Chemistry 3070-001

Spring Semester, 2006

INSTRUCTOR: Dr. Edward M. (Ted) Eyring, Professor of Chemistry; 2428 S HEB, 581-8658; Fax: 587-9919
Office Hours: M W F 8:25-9:25 a.m. at 2428 HEB or by appointment (581-8658)
E-mail: <eyring@chem.utah.edu> Please do not send confidential material or assignments to this e-mail address.
Executive Secretary: Cheryl Gabbott, 2420 S HEB, 581-4191

LECTURES: M W F 9:40 a.m. to 10:30 a.m., HEB 2006

TEXT: D.A. McQuarrie & J.D. Simon, *Physical Chemistry: A Molecular Approach*, University Science Books, Sausalito, CA, 1997 (Required)

DISCUSSION: Tuesday and Thursday, 7:30 – 8:20 a.m., ST 214 (Section 3070-002)
Tuesday and Thursday, 9:40 – 10:30 a.m., ST 215 (Section 3070-003)

The first Discussion meeting will be held on Tuesday, January 10th.
The Teaching Assistant's name is Moussa Barhoum.
His e-mail address is mbcom@chem.utah.edu

E-mail: Every student must have a functioning e-mail account. Important information will be exchanged this way. Please give your Teaching Assistant a working e-mail address A.S.A.P that you access frequently.

INSTRUCTIONS FOR ALL STUDENTS:

Students will attend two Discussions each week. The required textbook, McQuarrie & Simon, is quite different in content and emphasis from our previous required textbook, Atkins & de Paula, Seventh Edition. Students are advised against trying to limp along with a copy of the Atkins & de Paula textbook or with a paperback copy of McQuarrie & Simon that does not have all the chapters of the hardback textbook.

The McQuarrie & Simon text assignment should be read before the lecture. All **EXERCISES** and **PROBLEMS** assigned in the syllabus should be attempted before the recitation section session.

A student's lowest *exam* score (including the final exam total score, if this is the lowest) will be dropped. **No make-up examinations will be given in the course**, as it is impossible to write an examination that will be exactly equivalent. In case of an illness or a dire emergency, a student may be excused from one midterm examination if contact is made with Ted Eyring **prior** to the examination. If excused, the score for the missed examination will be the average of all the other Chem. 3070 midterm examinations for the semester taken by the student.

Examination papers will only be considered for re-grading if they are submitted to Dr. Eyring or his secretary within two weeks after the date of the examination. Trivial resubmissions are discouraged and will result in the entire exam being re-graded.

Americans with Disabilities Act of 1990

The University of Utah seeks to provide equal access to its programs, services and activities for people with disabilities. If you will need accommodations in the class, reasonable prior notice needs to be given to the Center for Disability Services, 162 Olpin Union Building, 581-5020 (V/TDD). CDS will work with you and the instructor to make arrangements for accommodations. All written information in this course can be made available in alternative format with prior notification to the Center for Disability Services.

Your letter grade for Chem 3070-001 will be assigned on the basis of the following possible point scores:

First Hour Exam, Wednesday, Feb. 1, 9:40 a.m.	100 points
Second Hour Exam, Wednesday, Feb. 22, 9:40 a.m.	100 points
Third Hour Exam, Wednesday, March 22, 10:45 a.m.	100 points
Fourth Hour Exam, Wednesday, April 12, 10:45 a.m.	100 points
Final Exam, Monday, May 1, 8:00 a.m. – 10:00 a.m.	100 points
Possible Number of Discussion Points	150 points *
Total Possible Points	550 points (dropping low exam)

*The overall class average for discussion will be approximately 62%. The T.A. will give quizzes and graded homework assignments during the semester. (The average score on midterms in Fall 2004 was 67.9% and the average score on the final exam was 67.2%.)

Study Groups and Homework Assignments:

You will be asked to form study groups of 3-5 students each. Study groups will work on problems together during discussion in class, and will present solutions on the board. Discussion grades will be based on quizzes, homework assignments, and participation. Each student must write homework solutions out by hand in order to receive credit for the assignment. No photocopies or mass-produced copies will be accepted for grading. If you collaborate on homework, please write the names of your collaborators on your paper. Study groups are encouraged to meet outside of class to prepare together for exams. Assigned homework problems are due in your Discussion Section on the day stipulated by your T.A. No late homework assignments will be accepted for grading.

Midterms and Final Exams

Each exam will consist of two parts: The first part will be “closed book,” and the use of a pocket calculator will usually not be permitted. The second part of each exam will be “open book.” For the “open book” portion of the exam you may bring any calculator, books, notes, or other written material that you think you may find useful. The examinations given in Fall, 2005 are available at the Reserve Desk of the Marriott Library in the same loose leaf binder in which lecture notes will be posted.

