Chem 103: Foundations of Physical Chemistry
Fall 2011

Course Description:
A study of foundational principles in chemical thermodynamics, kinetics, quantum mechanics, and spectroscopy. Topics include the first and second laws of thermodynamics describing the state functions: internal energy, enthalpy, entropy, free energy; physical and chemical equilibria; rate laws and their determination; theories of reaction rates, mechanisms and catalysis; postulates of quantum mechanics; molecular vibrations; and atomic and molecular structure. Laboratory experiments emphasize the use of spectroscopy and computational calculations to measure the thermodynamic and kinetic properties of select chemical systems. Co- or prerequisites: CHEM 26, MATH 8, and PHYS 11.

Meeting Time:	M/W/F 10:40 – 11:45 am (in BC 215) Th 1:15 – 4:15 pm
Instructor:	Dr. Ryan Z. Hinrichs Office: S-210 rhinrich@drew.edu
Office Hours:	Tuesday 10:00-11:00 am, Wednesday 2:00-3:00 pm Or by appointment. Open door policy: if my door is open, stop by.
Materials:	A Physical Chemistry textbook published since 2000 (recommended authors: Atkins, Ball, Engel and Reid, Levine, or McQuarrie). *Chemical Kinetics and Reaction Dynamics*, Paul Houston, Dover Pub. *Intro to Molecular Thermodynamics*, Hanson & Green, Univ. Sci. Books. Scientific calculator; laptop with Excel, MathCAD, Gaussian and IgorPro.
Lab Materials:	Bound laboratory notebook Safety glasses ($10, if needed, purchase from Jackie in S-218)

Student learning objectives:

Upon completion of this course, you should be able to:

- explain the postulates of quantum mechanics and apply them to chemically relevant systems, such as the particle in a box, the harmonic oscillator, the hydrogen atom, and electronic structure calculations.
- use the central concepts of statistical mechanics to relate atomic and molecular energy levels to macroscopic thermodynamic properties, including chemical equilibria.
- apply theories of chemical kinetics to analyze reaction rates to elucidate complex chemical mechanisms and reaction energetics.
- use the laws of thermodynamics to predict when and explain why certain chemical processes are favorable while others are not.

What I expect from you:

- attend all classes (**attendance is mandatory**) and arrive on time;
- complete assignments on time;
- read the textbook material associated with the current topic thoroughly;
- ask questions (I suggest you write down any questions as you study outside of class).

If you miss class, you are responsible to find out what material we discussed and you are expected to be prepared for the following class. If you miss more than two classes, you must schedule a meeting with me to discuss this issue.

Your work in this course will be evaluated on the following:

Participation & Quizzes	100
HW Problems (35×10)	350
Exams (3×100)	300
Laboratory	250
Total	**1000**

Participation & Quizzes: (100 points) On occasion, class will start with a brief 5 minute quiz covering basic concepts from the prior class. **There will be no make-up quizzes**. If you arrive late to class and miss a quiz, you will receive a zero.

Problem Sets: (350 points; approx. 20 assignments, 10-20 points each) Homework problems will assigned on a regular basis. Assigned problems will be handed out in class or placed in the Chem103 folder on the Drew network by the end of the prior class. **You must write up your answers individually**. If you have questions regarding a problem, please don't hesitate to contact me via email or stop by my office. *I have an open door policy - please feel free to drop by my office at anytime*.

Policy for Late Assignments: Unless you receive written permission from the course instructor at least 24 hours before an assignment is due, the following policy is in effect:
Assignments turned in **one day** late will be graded with a maximum grade of **90%**.
Assignments turned in **two weekdays** late will be graded with a maximum grade of **80%**.
Assignments turned in **three weekdays** late will be graded with a maximum grade of **70%**.
Assignments turned in **four weekdays** late will be graded with a maximum grade of **60%**.
Assignments turned in **five or more weekdays** late will be graded with a maximum grade of **50%**.

Three Exams: (100 points each) Two semester exams are scheduled for Wednesday, October 5 and Friday, November 4. The third exam will be in-class during the time scheduled for the "Final Exam" by the University Registrar. Details regarding the structure of these exams will be discussed in class at least one week prior to the date. Exams will consist of an in-class portion and a take-home portion. You must work on these exams by yourself, and I encourage you to review Drew University's policy on Academic Integrity.

Laboratory: (250 points) You are expected to keep a bound professional laboratory notebook, which I may occasionally collect. Notebooks should be written in ink and be properly dated and signed. All critical experimental details (e.g., procedures and results) and calculations should be included in your notebook. Individual experiments will also require additional documents as detailed in the lab manual. For instance, some weeks will simply require formatted graphs with captions while other labs will require a complete write-up in the format of a scientific article. All relevant data must be presented in tables and/or figures where appropriate and all references must be properly cited. Advice on scientific writing may be found in *Physical Chemistry: Methods, Techniques, Experiments* by Rodney Sime; an electronic version of this reading is located in the Chem 103 folder.

