Chemistry 326

"Chemical Kinetics"

Spring 2023 (13 March 2023)

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Office Hours: Immediately after class, in class, Tuesdays and Thursdays. If these times are inconvenient, please

contact me to schedule another meeting.

Grader: Dorian Twedt Gutierrez: dtwedt@iastate.edu

Meeting Times and Place: Tuesdays and Thursdays, 4:10-5 p.m., starting 21 March; 2354 Gilman. There is no class on Tuesday, 11 April.

Student Learning Outcomes. Students completing Chemistry 326 are expected to understand at an intermediate level: rate laws, temperature dependence of rate constants, reaction mechanisms, kinetic isotope effects, and (time permitting) Michaelis-Menten kinetics, transition-state theory, and Marcus theory.

Prerequisites. Chemistry 167 or 177 or 178 or 201; Math 166. Chemistry 324 and 325 are recommended.

Course Materials. Class notes are posted on Canvas. The main text is *Chemical Kinetics and Reaction Dynamics* by Paul L. Houston. Other useful, but not required, references are:

Physical Chemistry, a Molecular Approach, McQuarrie and Simon, which many of you may already have if you have taken Chemistry 324 or 325. (This is the "big red book," not the partial texts that treat only quantum mechanics or statistical thermodynamics.) Chapters 27-29 cover much of the material that we treat in this course.

Enzyme Structure and Mechanism, Fersht, Chapters 3 and 4. Although this book is intended to address enzyme kinetics, it provides a thorough, clear, and complementary treatment of much of the material in Chapter 2 of Houston.

Excerpts from M&S and Fersht are posted on Canvas.

Mathematical software such as Desmos, MathCAD, MATLAB, etc. will be necessary for understanding many of the discussions in the text as well as for working problems. Numerical computation, fitting of data, and plotting of results is required in order to obtain credit for problems. Some examples using MathCAD code are provided on Canvas.

Course Grade. This will be based upon four problem sets (5% each, representing 20% of the final grade), a midterm examination (30% of the final grade), and a cumulative final examination (50% of final grade).

The midterm and the cumulative final will be based completely upon your understanding of the problem sets. You are permitted one 8.5 x 11" cheat sheet for these examinations. It must be handed in with the examinations. The calculator should be able to do exponents and logarithms.

Schedule of Problem Sets and Examinations.

set 1, Sunday, 2 April, 11:59 p.m. on Canvas. **set 2**, Sunday, 9 April, 11:59 p.m. on Canvas.

Midterm, Thursday, 13 April, in class.

set 3, Sunday, 23 April, 11:59 p.m. on Canvas.

set 4, Sunday, 30 April, 11:59 p.m. on Canvas. Understanding the solution to this problem is one of the most valuable outcomes of the course. It synthesizes many of the fundamental principles covered. The problem is difficult. Do not attempt it the night it is due.

Cumulative final, Thursday, 4 May, in class.

Problem sets are to be submitted as PDF files *via* Canvas. Problem sets handwritten on paper should be neatly scanned, such as by using a smartphone scanning app. (Scanners are also available at Parks Library.) Blurry or otherwise difficult to read photos or scans will not be graded. Feedback on problem sets will be provided *via* Canvas. Late problem sets will not be accepted.

1. Problem sets are to be turned in on or before their deadlines. Students may work together, but they must express their responses in their own terms. Identical (*i.e.*, copied) papers will be graded as zero. **Problem sets must be legible and neatly presented.** It is reasonable to rewrite one's responses once they have been formulated.

All work must be shown on a problem set, and sufficient explanation must be provided to indicate that you know how to solve a problem. Many problems require the use of a computer program to generate the answer. Explanation of the solution with equations and words (complete sentences) is required to receive credit for your answer.

