CHM4411

Physical Chemistry: Thermodynamics and Kinetics Fall 2023

The Information listed below is subject to change.

Canvas e-learning site:

https://ufl.instructure.com/courses/494830

All communications must be done through the e-learning site, including homework, deadlines, grades and announcements.

Please do not email the instructors (or the TAs) personal email accounts.

It is your responsibility to check the canvas site for updates.

Schedule:

T,R | Period 3 – 4 (9:35 AM - 11:30 AM)

LEI207

Professor:

Dr. Adrian E. Roitberg

Office Hours: TBA

Teaching Assistants:

Ignacio Pickering

Office Hours: TBA

Dinushika Kotudura Arachchige

Office Hours: TBA

Ethan Wilner

Office Hours: TBA

Prerequisites: MAC 2313.

Textbook:

There is no required textbook, but you MUST have an undergraduate Physical

Chemistry Book that includes thermodynamics and kinetics. Show any of the instructors which

book you have, and they will tell you if it is ok.

Course objectives

By the end of the course the students should be able to

Understand and use the four laws of thermodynamics.

Understand and use the principles of chemical and biological kinetics.

Course Itinerary

(Tentative)

Note: Items marked with an asterisk (*) will depend on the time available.

Why Physical Chemistry?

The First Law: Energy Is Conserved.

Energy Conversion and Conservation.

Describing the State of a System.

Phase Changes. Chemical Reactions.

The Second Law: The Entropy of the Universe Increases.

A New State Function, Entropy.

The Second Law of Thermodynamics: Entropy Is Not Conserved.

Chemical Reactions. Third Law of Thermodynamics.

Gibbs Free Energy. Helmholtz Free Energy. Noncovalent Reactions.

Free Energy and Chemical Equilibria.

Chemical Potential (Partial Molar Gibbs Free Energy).

Reactions of Gases: The Ideal Gas Approximation.

Nonideal Systems.*

The Eq. Constant and the Standard Gibbs Free Energies of the Reactants and Products.

Biochemical Applications of Thermodynamics

Kinetics: Rates of Chemical Reactions.

Kinetics. Reaction Mechanisms and Rate Laws. Temperature Dependence.

Transition-State Theory. Electron Transfer Reactions: Marcus Theory.

Ionic Reactions and Salt Effects. Isotopes and Stereochemical Properties.

Very Fast Reactions. Diffusion-Controlled Reactions.

Photochemistry and Photobiology. Photosynthesis.

Enzyme Kinetics. Michaelis-Menten Kinetics. Competition and Inhibition.

Homeworks:

There will be homework assigned nearly every week. Homework is usually due one week after it is assigned. It must be turned in at the beginning of class on the due date. Computer-typed is preferable.

Each problem must be solved in a different page. Answers should be turned in on time and should be neat and legible. Write your name and UFID clearly on each page. Neatness is crucial. Think about future employers reading your work. If they do not find it clear and easy to read and understand, they would not hire you or rate your work very high.

Each homework problem must show a full derivation of equations, explanation about every step you took, and any assumptions you have made. No points will be given for a final result without justification.

Units and numerical results will be checked and graded. Several of the homework assignments involve interpretation of computational and experimental data. When preparing graphs, you must use Excel or a comparable graphing program. If you are doing a curve fit, you must justify the choice of fitting function.

There will be no partial credit for late homeworks. If not turned in before or at the deadline, the grade will be zero.

The homeworks will be graded and returned. Solutions will be provided after the deadline.

While you might work in groups, the homework assignments must be turned in individually, thus you must turn in your own work to receive any credit!

Any sort of plagiarism will not be tolerated. Failure to adhere to these requirements will result in zero credit for the assignment.

I do have access to the same web sites where UF students go looking for help. If I find that you have copied directly from one of those sites, you will be reported immediately for plagiarism. I work on computers all day and can trace your IP and usernames without much trouble, so please do not do it!

Exams: There will be two progress exams. Conflicts with these exams' dates should be resolved with the instructor no later than one week prior to the exam date. There will be no make-up exams. The exam dates will be announced shortly.

Grading: The grade will be determined by Homeworks (40%), 2 progress tests (40% total) and a final exam (20%).

The grades are absolute, there will be no curve grading.

Students can decide not to take the final exam. If they do not take the final, then their final grade will be computed by Homeworks (40%) and 2 progress tests (60% total). This decision can be made as late as the last week of classes.

If a student decides to take the final, their grades could go up or down, so they should choose carefully. We will not take the better of the grades.

Grading scale:

- A > 90
- A- 87.5 to 89.99
- B+ 82.5 to 87.49
- B 77.5 to 82.49
- B- 75 to 77.49
- C+ 72.5 to 74.99
- C 67.5 to 72.49
- C- 65 to 67.49
- D+ 62.5 to 64.99
- D 57.5 to 62.49
- D- 55 to 57.49
- E <60

Attendance: Lecture attendance is essential for your success in this class. However, we will not take roll.

Course Evaluations: Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at https://evaluations.ufl.edu. Evaluations are

typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at https://evaluations.ufl.edu/results/.

HONOR CODE The student honor code can be found at:

http://www.registrar.ufl.edu/catalog/policies/students.html

The students, instructor and TAs are honor bound to comply with the Honors Pledge:

We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

On all work submitted for credit by students at the university, the following pledge is either required or implied: On my honor, I have neither given nor received unauthorized aid in doing this assignment.

Students with disabilities: Students requiring special accommodations need to register at the Dean of Student Offices and bring the documentation to the instructor.

Counseling services are available at http://www.counsel.ufl.edu . or call (352)-392-1575 during regular service hours (8am-5pm). For other hours or weekends call the Alachua County Crisis Center (264-6789). Students may also call the clinician on-call at Student Mental Health for phone callback and consultation at (352)-392-1171