of chapter problems in the text. The goal is to help you figure out what you need to ask about in class.

Problems: These problems will be a little more challenging and based on material discussed in the previous classes.

Exams: There will be 220 available points on each exam. However, exams will be scored out of 200 points (20 pts of extra credit distributed throughout the exam). The material requires that exams be cumulative, but primary emphasis will be on the chapters covered since the previous exam. The goal of this course is not to memorize formulas, but to learn how to use models to make predictions. You will be provided with an equation sheet for each exam consisting of the fundamental equations of each model. Additionally, you will be allowed to bring a 3" x 5" card of ***handwritten*** notes to the exam. <u>There will also be a 90 minute laboratory exam (see the lab section of the syllabus for more details).</u>

Grading:

Homework & in class worksheets:		25%
Exams:	3 x 200 pts	50%
Lab:		<u>25%</u>
Total:		100%

Grade Cutoffs: A/A- > 87%, B+/B/B- > 77%, C+/C/C- > 67%, D+/D > 60%, F ≤ 60%. The cutoffs will not be adjusted upwards, but the instructor reserves the right to lower them.

Additional Resources:

WEB RESOURCES: This syllabus, copies of homework assignments and answer keys will be available at the course D2L site. Useful links will be provided within D2L, but can also be accessed from the instructor's home page: http://www.uwosh.edu/facstaff/gutow.

CLASS DISCUSSION LIST: A private Google group has been set up for this class. Registering for the class adds you to the group. The e-mail address for this group is uwo_chem371s15@googlegroups.com. This e-mail discussion group will be used by the instructor to distribute notices and links to assignments. You should use this group to ask questions of fellow students. The instructor monitors the list and will try to address any unanswered questions after 24 hours. If you want to access the group on the web the direct link is: https://groups.google.com/forum/#!forum/uwo_chem371s15.

SYMBOLIC MATH PACKAGES: These can help you do algebra and calculus. The open source SAGE math package is available on the Chem SAGE Server or can be downloaded from the SAGEmath web site and installed on your personal computer. Information on user accounts on the Chem SAGE Server will be provided in class. MAPLE™ is available on the computers in the open access labs in Halsey.

GAMESS QUANTUM PACKAGE: The GAMESS package is available on the computers in P-Chem lab.

TEXTS: The following books are on reserve in in the Halsey Resource Center (HS-289). You may find it useful to see difficult concepts described a number of ways. Homework assignments may suggest sections of these texts to look at for additional help.

Atkins, *Molecular Quantum Mechanics*, QD462.A84 1997. This text expands on the quantum mechanics discussed in the course text.

Atkins, *Quanta*. This is essentially a dictionary of quantum mechanical terms. You may find it useful because it explains the significance of most things with very little mathematics. A good way to get an overview.

Barrante, *Applied Mathematics for Physical Chemistry* QD455.3.M3 B37. A good review of chemical applications of graphing and calculus.

Jorgensen and Salem, *The Organic Chemist's Book of Orbitals*, QC461.J68. This book has lots of nice electron density maps for the various orbitals of common molecules calculated using molecular orbital theory.

Warren, *The Physical Basis of Chemistry*, QD475.P47. This book has nice simplified, but accurate, descriptions of many of the quantum, spectroscopic and thermodynamic concepts we will discuss.

Tentative Lecture Schedule (S15):

Topic (VOLUME.CHAPTER, T = Thermo volume, Q = Quantum volume)	Lectures
I. Theory of Molecular Structure	
Introduction to Quantum Mechanics (Q.1, Q.2)	2/2, exercises in lab, 2/4, 2/6
One Electron Atoms (Q.3, skip Q.3.4)	2/9, 2/11, 2/13
Many Electron Atoms (Q.4, skip perturbation theory, skip Q.4.4)	2/16, 2/18, 2/20
Molecular Structure (Q.5.1 – Q.5.4, pictorial orbital handout, Q.7.3, Q.13.4)	2/23, 2/25, 2/27, 3/2
Review	3/4
Exam 1 (Unit I)	**March 6, 2015**
II. Spectroscopy and Kinetics I	
Electronic Spectroscopy/Lasers (Q.7.4, skip transition metals, T.6.3 – T.6.5)	3/9, 3/11, 3/13
Vibrational & Rotational Spectroscopy (Q.8, Q.9)	3/16, 3/18, 3/20, *Spring Break,* 3/30
Molecular Transport (T.5.1 – T.5.3)	4/1, 4/3
Elementary Reactions and Reaction Dynamics (T.13)	4/6, 4/8, 4/10
Review	4/13
Exam 2 (Unit II)	**April 15, 2015**
III. Kinetics II (Mechanisms)	
Multistep Reactions (T.14.1 – T.14.3)	4/17, 4/20, 4/22
Catalysis (T.14.4)	4/24, 4/27, 4/29, 5/1
Kinetic Modeling (handout)	5/4, 5/6, 5/8, 5/11
Review	5/13
Exam 3 (Unit III)	**May 15, 2014**

Laboratory

Laboratory Notebooks: Notebooks should be records of everything a scientist does. They are used as legal evidence that an experiment was performed in patent claims and are often referred to by other scientists working on related experiments. Entries should be made in permanent ink. *Notes from pre-lab lectures should not be recorded in your notebook*, but all calculations and data analysis should be. A minimum checklist of what should be in your notebook is available on the class web site. Pages should be numbered consecutively and a table of contents included. Date each page as it is used and start a new page on each day; do not tear out pages, simply draw a line through errors. Lab notebooks will be checked each day and initialed by your instructor. You will turn in your duplicate pages with each report to assist in grading.

