Physical Chemistry Laboratory II

Chemistry 357, Spring 2024

Course Information

Class time: Tuesday, 8:30am–11:20pm
Class location: North Building, 1412B
Course webpage: Microsoft Teams

Instructor

Dustin Wheeler, Ph.D.
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Office hours: By appointment only, in person or remote
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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). A bound (*not* spiral) notebook is also acceptable, though it should have pre-numbered pages. A USB flash storage drive will be necessary to retrieve data from various instrumentation.

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

Course communication, lectures, help sessions, and announcements will be posted on the course page in Microsoft Teams. All students should have been invited to the team prior to the start of the semester.

Computational work for the course will be performed with [JupyterLab][JupyterLab] on shared departmental resources. This server can be accessed at https://sugarcube.hunter.cuny.edu. Students will need to create an account using the “Sign up” link below the login window.

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.
- Cell phones should be silenced prior to coming in to lab. Please refrain from using phones during the lab session. Your attention should be focused on the work being performed, and distractions can be dangerous when working with some of the equipment.

Grading

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

- Attendance and participation in every laboratory period. You will work in groups of two on all experiments; your partner will remain the same all semester. (**30%** of semester grade)
- Practice exercises for lab-related skills, graded for completion (**15%** of semester grade)
- Summaries for four lab exercises, details given below. (**15%** of semester grade)
- Written lab reports for two labs, details given below. (**30%** of semester grade)
- 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 points of the grade for each summary or report. At the end of each lab period, you will be required to clean up your work and submit your notebook to the instructor for sign-off. Failure to do either of these will result in a loss of participation points for the lab and 10 points from the submitted report or summary.

Summaries are due *one week* after the completion of the lab, while full reports are due *two weeks* after completing the lab.

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	✓	✓
10	Intro/Objective		✓
10	Procedure	✓	✓
30	Results/Discussion		✓
10	Conclusion		✓
10	References	✓	✓
20	Appendix (raw data/calcs)	✓	✓
	Total points	50	100

- Prior to arriving for each experimental lab, a pre-lab should be completed. This should contain an outline or flowchart of steps to be taken in the lab. It should be written in such a way that you can follow each step quickly and accurately during the lab, without needing to refer back to some section of the lab guide. Another researcher looking at your notebook should be able to replicate your work with relatively little difficulty, and your pre-lab is the start to this "instruction set". All masses, volumes, etc. should be calculated ahead of time, and a list of necessary equipment should be included so you can come in to lab, collect your equipment, and begin working within a few minutes.
- Summaries should include Procedure and Appendix sections. The Appendix should include your data analysis and any resultant figures or tables, as well as a comparison to literature values (with references). Each summary will be focused on one particular component of the analysis work (*e.g.,* figure preparation, data manipulation, error analysis). Focus topics for each summary analysis are listed in the experiment descriptions below. Your summary should also include a rough outline of your discussion points, *e.g.,* answers to any questions posed in the lab manual, observations about trends shown in your data, commentary on any sources of error, etc.
- Lab reports 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. Lab reports should be written in the style of [*The Journal of Physical Chemistry A* (JPCA)][jpca-home]. 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 page and Author Guidelines (specifically the author guidelines section on *Manuscript Text Components*) may be helpful if you aren't sure how to structure a manuscript. Please structure the report section of your Jupyter notebooks accordingly (*i.e.,* header cells for each section, formatted text/equations, inline figures created from your analysis section, and formatted references listed at the end).

CUNY Policies and Statements

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 E1214B) 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.

Schedule for Spring, 2024

Week	Date	Groups 1/2	Groups 3/4	Groups 5/6
1	1/30	JupyterLab/Python Tutorial	JupyterLab/Python Tutorial	JupyterLab/Python Tutorial
2	2/6	Intro. to Plotting/Error Analysis	Intro. to Plotting/Error Analysis	Intro. to Plotting/Error Analysis
3	2/21	Fluorescence	Intro. to Computational Chemistry	Polymers
4	2/27	Fluorescence calcs	Fluorescence	Intro. to Computational Chemistry
5	3/5	Polymers	Fluorescence calcs	Fluorescence
6	3/12	Intro. to Computational Chemistry	Polymers	Fluorescence calcs
7	3/19	NMR (HN 1304)	NMR (HN 1304)	NMR (HN 1304)
8	3/26	NMR calcs	NMR calcs	NMR calcs
9	4/2	FRET measurements	Off	HCl/DCl measurements
10	4/9	HCl/DCl measurements	FRET measurements	HCl/DCl calculations
11	4/16	HCl/DCl calculations	HCl/DCl measurements	FRET measurements
12	5/7	Off	HCl/DCl calculations	Off
13	5/14	Final Presentations	Final Presentations	Final Presentations

Description of Experiments

Introduction to Data Analysis and Plotting

This one-week exercise will give you an introduction to the JupyterLab interface, the Jupyter notebook, basic plotting techniques using Matplotlib, and show you how to work with data in a variety of digital formats.

Instrumentation used: JupyterLab

Report type: Submit completed Jupyter notebook

Introduction to Computation Chemistry

This lab will introduce you to the Unix command line shell, 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

Report type: Summary, focus on discussion and appropriate presentation of numbers (*i.e.,* significant figures)

Introduction to Error Analysis

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

Instrumentation used: None

Report type: Submit homework problems

Fluorescence - The Kinetics of a Diffusion-Controlled Reaction

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

Report type: Summary, focus on figure preparation (clear labels, captions, presentation of data in a clear and compelling manner)

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

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

Report type: Summary, focus on discussion and presentation of data (tables/plots)

NMR - Determination of the Rotational Barrier in *N,N*-dimethylacetamide

Using nuclear magnetic resonance spectroscopy, you will determine the energy of the rotational barrier in *N,N*-dimethylacetamide. By investigating the NMR spectra over a series of temperatures, you will determine the equilibrium constant for the conversion.

Instrumentation used: NMR spectrometer, Gaussian16

Report type: Summary, focus on error analysis, plot creation

HCl/DCl - Vibrational-Rotational Spectra of HCl and DCl

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

Report type: Full report

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

In this 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

Report type: Full report

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.