Department of Chemistry
The University of Texas at El Paso
Physical Chemistry Laboratory

CHEM 3152 (CRN 20998) Spring Term, 2021

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COVID-19 Considerations

Due to the current conditions from the COVID-19 pandemic several changes have been instituted to this laboratory course when compared to other semesters. This laboratory course is listed as HYBRID. This means we have permission to attend lectures on campus at least once per week. We will not necessarily do so. Most of the laboratory practices have been adapted to be done virtually on a computer. We will hold pre-laboratory meetings using Microsoft Teams at the scheduled time. Please find and install this programs on your computer. All prelaboratory sessions will be recorded and stored within MS Teams, so while attendance to the prelaboratory meetings is necessary, you may be able to review the given instructions at any time. Attending online laboratories will be challenging. We encourage you to ask questions about the task so you will understand of the topics covered. Attending prelaboratory meetings in real time will allow you to ask and answer questions immediately. Office hours will be held online and by appointment. Depending on the current Emergency status in campus, in the state of Texas, and in El Paso, we may have face-to-face meetings. We will inform you of changes at least two weeks in advance. Prelab meetings will be held on Wednesdays 1:30 – 2:20 pm through MS Teams (or Zoom if necessary). For questions about the laboratory experiments and report guidelines, talk to the Teaching Assistants. Their office hours will be held virtually by appointment through MS Teams on Fridays.

Course Description

The objective of this course is to present and perform complementary experimental work to the Physical Chemistry course CHEM 3352 that focuses mainly in Quantum Theory, kinetics, spectroscopy, and magnetism from a chemical standpoint.

Textbook

No textbook will be required. Appropriate handouts will be provided for every experiment. All of these handouts will be uploaded to Blackboard which can be accessed through http://my.utep.edu.

Grading

The grade for this course will consist on the cumulative points obtained by individual laboratory practice reports averaged by the number of experiments in the course plus the result of quizzes

administered previous to the laboratory practice. The grade distribution will be: The grade distribution will be:

- 60% Lab reports
- 20% Pre-lab quizzes
- 10% Laboratory performance

Quizzes will be administered through Blackboard using the Respondus Lockdown Browser. Quizzes will be short and will test your understanding of the practice BEFORE the actual prelaboratory meeting. These quizzes will be timed and will be available for a short period of time before the prelaboratory meeting. You will have one attempt. You MUST be prepared to do the practice at the meeting time. "Prepared" means understanding the objectives of the practice and being familiar with the conceptual concepts to be discussed. "Laboratory performance" includes attendance, successful execution of the practice, and proper safety behavior. Even under virtual laboratory settings, proper safety is necessary. Reports are due one week after the completion of the laboratory practice. Reports must be submitted in Blackboard. Late reports may be accepted with a penalty of 20% per late day. If the report is not submitted at the due date and time the report will be considered late. It is your responsibility to make sure that the report was received, and that the electronic version is readable. Corrupted files (i.e. un-openable files) will not be tolerated.

Laboratory report format

The format of the experimental reports must follow the ACS style that can be found in any journal of the American Chemical Society. The format of JACS, Physical Chemistry A or Physical Chemistry B is recommended. Each individual report will be graded on the basis of the quality of the following sections:

1. Abstract: An abstract is a brief and concise summary of the experiment described in the report. It should include the general idea of the experiment, results obtained, and the conclusions drawn from those results.
2. Introduction: This section includes the background to the experiment. It must include the necessary theoretical framework required to understand the experimental work, and it must end with a clear statement of what will be investigated during the experimental practice.
3. Experimental Information: This section can be separated in two parts. a) A clear description of the experimental apparatuses, chemicals, or specialized computational programs utilized, and b) The exact experimental procedure followed during the practice. This section should be written in the "past tense", since this is a report of what was observed.
4. Results and discussion: A clear description of the results and any observations recorded during the experiment. Discussion of these results and how do they fit into the whole theoretical background discussed in the Introduction part.
5. Conclusion: This includes conclusions drawn from the experiment.
6. References: These should conform to the ACS style. Please refer to any JACS, Physical Chemistry A or Physical Chemistry B journals for further information. These journals can be accessed through any UTEP connection (including VPN connections from home) at http://pubs.acs.org.

