

Chem 330

PROBLEM SOLVING METHODS

For Physical Chemistry

Room 225, Monday 2 – 4 pm

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Office Hours: Ful. 116d

NOTICES

- Semester Grades are based on the point total computed from (HW/3 + FINAL/5). That is, 80% of total is contributed from homework and 20% from the final. Maximum total: $(240/3 + 100/5) = 100$.

Likely grade scale (downward adjustments only)

100-90%	A
89-75%	B
74-60%	C
<59	D

- Required Problems and Homework consists of
Mathematical review (Barrante) and Problems (not graded)
 - #1. Units, graphing and degree of confidence.
 - #2. Properties of Gases problems.
 - #3. First Law Problems,
 - #4. Second and Third Law Problems,
 - #5. Phase Equilibrium Problems,
 - #6. Chemical Reactions and Electrochemistry, Problems,
 - #7. Electrochemistry and Chemical Kinetics Problems.

- The final exam will be a take home. You should work this exam on your own. You can e-mail questions about the final to me and I'll decide whether it's fair to answer.

Notes: Cheating of any kind will not be tolerated. This includes the inappropriate use of solution manuals for homework sets, as well as the usual forms of copying, etc...

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.

Personal computing and the internet are changing the way science is taught as well as revolutionizing the way professionals do science. This course helps you to develop computing and internet skills and to solve physical chemistry problems.

Course Description

Chem. 330 Problem Solving in Physical Chemistry 1

Prereq. Chem 106 or 116; Math 172.

Quantitative methods of data analysis and chemical concept development; emphasis on multivariable, matrix, and computer methods.

Objectives

- To review and refresh your knowledge of mathematics and computational methods.
- To develop skills to use computer tools for computation and symbolic mathematics.
- And apply mathematical concepts and computing tools in physical chemistry problem solving.

Course learning resources

- Text: “Physical Chemistry using MathCAD” by Joseph H. Noggle [Pine Creek Publishing Co., 1997].
- Under the Help pull-down menu, find MathCAD’s built-in *MathCAD Help* and *resource center*.
- Mathsoft, MathCAD’s vendor, maintains a web site with resources and links: <http://www.mathsoft.com/>.
- Web sites dealing with physical chemistry topics: “[MathCAD Documents for Physical Chemistry](#)”; “[ftp site of MathCAD files for physical chemistry problems](#)”; “[IDEA site](#)” see special topics Chemical Kinetics Fundamentals, Oscillating Chemical Reactions, Temperature Programmed Desorption (TPD), Quantum Mechanical DE Solved .
- Book: “Applied Mathematics for Physical Chemistry” Third Edition by James R. Barrante [Pearson Education Inc., Pearson Prentice Hall].

Schedule of Topics and Homework

The topics will be covered every week. A problem set will be assigned each Monday and will be due at the latest that Friday before noon (Fulmer 208). The materials will be covered in scheduled class and laboratory sessions in 10 weeks. By meeting together as a class during these labs, you will benefit from personal help from fellow students, the TA and the instructor.

1. **Mathematical review.** *Work problems from Barrante.*
2. **Introduction.** (Read Noggle: Introduction)
The mathematical prerequisites. MathCAD: Getting Started.
3. **Units' conversion and graphs.** Homework Problems, set#1
4. **Properties of Gases.** (Noggle: Chapt.1)
Ideal Gas. Real gases. Virial equation, van der Waals' equation, Redlich-Kwong equation. Interpretation and visualization, graphs and plots. Isotherm, isobar, isochor. Kinetic Theory of Gases. *Reading assignment Noggle Chap.1 (to be done before class or lab meeting).*
Homework Problems, set #2
5. **The First Law.** (Noggle: Chapt.2)
 ΔU and ΔH , Heat capacities. *Reading assignment: Noggle Chap. 2 (to be done before class or lab meeting).*
Homework Problems, set #3.
6. **Second Law, Third Law.** (Noggle: Chapt.3)
Prerequisites. Mathcad's integration functions. Interpolation between data points. Definition of entropy as a differential, as an integral. Entropy change of an ideal gas during isothermal expansion/compression. *Reading assignment: Noggle Chap.3 (to be done before class or lab meeting).*
Homework Problems set #4.
7. **Phase Equilibrium.** (Noggle: Chapt.4)
Clausius-Clapeyron calculations. Boiling temperature of fluid via equal area rule.
Reading assignment: Noggle Chap.4. Complete this prior to meeting.
Homework Problems, set #5
8. **Chemical reaction, Electrochemistry.** (Noggle: Chapt. 6 (sect. 6.4), 8 (sect. 8.2))
Fugacity Coefficient. Conductivity. Thermodynamic Equilibrium constant K_{eq} , ΔH , ΔG , ΔS , and extent of reaction calculations.
Homework Problems, set #6
9. **Chemical Kinetics.** (Noggle: Chapt. 8 and 10)
Conductivity and EMF. Analysis of the order of a reaction. Mechanisms, Differential Equations calculations.
Homework Problems, set #7
10. **FINAL EXAMINATION** (Take-home Final)
Submit print-out one week after receiving it.