CHEMISTRY 391
EXPERIMENTAL PHYSICAL CHEMISTRY
Spring Semester 2015

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Lecture: MWF 10:30 - 11:20 am Lab: W 1:30-5:15 / R 12:15 - 4:45

Date	Lecture Topics	Laboratory
Jan. 12	Course Introduction	No Lab
Jan. 14	MathCAD (computer lab): variables, units, symbolic vs numerical operations	
Jan. 16	MathCAD (computer lab): functions, graphing, importing data, solve blocks	
Jan. 19	**MLK, Jr BREAK**	Calorimetry
Jan. 21	Method of least squares and weighted regression	
Jan. 23	Error analysis, goodness-of-fit, propagation of error	
Jan. 26	MathCAD (computer lab): regression, error analysis, propagation of error	Calorimetry
Jan. 28	MathCAD (computer lab): debugging programs	
Jan. 30	Preparing Quality Graphs (Excel and MathCAD)	
Feb. 2	Statistical Mechanics	Vapor Pressure
Feb. 4	probabilities, partition functions, calculating thermodynamic properties	
Feb. 6	Vibrational-Rotational Spectroscopy	
Feb. 9	SHO and rigid rotor, Morse oscillator, anharmonicity	Vapor Pressure
Feb. 11	Analysis of experimental data, properties of molecules	
Feb. 13	Computational Chemistry	
Feb. 16	the QM problem, orbitals, basis sets	Spectroscopy
Feb. 18	Hartree-Fock, perturbation theory, density functional theory	
Feb. 20	geometry optimization, thermochemistry, transition states	
Feb. 23	Computations using Spartan (computer lab)	Spectroscopy
Feb. 25	Transition-State Theory	
Feb. 27	enthalpy and entropy of activation, Eyring plot	
Mar. 2-6	**SPRING BREAK**	No Lab
Mar. 9	Fluorescence Spectroscopy and Luminescence Quenching	$Ru(bpy)_3^{2+}$
Mar. 11	UV-Vis/fluorescence/electrochemistry energy levels, lifetimes, quenching	
Mar. 13	dye-sensitized solar cells, cell efficiency	
Mar. 16	Electrochemistry: electrochemical cells, cell potential, cell potentials	$Ru(bpy)_3^{2+}$
Mar. 18	electrochemical potential, Nernst equation, membrane potential	
Mar. 20	Ion-Selective Electrodes: Donnan equilibria, membrane potentials	
Mar. 23	**ACS National Meeting**	Group Projects
Mar. 25	**ACS National Meeting**	
Mar. 27	glass membranes, liquid polymer membranes, solid-state devices	
Mar. 30	Group Meetings: presentation of projects	Group Projects
Apr. 1	Group Meetings: presentation of projects	
Apr. 3	Mass Transport Processes: transport equations, Fick's laws	

Apr. 6	**EASTER BREAK**	Group Projects
Apr. 8	Electrical Conductivity: mobility, conductance, applications	
Apr. 10	Voltammetry: flux, current, mass transport-limited currents, Nernst model	
Apr. 13	current-voltage curves, factors affecting the half-wave potential	Group Projects
Apr. 15	Chronoamperometry: semi-infinite linear diffusion, Cottrell equation	
Apr. 17	Normal Pulse Voltammetry: pulse experiments, current-voltage curves	
Apr. 20	Cyclic Voltammetry: analysis of cyclic voltammograms, effect of sweep rate	Group Projects
Apr. 22	electrochemical mechanisms (E, EE, EC, ECE)	
Apr. 24	cell resistance, interfacial capacitance	
Apr. 27	Group Meetings: presentation of results	Group Projects
Apr. 29	Group Meetings: presentation of results	& Lab Clean Up
May 1	Course Evaluations	

TEXTS (optional)

Carl W. Garland, Joseph W. Nibler, David P. Shoemaker

Experiments in Physical Chemistry, 8th ed., McGraw Hill: New York, 2009.

An analytical chemistry text and a physical chemistry text are also recommended.

COURSE WEB PAGES

Lecture Materials: http://www.chm.davidson.edu/dablauch/che391/

Laboratory Materials: http://moodle.davidson.edu/moodle2/

GRADE SCALE

		A	93 - 100%	A-	90 - 93%
B+	87 - 90%	B	83 - 87%	B-	80 - 83%
C+	77 - 80%	C	73 - 77%	C-	70 - 73%
D+	67 - 70%	D	60 - 67%		
F	< 60%				

COURSE GRADE

Experiments (four, 100 points each)	**400** points
Group Project	**200** points
Homework Assignments (five, 50 points each)	**250** points
Class Participation and Laboratory Performance	**50** points
Total	**900** Points

HOMEWORK ASSIGNMENTS

1.	Curve-Fitting (MathCAD)	Due Friday	February 6
2.	Computational Chemistry	Due Friday	February 27
3.	Transition-State Theory (MathCAD)	Due Friday	March 13
4.	Potentiometry and Ion-Selective Electrodes (MathCAD)	Due Friday	April 3
5.	Conductivity and Voltammetry (MathCAD)	Due Friday	May 1

Assignments due at 10:30 am on the indicated date. Late assignments are penalized 3% per day.