- a. Simply presenting the "code" used to generate the solution will result in no credit. Detailed explanation in complete sentences is required for all work submitted.
- b. Plots of fitted data are always required.
- 2. **Regrading Policy.** Any appeal regarding a grade must be made to the grader electronically no later than five "school days" after the problem set has been graded. Problem sets submitted for appeal may be subject to complete reevaluation.
- 3. +/- grading will be used. There is no curve for the course. Grades will *tentatively* be assigned as follows:

100-90: A 89-75: B 74-50: C 49-40: D <40: F

| Topic | Reading (class notes and) |
|---|------------------------------------|
| rates of reaction, rate constants, and rate laws; order of reaction; half life | M&S, Chap. 28*; Houston, pp. 34-37 |
| determining reaction order by measuring the change in conc. vs. time | Houston, pp. 37-47 |
| Arrhenius behavior; time dependence of equil., consec., and parallel rxns. | Houston, pp. 48-51 |
| steady-state approximation; Lindemann mechanism | Houston, pp. 51-56 |
| enzyme function; proper description of the equilibrium constant in terms of μ | Houston, pp. 56-63 |
| Michealis-Menten kinetics vs. Briggs-Haldane kinetics | Houston, pp. 64-67 |
| chain reactions: discussion of Houston 2.32 | Houston np 72-81 prob 2 32 |

^{*} The scanned chapter is provided on Canvas.

University Policy and Resources

Academic Integrity. Academic Integrity, based on the values of honesty, trust, fairness, respect, and responsibility, is a fundamental principle of scholarship in higher education. Iowa State's Academic and Research Misconduct Policy prohibits: plagiarism (using another person's writing or copying any work without proper citation); falsification; unauthorized collaboration during a test or on an assignment or substitution for another student to take an exam, course or test; and other forms of academic dishonesty. If you are to benefit from this class and be properly evaluated for your contributions, it is important for you to be familiar with and follow Iowa State's Academic Dishonesty and Research Misconduct policies. Students are also encouraged to review these Student Resources. Work that violates this policy will not be tolerated. Students who are found responsible for a violation of the Academic Misconduct Policy will have both a university process sanction and an academic outcome that could include a failing grade on the assignment or exam, or a failing grade for the course.

Accessibility. Iowa State University is committed to assuring that all educational activities are free from discrimination and harassment based on disability status. Students requesting accommodations for a documented disability are required to work directly with staff in Student Accessibility Services (SAS) to establish eligibility and learn about related processes before accommodations will be identified. After eligibility is established, SAS staff will create and issue a Notification Letter for each course listing approved reasonable accommodations. This document will be made available to the student and instructor either electronically or in hard-copy every semester. Students and instructors are encouraged to review contents of the Notification Letters as early in the semester as possible to identify a specific, timely plan to deliver/receive the indicated accommodations. Reasonable accommodations are not retroactive in nature and are not intended to be an unfair advantage. Additional information or assistance is available online at www.sas.dso.iastate.edu, by contacting SAS staff by email at accessibility@iastate.edu, or by calling 515-294- 7220. Student Accessibility Services is a unit in the Dean of Students Office located at 1076 Student Services Building.

Discrimination and Harassment. Iowa State University does not discriminate on the basis of race, color, age, ethnicity, religion, national origin, pregnancy, sexual orientation, gender identity, genetic information, sex, marital status, disability, or status as a U.S. Veteran. Inquiries regarding non-discrimination policies may be directed to Office of Equal Opportunity, 3410 Beardshear Hall, 515 Morrill Road, Ames, Iowa 50011, Tel. 515-294-7612, Hotline 515-294-1222, email eooffice@iastate.edu.

Free Expression. Iowa State University supports and upholds the First Amendment protection of <u>freedom of speech</u> and the principle of <u>academic freedom</u> in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.

Prep Week. This class follows the Iowa State University Prep Week policy, as noted in the ISU Policy Library and section 10.6.4 of the Faculty Handbook. Visit the <u>ISU Policy Library website</u> for policy wording.

Religious Accommodations. Iowa State University welcomes diversity of religious beliefs and practices, recognizing the contributions differing experiences and viewpoints can bring to the community. There may be times when an academic requirement conflicts with religious observances and practices. If that happens, students may request reasonable accommodation for religious practices. In all cases, you must put your request in writing. The instructor will review the situation in an effort to provide a reasonable accommodation when possible to do so without fundamentally altering a course. For students, you should first discuss the conflict and your requested accommodation with your professor at the earliest possible time. You or your instructor may also seek assistance from the <u>Dean of Students Office</u> at 515-294-1020 or the <u>Office of Equal Opportunity</u> at 515-294-7612.

Contact Information for Academic Issues. If you are experiencing, or have experienced, a problem with any of the above issues, email academicissues@iastate.edu