CHE 329, Fall 2014: Physical Chemistry (PChem) Laboratory

Syllabus Revision 9. Last updated: August 6, 2014

Location: NSC 350 (lab and lectures), North Campus
Laboratory: M/T/W for sections 1/2/3, 1:00 – 5:50 pm, per assigned group schedule
Orientations: August 25/26/27 (M/T/W) for Sections 1/2/3.

Instructor: Prof. Jochen Autschbach, jochena@buffalo.edu, 716-645-4122
Instructor's Office Hours: Mon 5 – 6 pm, NSC 313
Faculty mailboxes are located inside the Chemistry Department's main office, NSC 359

Teaching Assistants (TAs): TA mailboxes are located in the hallway outside of 359 NSC
Tom Duignan, NSC 345, tjduigna@buffalo.edu
Alex Marchenko, NSC 345, alexmarc@buffalo.edu
Robert Martin, NSC 345, rmartin9@buffalo.edu

Safety, Orientation meetings: Attendance at one of the three scheduled orientation meetings is mandatory. *You acknowledge that performing experiments in this laboratory course is a potentially hazardous activity. Always follow proper safety procedures. You must read and understand the Safety Regulations and Emergency Protocol handout.*

Important dates (please check with the official UB calendar):
Semester begins on Monday, August 25
Labor Day Observed: Mon, Sep. 1
Fall Recess: Wed, Nov. 26 – Sat, Nov. 28
Deadline for course resignation: Fri, Nov. 7
Last day of classes: Friday, Dec. 5

Course web site: UBLearns, https://ublearns.buffalo.edu. The course web site contains downloadable (PDF) versions of the syllabus, lab instructions, announcements regarding the course, and other material. The instructor and TAs use UBLearns to contact students via email.

Learning Outcomes

Goal	Assessment (see 'Course Grade' for further details)
Hands-on experience with PChem Lab techniques	Performing experiments as scheduled under supervision of TAs. Student demonstrated that he or she was prepared for the lab. Competency during lab hours.
Develop scientific writing skills	Lab. reports for each experiment
Knowledge of scientific background of each experiment	Pre-lab quizzes, Introduction section of written reports
Data analysis	Score of data analysis part of Lab. report,
Scientific reasoning, analytic thinking	Discussion in the Lab. report of results and conclusions obtained from the experiment

Course Content: Students perform five experiments (one of these is a computer simulation), submit a Lab Report for each of these, and attend related lectures if / when announced. Before each experiment, each student group has to take part in a pre-lab quiz in order to demonstrate that he or she is adequately prepared. If a student's preparation for the experiment is deemed unsatisfactory by the TA, the student will not be permitted to perform the experiment (and receive a score of zero points for the experiment *and* the lab report). If a student shows up late, there will be a point reduction for the lab report corresponding to the fraction of time needed for the experiment that the student missed, and no points will be given for the quiz. If a student is so late that already half of the experiment is complete, the score for the lab will be zero points. *Bottom line: show up on time!* There are no written exams. There is no 'extra credit' available; no exceptions. Regarding incomplete grades, see http://undergrad-catalog.buffalo.edu/policies/grading/explanation.shtml#incomplete . A documented medical emergency near the deadline for the last Lab Report might be one of the rare cases where an incomplete grade is given. Normally, a deadline extension (at the discretion of the instructor) should cover all exceptional situations that might arise.

Course grade: Each Lab Report will be assigned up to 100 points, with 100 points awarded to a perfect report and 50 points for a barely acceptable one. Up to 100 additional points (over the whole course) will be assigned to each student based on a joint instructor – TA general evaluation of a student's performance in the lab. The maximum number of points is therefore 600. A letter grade will be assigned at the end of the course, based on the final percentage score. The grading scheme used in the previous 3 years is as follows: below 40 percent is F. The cut-off percentages for higher grades are: 40=D, 45=D+ 50=C-, 56=C, 62=C+, 68=B-, 74=B, 80=B+, 86=A-, 92=A. The instructor reserves the right to modify the grading scheme if this year's class performs very differently from previous classes. Lab Reports that are assigned less than 50 points are unsatisfactory. If you receive less than 50 points for a lab report you should substantially increase your efforts for subsequent labs / lab reports. Points assigned for the various sections of the lab reports (see below) will used to assess whether the student has achieved the various Goals listed under 'Learning Outcomes'.

Textbook:
There is no required textbook. Notes and instructions for the experiments will be provided by the instructor or the TAs. For background information not provided in the handouts see your Physical Chemistry textbook that you use (or used) for CHE 319 / 320 or CHE 349.

Lab Reports: The preparation of the Lab Reports is an essential component of CHE 329 — equally important as performing the experiments. Lab Reports are examples of the kind of technical writing that is very likely going to be part of your future professional experience, whether you will work in industry, academia, or for the government. The data analysis part, and the discussion of the results, will help to develop your analytic thinking and scientific reasoning.