Software

We will use several computational modelling software programs. You will be required to be well versed on all of them. Spartan 18 and AMPAC both work on either Mac or PC but not on Chrome computers or tablets.

Spartan '18. We will use the Student version of Spartan '18 https://www.wavefun.com/spartan You will have to purchase this software ($50.00 for the student version) if you have not already done so.

AMPAC (Semichem). AMPAC is a molecular mechanics program that will be provided to you whenever we are ready to use it. We may use this program to aid us in setting up chemical calculations using Gaussian.

Gaussian 19. We will provide you with student accounts in the UTEP Supercomputing facilities. Having supercomputing accounts will require for you to abide by all the UTEP electronic and computational regulations. You will be responsible for any unauthorized use emanating from your account. This program can only be accessed through a terminal set up (on a Mac) or through a remote ssh connection using an additional program (i.e. PuTTy, for PCs). You will have to learn and be familiar on how to use these programs.

Syllabus

The following are the expected experiments we will perform this semester. Each experiment will have a timeframe of at least two weeks.

1. Spartan Student and Gaussian Tutorials
2. Calculating Redox Potentials (Electrochemistry)
3. Particle in a Box/ Particle in a Ring
4. Kinetics of Quantum Dots
5. SQHO: IR and Raman Spectroscopy
6. Spectroscopy: Absorption spectra of I_2.
7. Elements & Energy

If you need help performing any of these practices you MUST contact the TAs within the first few days of the assignment of the experiment. We will be unable to help you the day before the reports are due.

If we are able to move to the laboratory, we will have to accommodate the dates for every experiment due to the limited number of instruments available. We will try to schedule two or more different experiments per week. This means that the TA and instructor will be focusing on several things at the same time. Therefore, you must come well prepared to the laboratory practice to avoid wasting time. Students who are not well prepared will not be allowed to perform the experiment that week, and will have their grades affected.

Disability

If you believe you may qualify for special accommodations due to disability contact the Center for Accommodations and Support Services Office: http://sa.utep.edu/cass; 915-747-5148.

Safety

A separate safety instruction sheet will be provided if we enter the lab later in the semester. Students will be required to follow these laboratory rules at all times. Use of appropriate eyewear protection compliant to university rules is mandatory at all times during laboratory practice.

Course Drop Policy

All grades of Incomplete must be accompanied by an Incomplete Contract that has been signed by the instructor of record, student, departmental chair, and the dean. Although UTEP will allow a maximum of one year to complete this contract, the College of Science requests it be limited to month based upon completion data. A grade of Incomplete is only used in extraordinary circumstances confined to a limited event such as a missed exam, project, or lab. If the student has missed a significant amount of work (e.g. multiple assignments or tasks), a grade of Incomplete is not appropriate or warranted. Please add this to your spring syllabi.

Other considerations

Please ask questions and be ready to discuss the experiments before the practice.

Tentative Schedule

	Pre-Lab Date	Experiment	Programs Needed	Report Due
1.	1/27	Introduction	N/A	N/A
2.	2/3	Spartan Student and Gaussian Tutorial	Spartan Student, AMPAC, agui, Gaussian, putty or terminal, WinScp, access to HPC computers	2/10 (worksheet)
3.	2/10	Redox Potentials	Spartan Student	2/24
4.	2/24	Particle in a Box/Particle in a Ring	AMPAC, agui, Gaussian, putty or terminal, WinScp, access to HPC computers	3/10
5.	3/10	Laboratory Safety	N/A	N/A
	3/17	No Lab- Spring Break	N/A	N/A
6.	3/24	Quantum Dots	In-Person	4/7
7.	4/7	IR & Raman spectroscopy	In- Person & Spartan Student	4/21
8.	4/21	Spectroscopy: Absorption spectra of I_2	In-Person	4/28
9.	4/28	Elements & Energy	Spartan Student	5/5 Final Report