GRADES

When this course has been taught previously by Ted Eyring, the letter grade distributions for the semester length class have been the following:

	Spring 2001	Fall 2001	Spring 2002	Fall 2002	Spring 2003	Fall 2003	Spring 2004	Fall 2004	Spring 2005	Fall 2005
A	7	8	7	7	9	10	7	6	10	9
A-	8	3	10	7	5	6	8	7	9	8
B+	7	4	9	5	4	4	5	8	7	5
B	8	10	7	10	8	8	9	11	13	5
B-	5	4	13	3	3	4	6	5	10	3
C+	6	3	5	6	9	3	6	5	8	3
C	2	4	1	2	4	7	4	4	2	11
C-	2	0	3	0	3	1	2	1	0	0
D+	0	0	2	0	0	1	1	0	1	3
D	0	0	1	2	0	1	2	0	2	1
D-	0	0	0	1	0	1	1	0	1	1
E	2	1	1	1	1	0	1	2	3	2
I	1	0	0	0	0	0	1	0	0	0
Total	48	37	59	44	46	46	53	49	66	51

Chemistry 3070-001 (4 credits), Spring 2006

	Monday	Wednesday	Friday
January	Housekeeping Details **9** 16-1 Ideal Gases 16-2 Two-Parameter EOS's 16-3 …Cubic Equation… 16-4 Law of Corresponding States	16-5 2nd Virial Coeff. **11** MathChapter H. Partial Differentiation 17-1 Boltzmann Factor 17-2 Probability….	17-3 Avg. Ensemble Energy **13** 17-4 Heat Capacity 17-5 Pressure 17-6 Distinguishable 17-7 Indistinguishable 17-8 Decomposed
	16 MARTIN LUTHER KING, JR. HOLIDAY	MathChapter I. Series and Limits **18** 18-1 Translational 18-2 Electronic 18-3 Diatomic 18-4 Vibrational	18-5 Rotational **20** 18-6 Symmetry No. 18-7 Polyatomic 18-8 The Form…. 19-1 PV Work 19-2 State Function
	19-3 First Law of Thermo. **23** 19-4 Adiabatic Process 19-5 Reversible Expansion 19-6 Work/Heat 19-7 Enthalpy	19-8 Heat Capacity **25** 19-9 Heats of Transition 19-10 $\Delta_r H$ Additive 19-11 Heats of Formation	19-12 $\Delta H = \int C_p dT$ **27** Joule-Thomson Effect MathChap. J. Binom. Distrib. 20-1 Spontaneous Process
February	20-2 Evolve to Disorder **30** 20-3 Adiabatic Process 20-4 2nd Law 20-5 $S = k_a \ln W$	**1** **First Midterm Exam**	20-6 Calculating ΔS **3** 20-7 Heat to Work Carnot Cycle 20-8 Partition Function
	Shuffled Cards **6** 21-1 S Increases with T 21-2 3rd Law 21-8 Spectroscopic S 21-3 $\Delta_{trs}S$	21-4 Debye T^3 Law **8** 21-5 Absolute Entropies 21-7 Stand. Molar Entropies	21-9 Calculating $\Delta_r S°$ **10** 22-1 Helmholtz Energy A 22-2 Gibbs Energy G 22-3 Maxwell Relations
	Tobolsky's Method **13** 22-4 Ideal Gas Enthalpy 22-5 Natural Independent Variables	22-6 Hypothetical Ideal Gas **15** 22-7 Gibbs-Helmholtz Eq. 22-8 Fugacity Fischer-Tropsch Chem. Water-Gas-Shift Rxn.	23-1 Phase Diagram **17** 23-2 Gibbs Energy/Phase Diagram 23-3 μ in 2 phases Clapeyron equation
	20 PRESIDENT'S DAY HOLIDAY	**22** **Second Midterm Exam**	23-4 Clausius-Clapeyron **24** Liquid Surface Tension 23-5 μ from Partition Function 24-1 Partial Molar Volume
	24-2 Gibbs-Duhem Eq. **27** 24-3 μ same in each phase 24-4 Raoult's Law 24-5 Henry's Law Molecular Dynamics Simul.	24-6 Vapor Pressures **1** 24-7 Activity 24-8 Activities & Stand. States 24-9 $\Delta_{mix}G$	25-1 Solids Dissolved **3** 25-2 Nonvolatile Solute Activity 25-3 Colligative Properties Mass Spectrometry **Last day to withdraw**
March	25-4 Osmotic Pressure **6** 25-5 Electrolyte Solutions 25-6 Debye-Hückel Limiting Law 25-7 Higher Concentrations	2-component Phase Diag. **8** 26-1 Chemical Equilibrium 26-2 Equilibrium Constant 26-3 $\Delta G = -RT\ln K$	26-4 Minimum at Equilibrium **10** 26-5 Reaction Quotient 26-6 Reaction Spontaneity 26-7 Van't Hoff Equation 26-8 Partition Functions