Students work in pairs in the Lab and when preparing the Lab Reports. The two lab partners submit one jointly prepared report which is due two (2) weeks after the day the experiment is performed. Late reports involve a penalty of 20 points per week late (20 points for 1 to 7 days late, 40 points for 8 to 14, and so on). Lab reports will not be accepted past one week after the last day of classes. *Plagiarism and other cases of academic dishonesty will lead to severe penalties* (gen-

erally, zero points for the Lab Report, but in serious cases the instructor or grader will deduct an additional penalty and/or file an academic dishonesty report). Make sure you know the guidelines for academic integrity. See http://undergrad-catalog.buffalo.edu/policies/course/integrity.shtml . Lab Reports can be picked up from the TA offices at the end of the semester.

Lectures: Attendance is required at the scheduled lectures, and potentially when additional special lectures are announced on days for which a student is not assigned to perform one of the Lab experiments. Lecture subjects include physical chemistry background relevant to the experiments, and potentially some additional lectures on statistics and error analysis.

Required Experiments:

1. Carbon Dioxide Critical Point: Measure the critical temperature and density of CO_2 and the vapor–liquid coexistence curve in the region just below the critical point, and relate the result to Wilson's theory of critical exponents.

2. Virial coefficients of real gases: Measure the second and third virial coefficient of He or Ar, and CO_2, around room temperature.

3. Bomb calorimetry: Measure the heat of combustion using a Parr adiabatic calorimeter, and determine the related enthalpy changes.

4. UV-Vis absorption spectroscopy and the 'Particle in a Box': Principles of absorption spectroscopy. Quantum mechanical particle in a box, quantized energy levels, absorption and color, Beer's law.

5. Computer Simulation of the Vapor–Liquid equilibrium (VLE) of Carbon Dioxide using fitted data for the Virial coefficient (Virial-VLE module). This simulation links experiments 1 and 2 and demonstrates how attractive and repulsive potentials between molecules of a non–ideal gas influence its physical behavior.

Computer simulations: The software needed for the computational project (5.) is a Java program that can be executed from within a web browser, or you can run it on your own computer. You need the *Java run–time environment* (JRE), which can be downloaded from http://www.java.com/en/download/manual.jsp
If you don't have a computer you can use one of UB's public computers in the library or in one of the computer rooms listed here: http://ubit.buffalo.edu/sites/

Students with special needs: Please inform the instructor of any special needs and register with the Office of Accessibility Services (ODS) as soon as possible. See http://www.student-affairs.buffalo.edu/ods/ for details.

Structure of a Lab Report: Scientific writing is very *structured*. Your report should have *numbered* sections with short section titles such as 'Background', 'Experimental Setup', 'Results', 'Discussion', 'Conclusions', or similar, numbered figures *with captions*, and numbered tables with captions. The pages must also be numbered. A sample structure of a Lab Report is:

Cover page: Name of the experiment, name of students, date experiment was performed, date when the report is submitted.

Reports of more than six pages require a Table of Contents. Optional: Short abstract (150 words or less). Sections may be arranged as follows:
1. Introduction, Background: Why is this experiment important, what can be learned from it? Provide relevant equations and discuss the theoretical foundation of the experiment.
2. Experimental setup / Computational details: Describe the experimental setup and procedure, or the software used to perform calculations.
3. Results: Provide the results of the measurements that you obtained, and describe how the data was processed further. Experimental and calculated data, as well as results derived from them, have *units*, which must be provided. If you don't provide units for each number the Lab Report is going to receive a low score. For measured data and derived data also provide estimated error bars.
4. Discussion: Discuss the results of the measurement, and any additional questions, topics, and discussion points mentioned in the Lab instructions. Sometimes it is easier to have combined Results and Discussion sections, but if you combine them you need to be particularly careful about structuring them properly. Use subsections if appropriate.
5. Conclusions / Summary: Each technical report should end with some final conclusions or a concise summary of the results that were obtained (this is not a copy of the Abstract).

Figure and Table captions should give a short description so the reader has some understanding of their content without reading the text. For tables, the units for all data should be provided in the caption or in the column headers. Units for data plots should be included with the axis labels (axes always need to be labeled). Figure captions are usually placed below the figure, while table captions are above the table. An example for proper Table formatting is shown below:

Table 1: Density ρ of Compound *A* as a function of temperature.

T / K	ρ / g cm^{-3}
275	0.93
283	0.95
...	...

Make sure that each figure and each table that you provide is referenced by its number in the text and discussed appropriately.

Equations should be numbered consecutively as well, such as follows:

$$E = mc^2 \tag{1}$$

References in the text made to the equations should use these labels in parentheses.

It is very important that any source of data, or other references such as the textbook or on–line sources used to prepare the Background section are properly cited at the end of the lab report. If you quote from a source, clearly indicate this (e.g. by using quotation marks or italic font, with a reference to the source).