The University of Western Ontario
Chemistry 2384b – Winter 2017-2018
Microscopic Phenomena

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Office: Chemistry Building ChB071

Lectures: Mon, Wed, Fri 10:30 – 11:30 am, B&GS-0165
Office hours: Office hours will be every Monday and Wed. from 4:00 to 5:00 pm.

Course Prerequisite Requirements: Chem 2374a

Mandatory Notice from the Registrar: Unless you have either the requisites for this course or written special permission from your Dean to enrol in it, you may be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites.

Brief Description: The course discusses an introduction to statistical mechanics and its connection with thermodynamics, description of the kinetic theory of gas and liquid phases, chemical dynamics and diffusion and transport processes.

Laboratories: Laboratory times are: Tuesday, 9.30 am to 12.30 pm; Tuesday, 2.30 pm to 5.30 pm and Wednesday 2:30-5:30 pm (this lab might not open). Each student will perform 5 labs in total, therefore each student will write 5 lab reports. One laboratory experiment will take place every second week. A student must be enrolled in one of the lab sections in order to take this course. Laboratories start on Tuesday January 16, 2018 at 9:30 am. The list of lab sections and lab dates is found in this outline and more details will be posted in owl.

The written report from each performed laboratory must be submitted prior to the start of the next laboratory session. The template for the report is available on the OWL. Please strictly comply with this template. The report on the final laboratory experiment must be submitted to the same TA who was supervising your experiment in two weeks time, at the beginning of the next lab.
Course Learning Outcomes

Breadth and Depth of Knowledge: Be able to describe the fundamental scientific principles of the physical chemistry of microscopic phenomena and apply these principles in assignments, lab work, discussions on/off line.

Knowledge of Methods: (1) Obtain problem-solving skills in physical chemistry by assignments, on off-line discussions and lecture materials. (2) Obtain skills in laboratory work on physical chemistry experiments that will support solving chemical and research problems.

Application of Knowledge: (1) Be able to apply the knowledge in order to predict and rationalize the physical and chemical properties of systems.

Communication: Be able to prepare logical and concise written reports via training in the lab reporting, quizzes and assignments.

Awareness of Knowledge Limits: Recognize assumptions and limitations in the scientific models and their possible impact on the results by training on case studies, lectures, assignments, labs.

Autonomy and Professional Capacity: (1) Be able to work productively and collaboratively as a team member. (2) Be able to conduct laboratory experiments safely; evaluate the potential impact chemistry may have in society, health and environment.

Textbook:

- This book is recommended but it is not compulsory. Notes will be given and regularly uploaded to OWL. Other standard physical chemistry books can be also used.
- Chemistry 2384b Laboratory Manual (January 2018). Available at the Book Store.

Evaluation

Exams, Assignments and Weighting of Final Mark:

The overall course grade, out of 100, will be calculated as listed below. Listed next to the respective components are their maximum contributions toward the course grade.

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Mid-Term Test</td>
<td>25 %</td>
</tr>
<tr>
<td>Take-home Assignments (3 total)</td>
<td>5% each (15% total)</td>
</tr>
<tr>
<td>Laboratory Reports (5 total)</td>
<td>4% each (20% total)</td>
</tr>
<tr>
<td>Final Exam</td>
<td>40 %</td>
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</tbody>
</table>
• **Mid-Term Test**: February, 2018. The exact date is to be announced.

• **Final Exam** in April – TBA by the registrar.

• **3 Take-home Assignments** – at the end of lectures covering each main topic. The assignments should be delivered in the designated box at the beginning or end of the class. It is the responsibility of the student to ensure that the assignment has been placed into the box. Claims for lost assignments will not be accepted. Late assignments will have penalty. One day late 15% penalty, 2 days late 30 percent penalty, 3 days late 60 percent penalty, 4 days late zero value on the assignment.

• **Five Laboratory Reports**. This component is worth 20% of the total course mark. One day late report will have a penalty of 30 percent. A late report more than one day it is assigned the value of zero.

  Labs:
  1) Determination of the Sublimation Pressure of Iodine and Statistical Thermodynamic Analysis.
  2) Raman Spectroscopy: A Powerful Analytical Technique in Chemistry.
  3) Determination of the Diffusion Coefficient of Ferrocenemethanol using Rotating Disk Electrode Technique.
  4) Free Energy of Protein Unfolding.
  5) Measuring Rapid Kinetics by Stopped-Flow Spectroscopy

**Note 1**: It is Faculty of Science policy that a student who chooses to write a test or exam deems themselves fit enough to do so, and the student must accept the mark obtained. Claims of medical, physical, or emotional distress after the fact will not be considered.

