Physical Chemistry Lab. 334--Fall Semester 2014

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TEXT: Experimental laboratory: Experiments in Physical Chemistry by Shoemaker, Garland, and Nibbler; 7th or 8th ed. (McGraw-Hill)
Computational laboratory: Handouts by Louis Scudiero, Ben Shepler and Kirk Peterson
Handouts are available on \\diamond3\instruction\Pchem\Chem 334\

EXPERIMENTS: You will be required to complete six (6) out of the eight experiments listed in this handout. Experiments **35, 36, B, and C** are mandatory. The remaining 2 experiments can be chosen from the list. The AFM (exp. Ia) requires that you have already done H (deposition an organic film on mica).

COMPUTATIONS: You will be required to perform two (2) computational laboratories (SO_2, SH_2 and S_3, and decomposition of Acetyl Radical) using Gaussian 03 and GaussView 3.09. In addition to the computations, two data analyses using MathCAD will be required and are listed below. Two experimental labs require additional computational work (IR of SO_2 and Raman spectrum of CCl_4). This should be attached to the lab report. For the computational laboratories, we will meet every Thursday in Fulmer 124. For the data analysis part, students will have to schedule a time to meet with me, or the TA after the experiments have been performed.

REPORTS Your reports will consist of three types

1. One Oral Presentation: The report will be presented to your peers, the TA and me. It should be presented like original work at a scientific meeting. It should last no more than 20 minutes including time for questions. The oral should be given the week before the last week of the semester (*November 27, 2014 in Fulmer 101*). Decide ***as soon as*** you can and let the TA know which experiment you want to present.

2. Two (2) Written Presentations: Two (2) reports should be written, one for the experimental and one for the computational portion of this course (decomposition of Acetyl radical). These should be written as if there were going to be published. For guidance as to the format consult the text in Chapter I or look in the Journal of Physical Chemistry. It will be ***read*** and ***marked*** as if sent to a referee for comments so it should be done well. Use a computer so that you can ***correct the imperfections*** and ***return them for a final grade***. The first report (experimental) is due no later than Friday, *October 17, 2014.* The second is due no later than Friday, *November 21, 2014*.

3. Five (5) Reports in Notebook: (4 experiments including any computation sections and 1 computation reports)
Five (5) reports should be written up in a notebook (computer printouts will be accepted for grading, they should include the original or a copy of the datasheet that was signed by the TA or me). These should contain the data, calculations, discussions, and error analysis. It should also include anything that would help you to redo the experiment in the future. (eg, references, differences in the experiment, etc.) These are due two weeks after the experiment is finished as determined by the TA or instructor initials.

SCHEDULING: Use the sign-up sheet posted in the hall outside the lab between 218 and 219 to reserve an experiment. Sign up each week for the following week lab. This is critical so that the equipment is available for you.

DATASHEET: The datasheet must be kept current during the experiments. It must be dated and initialed by the TA or me when the experiment is done. (This is your responsibility)

STUDENTS LEARNING OUTCOMES: At the end of this lab course the student should be able to

1. Connect concepts of quantum mechanics and spectroscopy covered in lectures (Chem. 334) with experimental measurements and calculations performed in this lab course.
2. Write notebook reports in which only the purpose of the experiment, raw data, graphs, calculations, references and conclusions are reported
3. Write two complete formal reports following the format of the Journal of Physical Chemistry (A, B or C)
4. Give an oral presentation on any experiment of his/her choice in front of the class
5. Be introduced to computation chemistry by using Gauss View and Gaussian 03

ASSESSMENTS: Student learning will be assessed based on how well the student is able to report measurements and

perform calculations and his/her ability to share verbally results and concepts of spectroscopy and quantum mechanics with the class during the oral presentation.

GRADING:

Oral Reports	20%	**Scale**		
Written Reports	20%	**90 →A**	**80 →B**	**68 →C**
Reports in Notebook	50%	**87 →A-**	**76 →B-**	**62 →D**
Laboratory Habits + online Eval.	5 + 5%	**84 →B+**	**72 →C+**	**< 62 →F**

Students with Disabilities: I am committed to providing assistance to help you be successful in this course. Reasonable accommodations are available for students with a documented disability. Please visit the Disability Resource Center (DRC) during the first two weeks of every semester to seek information or to qualify for accommodations. All accommodations MUST be approved through the DRC (Admin Annex Bldg, Rooms 205). Call 509 335 3417 to make an appointment with a disability counselor.

Academic Integrity: I encourage you to work with classmates on lab reports. However, each student must turn in original work. No copying will be accepted. Students who violate WSU's Policy on Academic Integrity will receive an F for that report. Academic integrity is the cornerstone of the university. Any student, who attempts to gain an unfair advantage over other students by cheating, will fail the course. You must do your own work.

			Shoemaker, Garland & Nibler	Page	Room
	K	Exp. F	Photo dissociation of Ferric Thiocyanate (FeSCN)	handout	234
	S	**Exp. 35**	**I-R Spectrum of SO_2 to compare with calculations**	**382**	**218&N106**
	S	**Exp. 36**	**Raman CCl_4 to compare with calcualtions**	**397 Handout**	**N106**
Non Text Experiments					
	S	**Exp. B**	**EPR Spectrum (dpph, Mn^{2+} and Ca^{2+} doped MgO)**	**434 handout**	**234**
	S	**Exp. C**	**I_2 Visible Spectrum (UV-Vis)**	**422 handout**	**N106**
	S	Exp.E	UV-Vis Spectra of solvated Dyes	Handout	N106
		Exp. H	Langmuir-Blodget films of non-peripheral Octabutoxy Copper (II) Phthalocyanine	Handout	N107
	M	Exp Ia	AFM (Atomic Force Microscopy) characterization of LB films	Handout	N106

Students will work in pairs on each experiment. Sign up for each experiment on the sheet in the hall between 219 and 218 at least a week ahead. Read the lab handout or text before you come to do an experiment. **Students will work individually on each computational lab.**

Data analysis will be performed for the following two experiments using MathCAD
1. EPR of dpph and MgO doped MnO or CaO
2. UV/Vis spectrum of I_2

Computations using Gaussian and GaussView will be done for the following laboratories:
1. SO_2, SH_2 and S_3, IR spectra (M)
2. Decomposition of Acetyl radical (M)
3. Raman spectra of CCl_4