Pre-lab preparation: Read the description of the experiment and any additional assignment. The experiments are not described as a list of steps to be followed, so careful reading and reflection before lab will be required to develop a plan for the project.

In your notebook ***record a brief outline of the procedure you expect to follow*** and construct two tables of information: 1) reagents; 2) equipment. The reagents table should include: the chemical name, chemical formula, a drawing of the Lewis structure, the state in which it will be found (solid, liquid, gas, or in solution), and hazard information from the Material Safety Data Sheet(s), which are available online or in the stockroom. If solutions are to be prepared, calculate the amounts needed. The equipment list only needs to list equipment. However, you must try to make it complete. The list should contain every piece of glassware and equipment you think you will need. This includes, for example, pipets, spatulas, sensors, D/A interfaces and computers.

During lab: Procedures actually followed should be described in your laboratory notebook. Do not rely on a summary written before the lab, although you may just note deviations from your planned procedure. List lab partners. Include all experimental observations, data and calculations; you should tape in computer printouts and spectra (cut or fold to fit). If data is stored in computer files accurately record the data file names. Goggles and appropriate clothing (no sandals or shorts) must be worn at all times. Failure to wear safety goggles may result in ejection from lab and an F in the course.

Literature Search: After every experiment you will be required to turn in the results of a SciFinder Search. Credit will be given as follows:

> *Full credit*: Results on the same species that can be compared to yours even if collected using a different technique. This search result does not actually have to be used for comparison in your report.
>
> *Half credit*: Results using any technique to get the same information about a different molecule or information about the species you studied that is relevant to the handling of the molecule in your experiment.
>
> *Zero credit*: Anything that does not meet the criteria for full or half credit.

Lab Reports: Because scientists use many formats for communicating information, we will practice a variety of report styles this semester.

1. Formal laboratory reports: Your reports should be written as if for publication in *The Journal of Physical Chemistry.* Assume that your readers have studied physical chemistry but are not familiar with your handouts. A sample lab report is available on the class web site. **You will be required to use proper ACS formatting for your references this semester (examples in the JPC author guide and handouts on the course website).** Additional recommendations on word choice, grammar, reference format, notation and nomenclature may be found in *The ACS Style Guide*, Anne M. Coghill, Lorrin R. Garson Eds. http://pubs.acs.org/isbn/9780841239999 (link also provided on class web site).
2. Results and Discussion reports: If you score better than 75% on the introduction and experimental sections of the first formal report, you will only have to turn in results and discussion sections for latter formal reports. This goes into effect as soon as you turn in a formal report, where you get 75% or better on the introduction and experimental sections.
3. Web report presentation: You will prepare a web site to be posted on the Internet. The site should be eye-catching and informative. You must have: a title, authors' names, an

abstract, an introduction, a body, a conclusion and references. This is a web version of a formal report. Sample calculations and error analysis are not to be part of the article but should be turned in for grading.

4. Data & Question Reports: You will be turning in your lab notebook pages with your data, analysis and answers to question. This is the only time that your lab notebook pages will be graded. They will be graded for completeness, dates, name, the data analysis and answers to questions asked in the handout. Make sure to attach copies of graphs, spectra and so on to your duplicate pages as they will be needed for grading.
5. Peer Review: All articles published in the literature are reviewed by anonymous reviewers. They are only published after the reviewers are satisfied that they are accurate, well written and a new contribution to the scientific body of knowledge. Most articles are rewritten at least once in response to reviewers' comments. Often additional experiments are also done. You will review two of your peers' reports. You may rewrite formal reports based on the reviews returned to you.

Students may discuss the write-up and calculations with each other but every student must turn in an individual report. Reports must be computer word processed. Use of computers for data plotting and analysis is encouraged as is reference to the chemical literature for accepted values.

Reports will be graded out of 19 points. A copy of the grading cover sheet for formal reports and web site is available online.

The reviews will be due a week after the reports were originally due. You may rewrite the first formal report based on the reviews. If you get less than 75% overall or less than 75% on any section of the report you must rewrite it. If you turn in the rewritten report within one week of getting the reviews the grade will be replaced with the grade of the rewritten report. A copy of this first report will be kept for the student portfolio used by the department for program assessment. 75% or greater on the rewritten introduction and experimental sections will allow you to write only Results & Discussion Reports for the last two "formal" reports.

Reports are due to the online dropboxes before class the week following completion of the project. Late reports will be marked down 10%/day. Incomplete reports will be returned and the late penalty assessed.