**Note 2**: In order to pass Chemistry 2384B it is necessary to obtain a passing grade on BOTH the laboratory component and the combined marks from the home assignments, midterm test and the final examination. One should write the midterm and final exam to pass the course. Obtaining a good average grade in the assignments and midterm is not sufficient to pass the course. Note also that, since there are no lab make-up labs (see below), one will fail automatically if one misses more than 2 labs even with valid medical or compassion reasons, or submit less than 3 lab reports.

**Laboratory Sections and Times**

<table>
<thead>
<tr>
<th>Section 021</th>
<th>Section 022</th>
<th>Section 023</th>
<th>Section 024</th>
<th>Section 033</th>
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</thead>
<tbody>
<tr>
<td>Jan 30 9:30-12:20</td>
<td>Feb 6 9:30-12:20</td>
<td>Jan 30 2:30-5:20</td>
<td>Feb 6 2:30-5:20</td>
<td>Jan 31 2:30-5:20</td>
</tr>
<tr>
<td>Feb 13 9:30-12:20</td>
<td>Feb 27 9:30-12:20</td>
<td>Feb 13 2:30-5:20</td>
<td>Feb 27 2:30-5:20</td>
<td>Feb 14 2:30-5:20</td>
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</table>

You will work with a partner. Your partner in the lab will be announced.
**General information about labs**

We have switched the lab notebooks the students use to the Hayden McNeil Organic Chemistry notebook, with carbonless copy pages. This way the students can hand in their notebook pages for grading. These should be in the bookstore.

The students are required to take the WHIMIS and Lab Safety Courses.

We are requiring that lab reports be submitted electronically, in addition to a hard copy.

**Missed Course Components**

If you are unable to meet a course requirement due to illness or other serious circumstances, you must provide valid medical or supporting documentation to the Academic Counselling Office of your home faculty as soon as possible.

If you are a science student, the Academic Counselling Office of the Faculty of Science is located in WSC 191, and can be contacted at 519-661-3040 or scibmsac@uwo.ca. Their website is http://www.uwo.ca/sci/undergrad/academic_counselling/index.html.

A student requiring academic accommodation due to illness must use the Student Medical Certificate (https://studentservices.uwo.ca/secure/medical_document.pdf) when visiting an off-campus medical facility. For further information, please consult the university’s medical illness policy at http://www.uwo.ca/univsec/pdf/academic_policies/appeals/accommodation_medical.pdf.

If the midterm is missed for valid reasons, as confirmed by the Academic Counselling Office, the weighting will be transferred to the final examination. In such case the total weight of the final will be 65%. Those students who cannot write the midterm test on the date indicated because of religious or class conflicts could be accommodated.

If you miss the Final Exam, contact your faculty’s Academic Counselling Office as soon as possible. They will assess your eligibility to write the Special Exam (the name given by the university to a makeup Final Exam).

You may also be eligible to write the Special Exam if you are in a “Multiple Exam Situation” (see http://www.registrar.uwo.ca/examinations/exam_schedule.html).

Similarly, if you cannot attend a lab for valid reasons, you must provide the documentation to your Academic Counselling Office. **You will not be able to do the missed lab at another time!** In this case, if the Counselling Office approves, the marks for the remaining labs will be re-weighed. For instance, if you miss one lab, the marks for the rest of your lab reports will be worth 5% each (4 labs, 20% lab component total). Please note that you still need to attend at least 3 labs and submit 3 lab reports, that is, you cannot miss all 5 labs even if you have valid reasons.
**Course Website**

Students should check OWL (http://owl.uwo.ca) on a regular basis for news and updates. This is the primary method by which information will be disseminated to all students in the class. The missing of critical information due to your failure to check OWL cannot be used as a basis for appeal.

**Accessibility**

Please contact the course instructor if you require lecture or printed material in an alternate format or if any other arrangements can make this course more accessible to you. You may also wish to contact Services for Students with Disabilities (SSD) at 661-2111 ext. 82147 if you have questions regarding accommodation.

**Support Services**

Learning-skills counsellors at the Student Development Centre (http://www.sdc.uwo.ca) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counselling.

Additional student-run support services are offered by the USC, http://westernusc.ca/services.

The website for Registrarial Services is http://www.registrar.uwo.ca.

