Chem 105: Atmospheric Physical Chemistry
Dr. Ryan Z. Hinrichs
Spring 2010

Meeting Time:	T/Th 9:00 – 10:15 am (in S-139) Th 1:15 – 4:15 pm
Instructor:	Dr. Ryan Z. Hinrichs Office: S-210 rhinrich@drew.edu Phone: 973.408.3853
Office Hours:	Open door policy: if my door is open, stop by. You may also schedule a time.
Required Materials:	Engel and Reid, *Physical Chemistry*, 2nd Ed., Prentice Hall, 2010 with Scientific calculator; laptop computer with Excel, MathCAD & Gaussian.
Lab Materials:	Laboratory notebook Safety glasses ($10, if needed, purchase from Jackie in S-218)

Course Description:
An in-depth study of chemical thermodynamics, kinetics, quantum mechanics, and spectroscopy with application to atmospheric chemistry. Topics include the quantum mechanics of translation, vibration, and rotation; electronic, vibrational, and rotational spectroscopy; thermodynamics of solutions and interfaces; statistical thermodynamics; molecular reaction dynamics; elementary nuclear magnetic resonance spectroscopy; and advanced electronic structure calculations. Laboratory experiments seek to determine the thermodynamic and kinetic behavior of systems using spectroscopic techniques and computational calculations.

What I expect from you:

- attend all classes (**attendance is mandatory**);
- arrive on time (I know it's early, but that is not an excuse);
- if an emergency forces you to miss class, please make a reasonable effort to contact me prior to the start of class;
- complete assignments on time (**late work will not be accepted**);
- read the textbook material associated with the current topic thoroughly;
- ask questions (I suggest you write down any questions as you study outside of class).

If you miss class, you are responsible to find out what material we discussed and you are expected to be prepared for the following class. If you miss more than two classes, you must schedule a meeting with me to discuss this issue.

Your work in this course will be evaluated on the following:

Participation	100
HW Problems (10×15)	150
Article Reports (6×25)	150
Exams (2×100)	200
Laboratory	200
Total	**800**

Participation: (100 points) On occasion, class will start with a brief 5 minute quiz covering basic concepts from the prior class. **There will be no make-up quizzes**. If you arrive late to class and miss a quiz, you will receive a zero.

Problem Sets: (150 points; approx. 10 assignments, 15 points each) Homework problems will assigned weekly. Assigned problems will be handed out in class or placed in the Chem105 folder on the Drew network by the end of the prior class. **You must write up your answers individually**. If you have questions regarding a problem, please don't hesitate to contact me via email or stop by my office. *I have an open door policy - please feel free to drop by my office at anytime*.

Article Reports: (150 points; approx. 6 articles, 25 points each)

Two Exams: (100 points each) Two semester exams are tentatively scheduled for Tuesday March 2 and Tuesday April 20. Details regarding the structure of these exams will be discussed in class at least one week prior to the date. Both exams will consist of an in-class portion and a take-home portion. You must work on these exams by yourself, and I encourage you to review Drew University's policy on Academic Integrity.

Laboratory: (200 points) You are expected to keep a professional laboratory notebook, which I will occasionally collect. Notebooks should be written in ink and be properly dated and signed. All critical experimental details (e.g. procedures and results) and calculations should be included in your notebook. You should also include a brief summary/conclusion at the end of each experiment. Individual experiments will also require additional documents as detailed in lab. For instance, some experiments will simply require formatted graphs with captions while other labs will require a complete write-up in the format of a scientific article. All relevant data must be presented in tables and/or figures where appropriate and all references must be properly cited. Advice on scientific writing may be found in *Physical Chemistry: Methods, Techniques, Experiments* by Rodney Sime; an electronic version of this reading is located in the Chem 105 folder.

Academic Accommodations:
Should you require academic accommodations, you must file a request with the Office of Educational Affairs (BC 114, extension 3327). It is your responsibility to self-identify with the Office of Educational Affairs and to provide me with the appropriate documentation from that office at least one week prior to any request for specific course accommodations. There are no retroactive accommodations.

T	1/26	Kinetic theory of gases; structure of atmosphere	Lab $HCCl_3$ overtone spectroscopy
Th	1/28	UV-visible photochemistry	
T	2/2	Article: The "Ozone Deficit" Problem: $O_2(X,v\geq26) + O(^3P)$ from Ozone Photodissociation, *Science, 265*, 1831-1938, 1994.	Lab HONO UV-vis spectroscopy
Th	2/4	Atmospheric photochemistry and photolysis rate constants.	
T	2/9	Article: Atmospheric Photochemistry via Vibrational Overtone Absorption, *Chem. Rev.*, *103*, 4717-4729 (2003).	Lab Infrared spectroscopy: GHG
Th	2/11	Quantum Mechanics: Rigid Rotor and Molecular Rotations	
T	2/16	Ro-vibrational spectroscopy	Lab IR: HCl, HBr, DCl, DBr
Th	2/18	Article: Atmospheric Lifetimes and Global Warming Potentials of Hydrofluoroethers, *J. Phys. Chem. A*, *103*, 9770-9779 (1999).	
T	2/23	Calculating greenhouse gas potentials	Lab IR: HCl, HBr, DCl, DBr
Th	2/25	Probability and an introduction to partition functions	
T	3/2	**Exam**	Lab IR: C_2H_2 and C_2D_2
Th	3/4	Ensemble and molecular partition functions	
Spring break			
T	3/16	Statistical mechanics	Lab Ozonolysis research
Th	3/18	Statistical mechanics	
T	3/23	Article 1: Formation of Microcrystals, Micropuddles and Other Spatial Inhomogenieties of Surface Reactions, *Langmuir*, *21*, 8793-8801 (2005). Article 2: Reactivity of Ozone with Solid Potassium Iodide Ivestigated by Atomic Force Microscopy, *J. Phys. Chem. C*, *112*, 8110-8113 (2008).	Lab Ozonolysis research
Th	3/25	Ideal solutions and Rault's Law.	
T	3/30	Solid-liquid phase equilibria and surface tension.	Lab Ozonolysis research
Th	4/1	Article 1: Molecular Structure of Salt Solutions, *J. Phys. Chem. B*, *105*, 10468-10472 (2001). Article 2: Enhanced Surface Photochemistry in Chloride-Nitrate Ion Mixtures, *Phys. Chem. Chem. Phys.*, *10*, 5668-5677 (2008).	
T	4/6	Ideal solutions: osmotic pressure and electrolytes	Lab Ozonolysis research
Th	4/8	Electrolyte thermodynamics and equilibria	
T	4/13	Transition state theory	Lab Ozonolysis research
Th	4/15	Reaction dynamics	
T	4/20	**Exam 2**	Lab Ozonolysis research
Th	4/22	Article presentations.	
T	4/27	Article presentations.	Lab Ozonolysis research
Th	4/29	tbd	