HONOR CODE

Students may discuss the homework, experiments, data, and data analysis with other students, but each student must perform the following tasks on his/her own **without consulting the work of any other student**: preparing graphs and tables, writing the formal report, performing calculations, completing homework, and writing MathCAD files. Students may **not copy** experimental data from other groups or any part of another individual's report. Reference to the laboratory reports of other students is not permitted except as required by the instructor. A student may **not examine** the MathCAD file, lab report or homework of another student.

LABORATORY PROGRAM

Laboratory Sessions

Your laboratory section will meet one afternoon a week (Wednesday from 1:30 to 5:15 pm or Thursday from 1:00 to 4:45 pm). There are no pre-lab sessions. Students will work in groups of two or three. All students are required to wear safety glasses and suitable attire while in lab. At the end of the semester, you will receive a laboratory charge for expendable items and for any breakage.

MATHCAD REPORTS

For experiments in which a MathCAD report is required, all data analysis will be performed in a MathCAD worksheet. MathCAD worksheets and should be submitted via **e-mail**.

Data Entry

- Raw data should be entered directly into the worksheet or read from data files. Data files should be placed in your group folder under **\\louise\public\Chemistry\CHE391** and read directly into MathCAD.
- Define all key quantities, such as the standard state: P^o = 1 atm or 1 bar, for example.
- Raw data should be entered **once**; thereafter all values must be computed (no manual entry of results).

Computations

- Perform **all calculations** and prepare **all graphs** in MathCAD. Do **NOT** perform computations elsewhere and copy the results into MathCAD.
- All information should contain appropriate units. Where possible, use built-in unit management.
- Use variable names that follow common conventions. All variables should be defined when first introduced.

Graphs

- Plot experimental data as **individual points**, unless there are too many points to see each point clearly.
- Plot theoretical predictions or curve-fitting results as a **smooth curve** that extends to the limits of the graph.

Miscellaneous

- The worksheet should be **well-organized** and contain **brief explanations** to guide the reader through the analysis process. Use **headings** to divide the worksheet into sections. Include your name and the experiment or assignment title at the top of the worksheet.
- Values should be formatted to display the correct number of significant figures.
- Place the answer to a question in a **text box**.
- Include **full citations** to all information obtained from other sources.

EXPERIMENTS

Background, experimental details, and report requirements are posted on the course web site. **Prior** to arriving for a laboratory session, each group should plan the experimental work for the afternoon.

Topic	Title	Report Due Date*
Calorimetry	Heats of Combustion	Feb 6
Vapor Pressure	Vapor Pressure of a Pure Liquid	Feb 20
Spectroscopy	Vibrational-Rotational Spectra of HCl and DCl	Mar 13
$Ru(bpy)_3^{2+}$	Excited State Lifetime of *Tris*(2,2'-bipyridine)ruthenium(II)	Apr 10
Group Project	To be decided by each group	May 8
Lab Clean Up**		

***** Laboratory reports are due by 11:00 pm on the assigned date. Late reports are penalized 3% per day.

****** Participation in laboratory clean-up is mandatory for all students.

GROUP PROJECTS

The goal of the group projects is to develop new experiments for future use in the physical chemistry laboratory program. The time line and due dates for the various stages of the project are provided below. Each member of the group must fully participate in all aspects of the project, including writing the Project Proposal and Project Report.

1. Selection of Project — Due Jan 30

   Each group will select an experimental topic for the projects. The topic will be a laboratory experiment that can be completed in one to three afternoons by students in either CHE 260 or CHE 360.

2. Project Proposal — Due Feb 27

   The topic should be refined to identify specific chemical systems and techniques that will be tested and developed into a viable educational unit. The proposal should identify the specific concepts and experimental techniques to be addressed and the expected nature of the experimental manipulations and measurements as well as the data analysis. The proposal should also include a list of equipment, chemicals, and materials required for the experiment. At least six relevant scientific articles from journals should be cited.

3. Experimental Work — Mar 23 to May 1

   Each group will test and refine the experiment in the laboratory. The experiment should be developed to be reproducible and feasible for the target course. Sample data will be obtained and analyzed.

4. Project Report — Due May 8

   The final report will consist of two documents, submitted as computer files (Word, Excel, MathCAD).

   The first document is the Experiment Module, which will be made available to future CHE 260 or 360 students who will perform this experiment. This module should provide background on the physical chemistry concepts and experimental techniques, an experimental procedure appropriate for the level of the course, and an explain of the data analysis and interpretation. Citations to relevant scientific articles should be provided. A set of discussion questions should also be provided.

   The second document is Instructor Notes, which provide information to the instructor or lab manager on preparing for the experiment. A list of resources (chemicals, materials, equipment) should be provided as well as advice on possible problems and their remedy. The Instructor Notes should also include experimental data and analysis and interpretation of the data, as well as a discussion of the questions included in the Experiment Module.