Students who are in emotional/mental distress should refer to Mental Health@Western http://www.health.uwo.ca/mental_health/ for a complete list of options about how to obtain help.

**Code of Conduct**

To foster a supportive and enriching academic environment that is conducive to learning and free inquiry, Western has a Student Code of Conduct (http://www.uwo.ca/univsec/board/code.pdf).
Important Legalities

It is Department of Chemistry policy that any student repeating a chemistry course must repeat the entire course, including the lab component. There are no lab exemptions.

It is Faculty of Science policy that a student who chooses to write a test or exam while ill is deemed medically fit to write and the student must accept the mark obtained. If you become ill during a test or exam, please contact an academic counsellor in the Dean’s Office of your Faculty immediately after the test or exam.

There is no opportunity for a reweight of the other course components after the test or exam has been written. The reason of “I did not want to write a heavily weighted final” is not a valid reason for writing the midterm test while ill.

No electronic devices may be in your possession during tests and exams. Aside from the specified calculator, no other electronic devices (phones, iPods, etc.) may be in your possession during tests and exams, even for timekeeping purposes.

It is university policy that a regularly scheduled class (lecture, lab, or tutorial) takes precedence over tests and exams. Therefore, if another course schedules a test or exam that takes place during your lab or tutorial, the instructor for that course must accommodate you.

Plagiarism

Plagiarism is a serious Scholastic Offence. Students must write their essays and assignments in their own words. Whenever students take an idea, or a passage from another author, they must acknowledge their debt both using quotation marks where appropriate and by proper referencing such as footnotes or citations. Scholastic offences are taken seriously and students are directed to the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf.

Social Media

Twitter - Follow us @westernuchem
Facebook - www.facebook.com/ChemistryatWestern

Important dates:
Monday, January 8, 2018 - classes resume
January 16, 2018 - Last day to add a second-term half course or a second-term full course
Monday, February 19, 2018 - Friday, Feb. 23 - Reading week
March 7, 2018 - Last day to drop a second-term half course, or a second-term full course without academic penalty.
Friday, March 30, 2018 - Good Friday
Wednesday, April 11, 2018 – classes end
Tentative topics to be covered in Chem 2384b

**Short abstract:** An introduction to statistical mechanics will provide the connection between molecular stats and macroscopic behaviour. The microscopic states of a system will be introduced as well as the Boltzmann distribution of the energy states of independent particles considering their partition function. The calculation of the thermodynamics properties for an ideal gas will be introduced from a statistical mechanics point of view and related with classical thermodynamics previously taught.

Description of the kinetics of gas particles will be described using the Maxwell-Boltzmann distribution of the velocities of molecules. Various parameters associated with a perfect gas molecule kinetics (collisions, mean free path) will be described in detail and linked to their macroscopic properties (pressure). The rate and order of complex reactions (reversible, consecutive reactions) will be developed and few examples will be given. The kinetics in the liquid phase will introduce new reactivity limiting parameters such as viscosity and diffusion that control the transport of reacting species.

**Tentative topics:**

1- **Statistical mechanics**
   - Microscopic state of a system
   - The Boltzmann distribution
   - Evaluation of the partition function
   - Molecular partition function for an ideal gas
   - Translational contributions to the thermodynamics of ideal gases
   - Vibrational contributions
   - Rotational contributions
   - Electronic contributions
   - Real gases

2- **Kinetic theory of Gases**
   - Probability density for molecular speed of gases
   - Velocity distribution
   - Maxwell distribution
   - Types of average speed
   - Pressure of an ideal gas
   - Collisions with a surface and effusion
   - Collision s of hard sphere molecules
   - Mean free path
   - Effects of molecular interactions on collisions
   - Transport phenomena in gases. Diffusion.
   - Viscosity of a liquid
   - Diffusion (Fick’s laws)
   - Mobility of an ion
3- **Experimental Reaction Kinetics**
- Rate of reaction
- Order of reaction
- Reversible first order reaction
- Consecutive first order reactions
- Microscopic reversibility and detailed balance
- Effect of temperature
- Mechanisms of chemical reactions
- Relation between rate constants for the forward and backward reaction
- Bimolecular reactions
- Unimolecular and trimolecular reaction
- Unbranched and branched chain reaction

4- **Chemical dynamics**
- simple collision theory of bimolecular reactions
- Potential energy surfaces
- Theoretical calculation of a rate constant
- Transition state theory

*Updated Dec 15, 2017*