Physical Chemistry Laboratory II

Chemistry 357, Spring 2020

Instructor

Dustin Wheeler, Ph.D.
Office: HN1313B
Office hours: By appointment only
Email: dustin.wheeler@hunter.cuny.edu

Course goal

Chemistry 357 is a laboratory course in physical chemistry. By the end of this course, you will have experience with a variety of instrumental and computational techniques designed to help you understand fundamental processes related to kinetics and quantum chemical phenomena.

This course is intended to help you grow as a scientist by:

1. exposing you to a variety of chemical modeling and characterization techniques, and
2. developing your reasoning and critical thinking skills for better problem solving.

Course Materials

Required: One carbon copy laboratory notebook (available in the Hunter College bookstore). There is no textbook for this course. I will provide handouts or post the relevant material on Blackboard for you. You should print out each lab and *must* complete a summary of the lab procedure in your notebook before you come to class.

If you are interested in purchasing a physical laboratory book (entirely optional), many of our experiments will be modified from the standard physical chemistry laboratory lab manual by Garland, Nibler, and Shoemaker: *Experiments in Physical Chemistry,* 7th Ed., 2003, McGraw-Hill, New York, NY.

Web site

Instructions on how to access the course website on Blackboard can be found on the Hunter College BlackBoard Announcement page (http://bb.hunter.cuny.edu) . In addition to instructions for individual labs, announcements and additional resources will occasionally be posted on Blackboard.

Attendance and Tardiness

Your attendance in each and every lab is mandatory. There will be no makeup labs offered for this course. For safety reasons, if you are **more than 15 minutes late** for class, you will not be permitted to perform the lab and you will lose participation points for the session.

Lab Safety

- First and foremost you will be **required** to wear safety goggles at **all** times when in the laboratory. If you are caught without safety glasses on more than one occasion you will be asked to leave the lab.
- Open-toed shoes are not permitted in the laboratory.
- No food or drink is allowed in the laboratory at any time.
- Do not sniff or taste **any** of the chemicals you will be using.
- Toxic substances must be used only under the hood. You will be responsible for looking up and understanding the MSDS of **all** chemicals used in the laboratory.
- All cell phones, pagers, CD players, MP3 players, etc. must be turned off (or at least on silent) while in the laboratory.

Grading

Your grade for this course will be based on the following factors:

- Attendance and participation in every laboratory period (**40%** of semester grade)
- A series of laboratory summaries (5) to be completed at home (**20%** of semester grade)
    - Pre-lab preparation (10% of each lab report)
    - Summaries should include Procedure, Results/Discussion, and Appendix sections (60 points total)
- A series of laboratory reports (3) to be completed at home (**30%** of semester grade)
    - Pre-lab preparation (10% of each lab report)
    - Lab reports should be written in the style of *The Journal of Physical Chemistry A* (JPCA). If you are unfamiliar with this style, please look up a few articles in a recent issue to familiarize yourself with the format. The Information for Authors (https://pubs.acs.org/page/jpcafh/submission/authors.html) page and Author Guidelines (https://publish.acs.org/publish/author_guidelines?coden=jpcafh) (specifically the author guidelines section on *Manuscript Text Components*) may be helpful if you aren't sure how to structure a manuscript. Templates (MS Word and LaTeX) are available for download on the course Blackboard page.
- A final group presentation based on one of the labs performed during the semester. More details will be given later in the semester. (**10%** of semester grade)

Pre-lab preparation is worth 10% of the grade for each summary or report. Summaries are due one week after the completion of the lab, while full reports are due two weeks after completing the lab. Write-ups should be clear, concise evaluations of the experiment, including any observations, experimental procedures, instrumental methods and instrumentation used, computational methods and results, and any additional analyses you performed. Please see the JPCA author guidelines for details on these sections.

The table below shows which sections should be included in each assignment and how many points each section is worth.

Lab Report Grading Rubric

Points	Section	Summary	Report
10	Pre-lab	✓	✓
5	Title/Author/Date	✓	✓
10	Intro/Objective		✓
10	Procedure	✓	✓
30	Results/Discussion	✓	✓
10	Conclusion		✓
5	References		✓
20	Appendix (data/calcs)	✓	✓
	Total points	75	100

Academic Integrity Statement

Hunter College regards acts of academic dishonesty (*e.g.*, plagiarism, cheating on examinations, obtaining unfair advantage, and falsification of records and official documents) as serious offenses against the values of intellectual honesty.

The college is committed to enforcing the CUNY Policy on Academic Integrity and will pursue cases of academic dishonesty according to the Hunter College Academic Integrity Procedures.

