

**Syllabus for CHEM 8565
Chemical Reaction Dynamics
University of Minnesota
Spring Semester, 2016
12:20–13:10, Monday, Wednesday, Friday
Room 364 Vincent Hall**

General Information and Description:

CHEM 8565 is a 2 cr. course that takes place during the first half of the semester (up to Spring Break). The course will cover chemical kinetics and reaction dynamics, with an emphasis on many of the microscopic details that dictate macroscopic reaction rates. This includes molecular collisions, intermolecular potentials, potential energy surfaces, transition state theory, molecular energy transfer, electron transfer, dynamics of reactions in solution, the influence of solvation, and Kramers theory.

Prerequisite:

A year of undergraduate physical chemistry that includes quantum mechanics, thermodynamics, and an introduction to statistical mechanics, equivalent courses in physics or chemical engineering, or instructor permission.

Instructor:

Professor David Blank
213 Smith Hall
blank@umn.edu
Office hours by appointment or drop-in

Course web pages:

The course Moodle site can be accessed by going to your myu page at <https://www.myu.umn.edu/>. After you login, click on the My Courses tab and then on the appropriate link for the course Moodle site (CHEM 8565 section 001). This site will be used for posting announcements, course related materials, and grades.

Grading and Evaluation:

The final course grade will be determined by grades on the quizzes and the homework assignments. The combined score on the quizzes will constitute 60% of the final grade and the combined score on the homework will constitute 40% of the final grade. There will be no final exam.

Quizzes:

There will be five 25-minute quizzes during the scheduled lecture time on the dates listed in the schedule below. *The quizzes will begin promptly at the beginning of class, 12:20 pm.*

Missed quizzes: A student can be excused from a quiz for a true emergency, serious illness, or University sponsored activity. The student should contact the instructor as soon as circumstances allow and appropriate documentation must be provided. If the circumstances are deemed as appropriate for missing a quiz, the unweighted average score of all other quizzes will be used in place of the missed quiz. If circumstances lead to a student missing more than one quiz, the student should immediately schedule a meeting with the instructor to discuss any available options.

Homework:

There will be five homework assignments that will be due at the beginning of class on the dates indicated in the schedule below. Each assignment will be spot checked and graded on a scale of 0–4. The grade will reflect the degree of completion, number of correct solutions with emphasis on the approach taken rather than the final value, *AND the clarity, legibility, and organization of presentation*. Your homework should be clearly marked with your name, the assignment number, and a page number on every page. Each problem should be clearly numbered and the assignment should be well organized. All pages must be mechanically fastened together (staple or equivalent) in the correct order. Complete solutions will be posted on the the course Moodle page soon after the due dates.

Textbook:

There is no *required* textbook for the course. Detailed notes from the instructor will be posted after every lecture on the course Moodle page. However, there are a number of valuable references that can be consulted for students that would like additional resources, and examples are listed below. The text by Paul Houston can serve as a good primary reference for those that prefer to own a course-specific text. The text by Steinfeld, Francisco, and Hase is recommended as a more detailed source (although note that it has recently become very expensive for reasons that are not known to the instructor – it is available in the library).

Primary reference:

- “Chemical Kinetics and Reaction Dynamics” by Paul L. Houston (ISBN 978-0486453347, 0486453340). Currently available via Dover for less than \$30.

Additional suggested references:

- “Chemical Kinetics and Dynamics” by Jeffrey I. Steinfeld, Joseph S. Francisco, and William L. Hase (2nd ed., Prentice Hall, 1999).
- “Chemical Kinetics” by Keith J. Laidler (3rd ed., Harper Collins Publishers Inc., 1987, ISBN 0-06-043862-2).
- “Reaction Dynamics” by M. Brouard (Oxford University Press, 1998, number 61 in the Oxford Chemistry Primers series)
- “Molecular Reaction Dynamics” by Raphael D. Levine (Cambridge University Press, 2005, ISBN 0 521 84276 X)

Schedule:

DATE (2016)	TOPIC	Chapter Houston	Chapter SFH
Jan 20	First day of class. Go over the rules. Informal discussion.		
Jan 22	Introduction example, $F_2 + I_2$		
Jan 25, 27, 29; Feb 1	Macroscopic rate laws	2	1–3, 14, 15
Feb 3	25 min QUIZ, HW 1 is DUE		
Feb 3	Intermolecular interactions		
Feb 5	Potential energy surfaces	3	7
Feb 8	Kinetic theory of gases	1	
Feb 10	25 min QUIZ, HW 2 is DUE		
Feb 10, 12, 15	Collisions and cross-sections	3, 8	6, 8, 9
Feb 17	NO CLASS		
Feb 19	Collisions and cross-sections	3, 8	6, 8, 9
Feb 22	25 min QUIZ, HW 3 is DUE		
Feb 22, 24	Transition state theory	3	10
Feb 26	TST, Electron transfer	5	12
Feb 29	Electron transfer	5	4, 12
Mar 2	25 min QUIZ, HW 4 is DUE		
Mar 2, 4	Reactions in solution	5	12
Mar 7	Literature examples - ET		
Mar 9	25 min QUIZ, Course evaluations		
Mar 11	HW5 is DUE, Last day of class, Lit- erature examples		
Mar 14–18	<i>SPRING BREAK</i>		

Scholastic Dishonesty:

The Board of Regents Student Conduct Code states that, “Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis.” For additional information see the student conduct code at http://regents.umn.edu/sites/default/files/policies/Student_Conduct_Code.pdf The Office for Student Conduct and Academic Integrity has compiled a useful list of Frequently Asked Questions pertaining to scholastic dishonesty: <http://www1.umn.edu/oscai/integrity/student/index.html>. The policy in this course is **zero tolerance**. The *minimum* action taken in a case of scholastic dishonesty in any portion of the work in this course will be a grade of F for the course.

Incompletes:

Students that have an excused absence from the final exam AND are passing the course based on all the work completed prior to the final exam may be eligible to receive a grade of “I” in the course. If these criteria are met, contact the instructor as soon as circumstances allow to discuss the possibility of an incomplete grade and the associated requirements for completion.

Student Mental Health and Stress Management:

As a student you may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance or reduce a student’s ability to participate in daily activities. University of Minnesota services are available to assist you with addressing these and other concerns you may be experiencing. You can learn more about the broad range of confidential mental health services available on campus via <http://www.mentalhealth.umn.edu/>.

Sexual Harassment:

The University policy on sexual harassment can be found at:
<http://regents.umn.edu/sites/default/files/policies/SexHarassment.pdf>.

Equity, Diversity, and Equal Opportunity:

The University policy on equity, diversity, and equal opportunity can be found at:
http://regents.umn.edu/sites/default/files/policies/Equity_Diversity_EO_AA.pdf.

Disability Services:

Students with special needs should contact the Disability Services Office
<https://diversity.umn.edu/disability/>, which will arrange with the instructor information on how those needs shall be accommodated.