University of Guelph

College of Engineering and Physical Sciences

Department of Chemistry

CHEM*4720: ORGANIC REACTIVITY (Credit: 0.5)

Winter Semester 2020

This course is an introduction to physical organic chemistry, including a discussion of reactive intermediates, substituent effects, medium effects, ring strain, electron transfer reactions and a theoretical description of the bonding in organic molecules.

Prerequisite: CHEM*3760 (may be taken concurrently). Recommended prerequisite: CHEM*2820 or CHEM*2880

Instructor: A. Houmam, Office MacN.123x56429. Email: ahoumam@uoguelph.ca

Office Hours: Mondays and Wednesdays from 1:00 to 2:30 PM.

I can be available outside of office hours. Please email me to arrange a meeting outside of these office hours.

Useful Textbooks (see other references at the end of this outline):

Advanced Organic Chemistry, Part A, 5th ed., by Carey and Sundberg.
Advanced Organic Chemistry Reactions and Mechanisms, 2nd ed. by Bernard Miller

These textbooks are useful references for some of the topics to be covered in the lectures. They DO NOT COVER ALL the chapters of this course. The Miller book is particularly useful if you are currently enrolled in CHEM*3760. Further references will be given where appropriate. Supplemental information in the form of class notes ARE REQUIRED. They will be available

on courselink.

Method of Presentation: Two lectures per week Tuesdays and Thursdays from 1:00 PM to 2:20 PM in MCLN, Room 101.

Method of Evaluation: The course grade will be based on one mid-term examination, a final examination and a number of problem assignments. The mid-term examination will be given on Thursday February 27, from 1:00 to 2:30 PM. The winter break this semester begins on Monday February 17 and ends on Friday February 21, so no classes are scheduled this week. The final examination will be given on April 8, 2020 from 7:00 PM to 9:00 PM (Room TBA).

The final grade will be calculated as follows:	Problem assignments	30%
	Mid-term examination	30%
	Final examination	40%

All midterm and examination questions are an exercise in problem recognition and solving. They are to be attempted and solved individually.

Course Outline:

1. Substituent Effects on Organic Rates and Equilibria

a) Qualitative description of substituent effects

b) Linear free energy relationship: the Hammett equation

2. Solvent Effects on Organic Rates and Equilibria

a) Basic relationships; solvents and solvation

b) Scales for ion solvating ability

c) Phase transfer catalysis

3. Angle Strain and Stereoelectronic Effects

a) Strained molecules and some reactivity

b) Radical clock reactions

c) Stereoelectronic requirements for reactions

4. Electron Transfer Initiated Reactions

a) Introduction to ET initiated reactions

b) Hush-Marcus theory vs dissociative ET theory

c) Factors controlling reactions mechanisms, kinetics and thermodynamics

5. The Hückel Molecular Orbital Method (mostly a self-study section)

a) Description of the method

b) Regularities in Huckel molecular orbitals

c) Aromaticity and NMR

E-mail Communication: As per university regulations, all students are required to check their <uoguelph.ca> e-mail account regularly: e-mail is the official route of communication between the University and its students.

When You Cannot Meet a Course Requirement: When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons, please advise the course instructor (or designated person, such as a teaching assistant) in writing, with your name, id#, and e-mail contact. See the undergraduate calendar for information on regulations and procedures for Academic Consideration.

Drop Date: The deadline for dropping a course is the last day of classes (April 3rd for the W20 semester). The regulations and procedures for Dropping Courses are available in the Undergraduate Calendar.

Copies of out-of-class assignments: Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

Accessibility: The University promotes the full participation of students who experience

disabilities in their academic programs. To that end, the provision of academic accommodation is a shared responsibility between the University and the student.

When accommodations are needed, the student is required to first register with Student Accessibility Services (SAS). Documentation to substantiate the existence of a disability is required, however, interim accommodations may be possible while that process is underway.

Accommodations are available for both permanent and temporary disabilities. It should be noted that common illnesses such as a cold or the flu do not constitute a disability.
Use of the SAS Exam Centre requires students to book their exams at least 7 days in advance, and not later than the 40th Class Day.

More information: www.uoguelph.ca/sas

Academic Misconduct: The University of Guelph is committed to upholding the highest standards of academic integrity and it is the responsibility of all members of the University community – faculty, staff, and students – to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring. University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of their location of study; faculty, staff and students have the responsibility of supporting an environment that discourages misconduct. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection.

Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it.

Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.

The Academic Misconduct Policy is detailed in the Undergraduate Calendar.

Recording of Materials: Presentations which are made in relation to course work—including lectures—cannot be recorded or copied without the permission of the presenter, whether the instructor, a classmate or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

Resources: The Academic Calendars are the source of information about the University of Guelph's procedures, policies and regulations which apply to undergraduate, graduate and diploma programs.

References available in the U of G Library

1. I. Fleming. Frontier Molecular Orbitals and Organic Chemical Reactions. QD 461.F53
2. T.L. Gilchrist and R.C. Storr. Organic Reactions and Orbital Symmetry. QD 476.G54 1979
3. B. Miller, Advanced Organic Chemistry Reactions and Mechanisms. QD251.2.M534 (maybe under Chem*3760)
4. F.A. Carroll Perspectives on Structure and Mechanism in Organic Chemistry QD476.C375 B.
5. E.V. Anslyn and D.A. Dougherty Modern Physical Organic Chemistry QD476 .A57 2006

Others include

1. T.H. Lowry and K.S. Richardson. Mechanism and Theory in Organic Chemistry, 3rd ed. QD 476.L68
2. N.S. Isaacs. Physical Organic Chemistry. QD 475.I846
3. F.A. Carey and R.J. Sundberg. Advanced Organic Chemistry Part A. QD 251.2.C36 1983
4. E.V. Anslyn and D.A. Dougherty. Modern Physical Organic Chemistry QD476.A57 2006
5. B. Halton, ed. Advances in Strain in Organic Chemistry QD 461.a33 1991
6. A. de Meijere and S. Blechert Strain and Its Implications in Organic Chemistry QD 461.S875
7. A. Greenburg. Strained Organic Molecules. QD 476.G66
8. K. Yates. Huckel Molecular Orbital Theory. QD 461.Y37
9. A. Streitweiser Jr. Molecular Orbital Theory for Organic Chemists. QD 255.S88
10. J.D. Roberts. Notes on Molecular Orbital Calculations. QD 476.R58
11. P.J. Garratt. Aromaticity. QD 331.G28 1986
12. R.B. Woodward and R. Hoffman. The Conservation of Orbital Symmetry. QD 461.W75
13. T.L. Gilchrist and C.W. Rees. Carbenes, Nitrenes and Arynes. QD 305.H7 G5
14. C.D. Johnson. The Hammett Equation. QD 502.J63
15. F.A. Carey and R.J. Sundberg. Advanced Organic Chemistry Part B. QD 251.2.C36 1983
16. A. Pross. Theoretical and Physical Principles of Organic Reactivity. QD476.P755 1995

References for Electron Transfer Reactions:

1. Grimshaw, J. *Electrochemical reactions and mechanisms in **organic** chemistry*. Elsevier, New York, 2000.
2. Nelsen S. F. Electron Transfer in Organic Chemistry. In *Electron Transfer Chemistry*. Balzani, V. (Ed.) Vol. 1, 2001.
3. Schäfer, H. J. Organic Electrochemistry. In *Encylopedia of Electrochemistry*. Vol 8. Wiley-VCH, Weinheim, 2004.
4. Torii, S. *Electroorganic Reduction Synthesis*. Wiley-VCH, Weinheim, 2006.
5. Savéant, J.-M. *Elements of Molecular and Biomolecular Electrochemistry. An Electrochemical Approach to Electron Transfer Chemistry*. Wiley & Sons, Inc., Hoboken, New Jersey, 2006.
6. Evans, D. H.; O'Connell, K. M. Conformation Changes and Isomerizations Associated with Electrode Reactions. In *Electroanalytical Chemistry*, Bard, A. J., Ed., Marcel Dekker: New York, 1985, Vol. 14, pp.113-207.
7. Eberson, L. Electron Transfer in Organic Chemistry. In *Advances in Physical Organic Chemistry*; Gold V. and Bethell D. Eds.; Academic press, London, 1982. vol. 18, pp. 78-185.
8. Houmam A. Electron Transfer Initiated Reactions: Bond Formation and Bond Dissociation, *Chem. Re*v. 2008.