Academic Accommodations:
Should you require academic accommodations, you must file a request with the Office of Educational Affairs (BC 114, extension 3327). It is your responsibility to self-identify with the Office of Educational Affairs and to provide me with the appropriate documentation from that office at least one week prior to any request for specific course accommodations. There are no retroactive accommodations.

CHEM 103 / Physical Chemistry I: Foundations **Tentative Course Schedule**

M 8/29	Introduction. The hydrogen atom – a historical perspective.	Pre-Lab. Safety, check-in, load software. MathCAD tutorial.
W 8/31	Quantum mechanics. Postulates of quantum mechanics.	
F 9/2	Quantum mechanics. Particle in a box; calculus review.	
M 9/5	Labor day. No class.	Lab 1. UV-visible spectroscopy of a particle in a box.
W 9/7	Quantum mechanics. Particle in a box; 2- and 3-D PIB.	
F 9/9	Quantum mechanics. 2-D PIB wavefuntions; classical harmonic oscillator.	
M 9/12	Quantum mechanics. Quantum harmonic oscillator; wavepackets.	Lab 2. Vibrational spectroscopy: analysis of overtones.
W 9/14	Quantum mechanics. Morse potential; infrared spectroscopy; Franck-Condon factors.	
F 9/16	Quantum mechanics. Hydrogen atom and atomic orbitals.	
M 9/19	Quantum mechanics. Radial distributions functions; many-electron atoms.	Lab 3. Absorbance and fluorescence spectroscopy of polycyclic aromatic hydrocarbons (PAH).
W 9/21	Quantum mechanics. Approximations using variational theory.	
F 9/23	Quantum mechanics. Spin and electronic configurations.	
M 9/26	Quantum mechanics. An introduction to electronic structure calculations.	Lab 5. Evaluating the impact of potential greenhouse gases.
W 9/28	Quantum mechanics. Electronic structure calculations. ***end of material for Exam 1***	
F 9/30	Statistical mechanics. Probabilities.	
M 10/3	Statistical mechanics. The Boltzmann distribution.	Lab 5. Evaluating the impact of potential greenhouse gases.
W 10/5	**Exam 1**	
F 10/7	Statistical mechanics. An introduction to partition functions.	

M 10/10	Reading day. No class.	Lab 5. Evaluating the impact of potential greenhouse gases.
W 10/12	Statistical mechanics. An introduction to partition functions.	
F 10/14	Statistical mechanics. Applications for chemical equilibria.	
M 10/17	Statistical mechanics. Applications for chemical equilibria.	Lab 5. Evaluating the impact of potential greenhouse gases.
W 10/19	Kinetics. Rates, transition states, and activated complex theory.	
F 10/21	Kinetics. Reversible and parallel, and sequential reactions.	
M 10/24	Kinetics. Integrated rate laws and numerical approaches.	Lab 6. Kinetic study of keto-enol tautomers: an NMR experiment and computational study.
W 10/26	Kinetics. Reaction mechanisms, potential energy surfaces, and kinetic isotope effects.	
F 10/28	Kinetics. Complex mechanisms and approximations. ***end of material for Exam 2***	
M 10/31	Chemical Thermodynamics Review. Spontaneous processes: ΔH, ΔS, ΔG; ΔG vs. ΔG°.	Lab 6. Kinetic study of keto-enol tautomers: an NMR experiment and computational study.
W 11/2	Chemical Thermodynamics Review. ΔG vs. ΔG°, K_c and K_p, assumptions.	
F 11/4	**Exam 2**	
M 11/7	Thermodynamics. First law, work.	Lab 6. Kinetic study of keto-enol tautomers: an NMR experiment and computational study.
W 11/9	Thermodynamics. Reversible vs. irreversible processes.	
F 11/11	Thermodynamics. Heat, heat capacity, and internal energy.	
M 11/14	Thermodynamics. Enthalpy.	Lab 7. Kinetic evaluation of antioxidants.
W 11/16	Thermodynamics. Thermodynamics of ideal gases.	
F 11/18	Thermodynamics. Temperature and pressure dependence of enthalpy.	

M 11/21	Thermodynamics. Second law and entropy.	No lab.
W 11/23	Thanksgiving break. Thermodynamics of cooking a turkey.	
F 11/25	Thanksgiving break. No class.	
M 11/28	Thermodynamics. Free energy definitions.	Lab 7. Kinetic evaluation of antioxidants.
W 11/30	Thermodynamics. Free energy applications.	
F 12/2	Thermodynamics. Chemical thermodynamics.	
M 12/5	Thermodynamics. Chemical thermodynamics.	