Class Web Site: https://www.uwosh.edu/facstaff/gutow/physical-chemistry-2 contains some publicly available class content (syllabus) and useful links. Most class content will be in CANVAS: https://uwosh.instructure.com/courses/388933.

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* both the Quantum and Thermodynamics volumes.

Chemistry 371 Lab Manual available at the University Bookstore.

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

Prerequisites: Physical Chemistry 1 (Chem 370), Analytical Chemistry 1 (Chem 311), calculus III.

Class times: Lectures: MWF 10:20 – 11:20 (HS 266); Lab (HS 428): M 1:50 – 5:10.

Instructor:

Name (Office)	E-mail	Class Sections	Online Office Hours (link)
Dr. Gutow (HS 412)	gutow@uwosh.edu	Lecture & Lab	MWF 11:30 – 12:30, TTh 10 – 11 *or by appointment*.

Assessment of learning: Homework, in-class exercises and exams will be used to assess your chemical knowledge and document your ability to:

- describe the structure and composition of matter;
- apply theoretical and mechanistic principles to the study of chemical systems employing both qualitative and quantitative approaches;
- use theories of microscopic properties to explain macroscopic behavior;
- explain the role of energy in determining the structure and reactivity of molecules;
- use mathematical representations of physical phenomena.

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

You are encouraged to discuss the homework with your classmates and instructor. The important thing is to understand the problems and exercises. Doing all the homework is the best way to understand the material and prepare for exams.

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

Homework will be *due before each class* and consist of up to three sections. The first two sections will focus on material we will be discussing during the class meeting for which the assignment is completed.

Critical Thinking Exercises/Discussion Questions: These are designed to help you learn how to use the textbook and other reference sources to prepare for class, as well as help you figure out what you need to ask about during class. These exercises might ask you 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 come primarily from the exercises section at the end of the chapter. The goal is to help you figure out what you need to ask about during class.

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

In Class Exercises will typically be worksheets/group exercises. You will receive 100% credit for putting in honest effort on the exercise during class.

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.

Grading:

Homework & in class worksheets:		25%
Exams:	3 x 200 pts	50%
Lab:		25%
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.

Approximate Lecture Schedule (S21):

Topic (X#.#, X = T: Thermo volume, X=Q: Quantum volume, #.# = chapter.section)	**Lectures**
I. Theory of Molecular Structure	
Introduction to Quantum Mechanics (Q1, Q2)	2/1, exercises in lab, 2/3, 2/5
One Electron Atoms (Q3, skip Q3.4)	2/8, 2/10, 2/12
Many Electron Atoms (Q4, skip perturbation theory, skip Q4.4)	2/15, 2/17, 2/19
Molecular Structure (Q5.1 – Q5.4, pictorial orbital handout, Q7.3, Q13.4)	2/22, 2/24, 2/26, 3/1
Review	3/3
Exam 1 (Unit I)	**March 5, 2021**
II. Spectroscopy and Kinetics I	
Electronic Spectroscopy/Lasers (Q7.4, skip transition metals, T6.3 – T6.5)	3/8, 3/10, 3/12
Vibrational & Rotational Spectroscopy (Q8, Q9)	3/15, 3/17, 3/19, *Spring Break,* 3/29
Molecular Transport (T5.1 – T5.3)	3/31, 4/2
Elementary Reactions and Reaction Dynamics (T13)	4/5, 4/7, 4/9
Review	4/12
Exam 2 (Unit II)	**April 14, 2021**
III. Kinetics II (Mechanisms)	
Multistep Reactions (T14.1 – T14.3)	4/16, 4/19, 4/21
Catalysis (T14.4)	4/23, 4/26, 4/28, 4/30
Kinetic Modeling (handout)	5/3, 5/5, 5/7, 5/10
Review	5/12
Exam 3 (Unit III)	**May 14, 2021**

Laboratory: This laboratory emphasizes the use of tools to study properties of chemicals. This semester we will focus on computational modeling and spectroscopic techniques. The tools you will apply include: the chemical literature; mechanical and electronic equipment, such as vacuum lines, lasers and spectrometers; quantum computation software; mathematical functions; error analysis; and written and oral communication.

The laboratory will be used to assess your chemical knowledge and document your ability to:

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

What will happen in lab? We will begin the semester with a review of mathematical principles needed for quantum mechanics and practice using software that can do some of the algebra and plotting for you.

