Physical Chemistry Laboratory II

Chemistry 357, Spring 2022

Instructor

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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).
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.

A USB drive for retrieving data from the various instruments used in the course.

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. To log in, use your CUNYlogin address (fname.lname##@login.cuny.edu). Please contact the course instructor and the Student HelpDesk if you have issues connecting to the course.

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 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. Since you will be writing your reports in JupyterLab, you need to make sure you follow the *content* conventions, not necessarily the format conventions (format is defined by the Jupyter export settings, set up by the instructor).
- 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.

Course Schedule

Schedule for Spring, 2021

Week	Date	Groups 1/2	Groups 3/4	Groups 5/6
1	1/31	Introduction, Python intro	Introduction, Python intro	Introduction, Python intro
2	2/7	Plotting, error analysis	Plotting, error analysis	Plotting, error analysis
3	2/14	Fluorescence†	Introduction to Computational Chemistry	Polymers†
4	2/28	Fluorescence calcs	Fluorescence†	Introduction to Computational Chemistry
5	3/7	Polymers†	Fluorescence calcs	Fluorescence†
6	3/14	Introduction to Computational Chemistry	Polymers†	Fluorescence calcs
7	3/21	NMR (HN 1304)†	NMR (HN 1304)†	NMR (HN 1304)†
8	3/28	NMR calcs	NMR calcs	NMR calcs
9	4/4	FRET measurements†	Off	HCl/DCl measurements
10	4/11	HCl/DCl measurements	FRET measurements†	HCl/DCl
11	4/25	HCl/DCl	HCl/DCl measurements	FRET measurements†
12	5/2	Off	HCl/DCl	Off
13	5/9	Final Presentations	Final Presentations	Final Presentations
14	5/16	Checkout	Checkout	Checkout

† – In-person lab

Description of Experiments

1. Introduction to Data Analysis and Plotting

This one-week exercise will give you an introduction to the JupyterLab interface, the Jupyter notebook, and the basics of the Python programming language. Additionally, you will learn to work with data in external files.

Instrumentation used: JupyterLab

Report type: Summary

2. Introduction to Plotting and Error Analysis

This one-week exercise will give you an introduction to basic plotting techniques using `matplotlib`, and show you how to work with data in a variety of digital formats. Additionally, you will be introduced to the principles of error analysis, propagation of error, and probability distributions.

Instrumentation used: JupyterLab

Report type: Summary

3. 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

4. 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: Fluorometer

Report type: Summary

5. 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

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

Using nuclear magnetic resonance spectroscopy, you will determine the energy of the rorational 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: Full report

7. 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

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

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, Fluorometer

Report type: Full report

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.