ADA Statement

In compliance with the ADA and with Section 504 of the Rehabilitation Act, Hunter College is committed to ensuring educational access and accommodations for all its registered students. Hunter College's students with disabilities and medical conditions are encouraged to register with the Office of AccessABILITY for assistance and accommodation. For information and appointment contact the Office of AccessABILITY (located in room E1214) or call 212–772–4857 or VRS 646–755–3129.

Hunter College Policy on Sexual Misconduct

In compliance with the CUNY Policy on Sexual Misconduct, Hunter College reaffirms the prohibition of any sexual misconduct, which includes sexual violence, sexual harassment, and gender-based harassment retaliation against students, employees, or visitors, as well as certain intimate relationships. Students who have experienced any form of sexual violence on or off campus (including CUNY-sponsored trips and events) are entitled to the rights outlined in the Bill of Rights for Hunter College.

1. Sexual Violence: Students are strongly encouraged to immediately report the incident by calling 911, contacting NYPD Special Victims Division Hotline (646–610–7272) or their local police precinct, or contacting the College's Public Safety Office (212–772–4444).
2. All Other Forms of Sexual Misconduct: Students are also encouraged to contact the College's Title IX Campus Coordinator, Dean John Rose (jtrose@hunter.cuny.edu, 212–650–3262) or Colleen Barry (colleen.barry@hunter.cuny.edu, 212–772–4534) and seek complimentary services through the Counseling and Wellness Services Office, Hunter East 1123. For more information, view the CUNY Policy on Sexual Misconduct (http://www.cuny.edu/about/administration/offices/la/Policy-on-Sexual-Misconduct-12-1-14-with-links.pdf) .

Course Schedule

Week	Date	Groups 1 & 2	Groups 3 & 4
1	1/27	Introduction, Plotting Tutorial	Introduction, Plotting Tutorial
2	2/3	Introduction to Error Analysis	Introduction to Error Analysis
3	2/10	Fluorescence	Fluorescence
4	2/24	Fluorescence	Fluorescence
5	3/2	Polymers	Polymers
6	3/9	NMR	NMR
7	3/16	NMR	NMR
8	3/23	Introduction to Computational Chemistry	Introduction to Computational Chemistry
9	3/30	HCl/DCl	FRET
10	4/6	HCl/DCl	FRET
11	4/20	FRET	HCl/DCl
12	4/27	FRET	HCl/DCl
13	5/4	Final Presentations	Final Presentations
14	5/11	Checkout	Checkout

Description of Experiments

1. Introduction to Data Analysis and Plotting (Summary)

This one-week exercise will give you an introduction to basic plotting techniques and show you how to work with data in a variety of digital formats.

Instrumentation used: Microsoft Excel

2. Introduction to Error Analysis (Summary)

This one week exercise will guide you through the principles of error analysis, propagation of error, and probability distributions.

Instrumentation used: None

3. Fluorescence - The Kinetics of a Diffusion-Controlled Reaction (Summary)

In this two-week experiment, you will determine the rate constant and collision diameter for a diffusion-controlled reaction using fluorescence quenching.

Instrumentation used: Fluorimeter

4. Polymers - Molecular Weight and Monomer Linkage Properties of Poly(vinyl alcohol) (Summary)

Using a viscometer, you will determine the average molecular weight of a polymer chain and the fraction of head-to-head monomer linkages in the polymer.

Instrumentation used: Ostwald viscometer

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5. NMR - Determination of Keto-Enol Equilibrium Constants via NMR Spectroscopy (Report)

Using nuclear magnetic resonance spectroscopy, you will determine the equilibrium composition of various keto-enol mixtures. By investigating a series of concentrations, you will determine the equilibrium constant for the conversion.

Instrumentation used: NMR spectrometer, GaussView6

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6. Introduction to Computation Chemistry (Summary)

This lab will serve to introduce you to the Linux operating system and Unix command line, after which you will learn to run some rudimentary quantum calculations using the Gaussian computational chemistry software package.

Instrumentation used: Command line shell, Python, Gaussian16, GaussView6

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7. HCl/DCl - Vibrational-Rotational Spectra of HCl and DCl (Report)

In this two-week experiment you will synthesize a gaseous mixture of hydrogen chloride and deuterium chloride to be analyzed using the FTIR spectrometer. You will then perform basic computations on the two molecules using the collected data.

Instrumentation used: FTIR, Gaussian16

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8. FRET - Emission Spectroscopy: Biophysics and Förster Resonance Energy Transfer (FRET) (Report)

In this two-week experiment, you will learn about quenching via Förster Resonance Energy Transfer, determine the free energy of unfolding a protein, and determine intramolecular distances in the partially-unfolded and fully-folded structures.

Instrumentation used: UV-Vis, Fluorimeter

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9. Final Presentations

Each group will be assigned a lab from the semester. Groups will create a detailed presentation related to the lab for their instructor and classmates. Presentations will be given at the end of the semester.