Laboratory Exam: There will be a 90 minute final exam based on work done in lab. You will be able to refer to your textbooks, lab reports, and lab notebooks on the exam. The 90 minutes allotted for the exam will not be enough to figure out what you did from your text and your lab reports. You will only have enough time to use them as references to get constants, formuli and relationships correct. You will need to review your laboratory reports and correct any mistakes you made in order to do well on this exam. You will also be responsible for material from the prelabs and assigned reading. A non-graded problem set will be distributed during the semester to assist your preparation for the exam.

Lab Grading

	10	Quantum/Math Exercises
6 X 1 =	6	SciFinder Searches
1.5*(1 X 19) =	28.5	First formal lab report
5 X 19 =	95	Lab Reports all formats
4 X 2 =	8	Reviews of first formal report and web report
6 X 5 =	30	Prelabs
	77	Lab Final
	254.5	Points total

Lab Schedule (S15):

		Due on lab day week of		
Week of	**Project**	**Written**	**Review**	**Rewrite**
2/3	Math and Quantum Mechanics	-	-	-
2/9	Spectroscopy of Conjugated Dyes	2/16 (formal)	2/23	3/2
2/16	Quantum Calculations	-	-	-
2/23	Quantum Calculations (continued)	-	-	-
3/2	Quantum Calculations (continued)	3/9 (web poster)	3/16	-
Rotate through 2 labs: HCl rovibrational spectroscopy and Raman Spectroscopy. Turn in: prelab + HCl (results & discussion) or Raman (data & answer questions in notebook).				
3/9	Spectroscopy A	-	-	-
3/16	Spectroscopy A	3/30	-	-
3/21	*no lab/Spring Break*			
3/30	Spectroscopy B	-	-	-
4/6	Spectroscopy B	4/13	-	-
Rotate through 2 labs: Solution kinetics and TBA kinetics. Turn in: prelab + Solution (results & discussion) or TBA (data & answer questions in notebook).				
4/13	Kinetics A	-	-	-
4/20	Kinetics A	4/27	-	-
4/27	Kinetics B	-	-	-
5/4	Kinetics B	5/11	-	-
5/11	90 min Lab Exam (exact time to be arranged)			

Why this is a Liberal Arts Course: As part of a good liberal arts curriculum this course has a number of goals. The primary goal, as described in the course overview, is to introduce you to modern chemical theory. This topic fits well into the liberal arts curriculum because it teaches skills which are generally useful and specific models that are widely applicable. Learning to use these theories is extremely good practice at solving difficult and unfamiliar problems as well as thinking analytically, critically and creatively. The models of chemical reactivity (kinetics) and structure (quantum mechanics) are fundamental to understanding much of what happens to matter in the universe. These models are used to understand the chemical reactions involved in living, to predict the shapes of biomolecules, to develop new drugs, design solid-state electronics, and understand environmental issues such as global warming. Lasers and photosynthesis are quantum phenomena. In lecture and lab you will practice using these widely applicable models and consider their limitations (more critical thinking). In many cases simpler models or direct experimentation can provide high accuracy results with significantly less effort. A secondary, but very important goal of the course, is to help you develop effective communication skills. You will work on communication skills primarily in lab where you will produce written and web-based reports on your work.

Assessment of Learning: As part of the department's assessment of its majors program, evidence will be added to your portfolios to demonstrate your ability to do a number of things.

From Lecture:

1. describe the structure and composition of matter;
2. apply theoretical and mechanistic principles to the study of chemical systems employing

both qualitative and quantitative approaches;
3. use theories of microscopic properties to explain macroscopic behavior;
4. explain the role of energy in determining the structure and reactivity of molecules;
5. use mathematical representations of physical phenomena.

From Lab:

1. read and follow experimental protocols;
2. properly set up and safely manipulate laboratory equipment;
3. plan and execute experiments, including the use of the chemical literature;
4. maintain accurate records of experimental work;
5. analyze data statistically and assess reliability of results;
6. prepare effective written scientific reports;
7. use mathematical representations of physical phenomena;
8. use and understand modern instrumentation;
9. use computers for chemical applications;
10. retrieve specific information from the chemical literature;
11. work cooperatively in problem solving situations.

Models you will learn to apply:

Model	Be able to apply to
Quantum Mechanics -Schrödinger equation -Born-Oppenheimer -Rigid-Rotor -Franck-Condon principle	Molecular and atomic structure Molecular and atomic energy levels Spectroscopy of gas phase molecules (electronic, vibrational, rotational and ro-vibronic) Liquid phase spectroscopy (electronic, vibrational) Fluorescence Spectroscopies (UV-Vis, Raman, IR, photoelectric) Physical properties (dipole moments)
Kinetics -Macroscopic (mechanistic) -Microscopic --Collision Theory of Reaction Rates --Collision Theory of Solution Reactions --Transition State Theory	First order reactions Mechanisms made of first and second order reactions Unimolecular gas phase reactions Michaelis-Menten (be aware of limited experimental conditions for applicability) Potential energy surfaces Modeling of simple reactions (liquid and gas phase) Radiation processes (photochemical reactions, lasers, fluorescence)