BIOPHYSICAL CHEMISTRY II LABORATORY (CHEM 361L)

Spring 2025

Experiments performed in this laboratory course are intended to complement the material presented in Biophysical Chemistry II. Spectroscopic methods, intermolecular interactions, and computational chemistry will be covered. Students who complete this laboratory are expected to be competent users of Gaussian, Gaussview, and the department's spectroscopic instrumentation.

The course grade will be a composite of report grades (80%) and laboratory technique. Attendance at all sessions is required. Laboratory reports for each experiment will be turned in the week after the experiment is completed. A penalty of **one letter grade per week (or part thereof)** will be assessed on late reports. No lab reports will be accepted after May 10.

The report must include an Introduction (a brief statement of experimental goals, in your own words), Experimental section (describing the methods used), Results section (data and calculations), and Discussion section (conclusions based on the results obtained).

One of the goals of this course is to introduce the student to the laboratory use of spreadsheet software. The departmental computers have a number of these (Excel is an example), as do many of the university PC's. If you are unfamiliar with these, seek help from the lab instructor or the course supervisor (Dr. Baumann). This syllabus and all lab handouts may be found on Dr. Baumann's home page (http://www.scranton.edu/faculty/baumann/).

Students with Disabilities

Students with disabilities may be eligible for reasonable academic and non-academic accommodations. Students are required to submit relevant and current documentation of their disability. Students are encouraged to contact the Office of Student Support and Success at disabilityservices@scranton.edu or (570) 941-4038 if they have or think they may have a disability and wish to determine eligibility for any academic accommodations. For non-academic accommodations, students should contact the Office of Equity and Diversity at non-academic-accom@scranton.edu or (570) 941-6645. Students can access accommodate by clicking here.

Writing Center Services

The Writing Center is a resource designed to help students at all academic levels become better writers. It is a safe space where students from any discipline can receive one-on-one feedback on written assignments from well-trained peer consultants who support students in any stage of the writing process. Students can make an appointment through the my.scranton portal: my.scranton.edu >OSSS Card >Writing Center Scheduler.

For more information, please contact writing-center@scranton.edu. For quick tips, user-friendly guides, and other writing resources, check out our blog at https://sites.scranton.edu/writingcenter.

Academic honesty:

The first time that a student is caught plagiarizing or using fabricated data in a report, he or she will receive a grade of zero points for that assignment. For further consequences of violating academic ethics please refer to the University of Scranton Student Handbook.

https://www.scranton.edu/academics/cte/acad-integ/acad-code-honesty.shtml

Date of Experiment	**EXPERIMENT**	Report Due
January 28	Computational Chemistry I: Structure of a Compound	February 4
February 4	Assignment of an IR Spectrum	February 18*
February 11	Computational Chemistry II: IR Spectrum of a Compound	
February 18	Measurement of Substituent Effects by IR Spectroscopy	March 4*
February 25	Computational Chemistry III: Substituent Effects	
March 4	Computational Chemistry IV: Structure of a Complex	April 1*
March 11, 25	Computational Chemistry V: Dynamics	
April 1	Kinetic Isotope Effect	April 8
April 8	Hydrogen Bonding: IR	
April 15	Hydrogen Bonding: UV Visible	April 29**
April 22	Hydrogen Bonding: Fluorescence	

* This report will be based on two experiments.

** This report will be based on three experiments.

Format for Laboratory Reports

The laboratory report for an experiment in this course must minimally contain the following:

1. Introduction:

A brief statement of the purpose of the experiment and the theory behind the experimental procedure.

2. Experimental:

A description of the experimental procedure, referenced whenever possible to the textbook or accompanying materials. Deviations from the reference procedures should be noted in this section.

3. Results:

Data should be presented in tabular and/or graphical form in this section. The use of spreadsheet software (such as Excel) will make this section much easier to complete. Explanations of calculations, including sample calculations, should be included, as should statistical computations and sample spectra.

4. Discussion:

A *brief* analysis of the results of the experiment, sources of error, and suggestions for improvement of the procedure. Comparison of experimentally obtained quantities with literature values should be made whenever possible.

5. References:

A list of all sources used in the laboratory report.

6. Appendix:

Copies of notebook pages, computer output, and spectra should be included in this section.

The SLO Track

In completing this course students should be able to:

1. build a molecule using Gaussview or Avogadro.
2. acquire an IR spectrum using an FTIR.
3. predict an IR spectrum of a compound using Gaussian.
4. measure the effect that an adjacent functional group has on the vibrational frequency of a chromophore using an FTIR.
5. predict the effect that an adjacent functional group has on the vibrational frequency of a chromophore using Gaussian.
6. predict the structure and stability of an intermolecular complex using Gaussian.
7. predict the structure and stability of an intermolecular complex using Gaussian.
8. predict the transition species for a chemical reaction using Gaussian.
9. measure the difference in the rate of a reaction upon isotopic substitution.
10. measure the effect of hydrogen bonding in IR, UV-visible, and fluorescence spectroscopy.