	Monday	Wednesday	Friday
March	**13** SPRING BREAK	**15** SPRING BREAK	**17** SPRING BREAK
	20 26-9 Thermo. Data Tables 26-10 Partial Fugacities 26-11 K and Activities Electrochemical Cells Half Reactions Reactions at Electrodes	**22** **Third Midterm Exam**	**24** Liquid Junction Potentials Cell Notation Cell Potentials Nernst Equation Concentration Cells Cells at Equilibrium Standard Potentials
	27 26-12 Solubility Calculations Deducing Reaction Entropy From Temp. Dependence Corrosion	**29** 27-1 Kinetic Theory 27-2 Maxwell-Boltzman Distribution 27-3 Molecular Speeds 27-4 Collision Frequency	**31** 27-5 Verification Expt. 27-6 Mean Free Path 27-7 Collisions & Chem. Reaction Rates 28-1 Rate Law Concept
April	**3** 28-2 Rate Law Determined Experimentally 28-3 First Order Reactions 28-4 Higher Order Reactions 28-5 Reversible Reactions	**5** 28-6 Relaxation Methods 28-7 Dependence of Rate on T	**7** 28-8 Transition-State Theory 29-1 Elementary Reactions 29-2 Detailed Balance
	10 29-3 Consecutive & Single Step Reactions 29-4 Steady-State Approx. 29-5 Rate Law Does Not Imply a Unique Mechanism 29-6 Lindemann Mechanism	**12** **Fourth Midterm Exam**	**14** 29-7 Chain Reactions 29-8 Catalysts 29-9 Michaelis-Menten Mechanism
	17 30-1 Hard Sphere Collision 30-2 Impact Parameter 30-3 Orientation 30-4 Internal Energy 30-5 Center-of-Mass Coord. 30-6 Crossed Beams	**19** 30-7 $F(g) + D_2(g) \rightarrow$ 30-8 Angular Distribution 30-9 Harpoon Michanism 30-10 Potential Energy Surfaces 31-1 Unit Cell 31-2 Miller Indices	**21** 31-3 X-ray Diffraction 31-4 Scattering Factors 31-5 Structure Factor 31-6 Physisorb or Chemisorb
	24 31-7 Adsorption Isotherms 31-8 Langmuir Isotherm 31-9 XPS, LEED 31-20 Volcano Curves	**26** **REVIEW**	**28** **FINAL EXAM PERIOD BEGINS**

FINAL EXAM: Monday, May 1, 2006, 8:00 – 10:00 a.m., HEB 2006

Chem. 3070 Discussion Homework

McQuarrie & Simon

-Chapter 16, The Properties of Gases
1, 3, 6, 9, 13, 15, 58, 59

-Math Chapter H, Partial Derivatives
2, 3, 7, 9, 12

-Chapter 17, The Boltzmann Factor and Partition Functions
2, 8, 17, 20, 34, 42, 43

-Math Chapter I, Series and Limits
3, 5, 9, 13, 14

Chapter 18, Partition Functions and Ideal Gases
7, 9, 16, 23, 24, 39

-Chapter 19, The First Law
1, 2, 4, 12, 15, 17, 18, 19, 23, 25, 34, 36, 40, 45

-Chapter 20, The Second Law
2, 6, 8, 9, 13, 15, 18, 19, 25, 26, 31, 32, 40

-Chapter 21, The Third Law
1, 2, 4, 6, 10, 16, 17, 20, 40, 41, 43, 45, 47

-Chapter 22, Helmholtz and Gibbs
1, 2, 3, 5, 8, 9, 11, 14, 19, 23

-Chapter 23, Phase Equilibria
1, 3, 6, 7, 8, 13, 20, 21, 23, 37

-Chapter 24, Solutions I: Liquid-Liquid Solutions
2, 3, 8, 10, 11, 12, 13, 16, 21, 23, 29

-Chapter 25, Solutions II: Solid-liquid Solutions
1, 2, 4, 24, 26, 29, 32, 40, 43, 48

-Chapter 26, Chemical Equilibrium
1, 2, 3, 4, 7, 10, 11, 14, 16, 21, 29, 43, 63, 64, 65

Atkins & de Paula

-Chapter 10, Equilibrium Electrochemistry
18(a), 23(a), 25(a), 27(a), 29(a), 32(a)

McQuarrie & Simon

-Chapter 27, The Kinetic Theory of Gases
1, 2, 3, 5, 11, 12, 17, 20, 27, 29, 32, 37, 49

-Chapter 28, Chemical Kinetics I: Rate Laws
1, 2, 3, 5, 6, 8, 13, 15, 17, 20, 33, 34, 38

-Chapter 29, Chemical Kinetics II: Reaction Mechanisms
1, 2, 4, 6, 7, 8, 12, 13, 14, 17, 18, 21, 31, 37, 47

-Chapter 30, Gas Phase Reaction Dynamics
1, 3, 4, 5, 6, 7, 9, 13, 16, 18, 21, 24, 39

-Chapter 31, Solids and Surface Chemistry
1, 2, 3, 4, 5, 7, 10, 14, 18, 23, 24, 47, 68