Six experiments have been chosen to illustrate principles studied in lecture:
quantum mechanics: Conjugated Dyes, Quantum Calculations
spectroscopy: Infrared Spectroscopy and Laser Spectroscopy
kinetics: Iodination of Ketone, Laser Induced Fluorescence

The laboratory schedule and grading specifications are included in the lab manual. In addition to in lab performance you will be evaluated on (see the lab manual for details):

- *Laboratory Notebooks*: These will include pre-lab, during the experiment and analysis notes.
- *Lab Reports*: You will be preparing formal reports (or parts of some), a poster, a website, and an oral report. You will have a chance to rewrite some of these to improve your grade.
- *Peer Reviews*: You will get credit for reviewing some of your peers' work in a timely manner so that your input can be used by your peers to rewrite their work.
- *SciFinder Searches*: You will do a number of literature searches to find articles related to the experiments you do.
- *Final Lab Quiz*: This will focus on your understanding of concepts from lab, and some simple data analysis including error propagation.

Additional Resources:

WEB RESOURCE: Class content will be in CANVAS: https://uwosh.instructure.com/courses/388933. Additionally, a copy of this syllabus and some of the useful links will be available on a public web page at: https://www.uwosh.edu/facstaff/gutow/physical-chemistry-2. Dr. Gutow also maintains useful information such as study hints and useful links for chemists on his website at: https://uwosh.edu/facstaff/gutow.

COMPUTER AIDES TO HELP WITH P-CHEM PROBLEM SOLVING: In this class you are encouraged to use computer assistance for algebra, calculus and numerical computations. There are lots of options (e.g. Maple™, MathCAD™, Mathematica™, SageMath, and others), but the *Python* programming language plus a web interface called *Jupyter* has recently been widely adopted for scientific computing and mathematics, so we will focus our efforts on that in class.

The software is available on a server at: https://math.gutow.uwosh.edu. You will be provided with server log-in information during the first meeting of class. This software is open-source and could also be installed on your own computer. Dr. Gutow will provide instructions for installation, if requested.

General Information

OFFICIAL BULLETIN COURSE DESCRIPTION: Physical Chemistry II: A continuation of Chemistry 370. Lecture topics include quantum chemistry, atomic and molecular spectra, and chemical kinetics. Laboratory includes experiments that are designed to illustrate the lecture material. Prerequisites: Mathematics 273, Chemistry 311, and Chemistry 370. 371/571 (3+3) Special fees may apply.

ACADEMIC MISCONDUCT: Representing the work of another as your own is considered academic misconduct. Any assignment (exams) which you are required to do individually should contain only your own work. Using ideas and writing from the work of others without proper attribution is considered plagiarism and could result in expulsion. See the Dean of Students office website for more information.

ABSENCES: You are responsible for informing your instructor of absences and making arrangements to make up any missed work. If an emergency (medical or exceptional personal circumstances) will cause you to miss more than three (3) days of class or prevents you from contacting individual instructors you should request an out-of-class letter from the Dean of Students office, which will go to all your instructors and provide you with one initial contact point.

ACCOMMODATIONS: The University of Wisconsin Oshkosh supports the right of all enrolled students to a full and equal educational opportunity. It is the University's policy to provide reasonable accommodations to students who have documented disabilities that may affect their ability to participate in course activities or to meet course requirements.

Students are expected to inform Instructors of the need for accommodations as soon as possible by presenting an Accommodation Plan from either the Accessibility Center, Project Success, or both. Reasonable accommodations for students with disabilities is a shared Instructor and student responsibility.

The Accessibility Center is part of the Dean of Students Office and is located in 125 Dempsey Hall. For more information, email accessibilitycenter@uwosh.edu, call 920-424-3100, or visit the Accessibility Center Website.

RESPECTING THE DIVERSITY OF OUR COMMUNITY: Diversity drives innovation, creativity, and progress. At the University of Wisconsin Oshkosh, the culture, identities, life experiences, unique abilities, and talents of every individual contribute to the foundation of our success. Creating and maintaining an inclusive and equitable environment is of paramount importance to us. This pursuit prepares all of us to be global citizens who will contribute to the betterment of the world. We are committed to a university culture that provides everyone with the opportunity to thrive. Therefore, all members of our community are expected to treat each other with respect and apply intellectually rigorous critical analysis to all their interactions with others (e.g. activities, discussions, arguments, etc...).

STUDENTS RIGHT TO KNOW ACT OF 1990: Students are advised to see the following URL for disclosures about essential consumer protection items required by the Students Right to Know Act of 1990: https://uwosh.edu/financialaid/consumer-information/.

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 models is extremely good practice at solving difficult and unfamiliar problems as well as thinking analytically, critically and creatively. The models discussed in this class are fundamental to understanding much of what happens to matter in the universe. 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 reports on your work.

Models you will learn to apply:

Model	Be able to apply to
Quantum Mechanics -Schrödinger equation -Born-Oppenheimer -Rigid-Rotor -Harmonic Oscillator -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, intermolecular forces, bulk electrical properties)
Kinetics -Macroscopic (mechanistic) -Microscopic --Collision Theory of Reaction Rates --Collision Theory of Solution Reactions --Transition State Theory -Numerical modeling	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)