

Course title: Physical Chemistry Laboratory I (2 credit hours)

Experiments in physical chemistry.

One three-hour laboratory and a single one-hour lecture a week.

Prerequisite, Chemistry 481; prerequisite or corequisite, Chemistry 482.

(Note: it is an Honor Code violation to register for a class for which you do not have the necessary prerequisites.)

Instructor: Carribeth Bliem

Office: A5 Venable Hall, 962-6194

Office hours: 1:30 pm Tuesday, and by appointment

Email: cbliem@unc.edu

I try to respond to email questions within 24 hours, and I will post useful questions on blackboard's discussion board.

Class meetings: Recitation, T, 12:30 pm, Chapman 125

Lab, one day/week, 2:00 – 4:50 pm, Morehead 213

Course mission

The purpose of this course is to provide students with opportunities to use computers to solve numerical problems in chemistry that would be too onerous to approach by hand. We will solve problems in thermodynamics and quantum mechanics.

To that end, we will use:

- Virtual Substance, a molecular dynamics simulation program that allows one to set parameters of a system and watch the dynamics unfold;
- Excel or another spreadsheet software;
- Mathcad, a mathematical software that enables general calculations; and
- PC Spartan, a molecule-building software that provides fundamental characteristics of molecules.

Course structure

Lab time (2:00-4:50) will be run as a help center. Each lab day, TAs will be available to assist students as they work to complete the lab protocol and think about the lab write-up. Lab write-ups will be due at the beginning of lab, with specific dates given with each lab module (typically one week after a module is completed); prelab questions (as applicable) should be handed in with the same lab's write-up.

Tuesday recitations will allow for general discussion of concepts, both chemical and computational.

Final Exam

The final exam will be held on Tuesday, December 11, at noon, in Chapman 125.

Textbook and materials

- Virtual Substance 081704.exe (required, available to download at <http://www.unc.edu/~jpapanik/VirtualSubstance/VGMain.htm>)
- Mathcad software or another mathematical software (required, Mathcad available to purchase at ChemStore, first floor of Venable)
- PC Spartan Plus software (required, will be installed in lab)
- Physical Chemistry, by Peter Atkins (recommended)

Blackboard

This class will use the Blackboard e-Education platform (<http://blackboard.unc.edu>) to post announcements, assignments, and suggested readings. Please check Blackboard daily because I will send class emails, post questions/answers, announcements, and assignments during the semester.

Course evaluation

Weekly lab write-ups (11 points each)	11 weeks x 20 points =	220 points
Final exam (20 points)	=	20 points
	Total	240 points

Total number points will be converted to a percentage score, and letter grades will be assigned as follows:

- A: 90-100%
- B: 80-89%
- C: 70-79%
- D: 60-69%
- F: < 60%

Weekly lab write-ups must be limited to five pages (single-spaced, 11 or 12 point font, 1 inch margins) including pertinent embedded graphs (4" x 4"). Each lab will address a set of research questions; your write-up should include the following:

- state those questions in your own words (2 pts);
- describe experimental protocols used to analyze the question (6 pts);
- discuss relevant findings (8 pts); and
- provide a conclusion section that answers the research questions (4 pts).

In the write-up, content is key but presentation matters as well. Therefore, you should answer all questions listed in the lab protocol using complete sentences, coherent arguments, and graphs as necessary to substantiate your claims. However, you should be succinct and only include remarks that pertain to the questions asked.

Attached to the five-page write-up, you should append the following:

- answers to applicable pre-lab questions, derivations;
- a presentation-quality Mathcad (or Excel) worksheet that documents your data analysis.

If you miss a lab period due to illness or other difficulty, you should contact me to schedule a make-up opportunity. Only under the most dire circumstances will lab write-ups be excused.

Computer upkeep

It is your responsibility to make sure that your laptop is running smoothly. Both Mathcad and Virtual Substance CAN run on the four-year old CCI computers you may have, but the laptops must be in good working order to have success. So, if your computer crashes regularly or if weird windows and errors pop up, take your laptop to the IT Response Center, located in the lower level of the R.B. House Undergrad Library (next to the Pit), for 24-hour technical support via phone (962-HELP). Walk-in support is offered Monday-Thursday, 7:30 am – midnight, Friday 7:30 am – 5:00 pm, and Sunday 3:00 pm – midnight.

First class

The first recitation meeting will be held Tuesday, September 4, in Chapman 125. We will review the course syllabus and talk about the role of computers in physical chemistry research as well as scientific ethics.

Course calendar

All lab weeks begin on Tuesday and end on Friday. Weekly lab write-ups are generally due one week after each lab is completed; specific due dates are listed on each lab module.

Week	Lab Module	Due Week of:
9/4	(1) Intro to Virtual Substance	9/11
9/11	(2) Maxwell Distribution	9/18
9/18	(3) Thermodynamic properties of gases	9/25
9/25	(4) Properties of real gases	10/2
10/2	(5) Structure of polymer chains	10/9
10/9	(6) Structure of solids and liquids	10/16
10/16	(7) Using mathematical software	10/30
10/23	No labs – Fall Break	
10/30	(8) Molecular Orbital treatment of H_2^+	11/6
11/6	(9) Potential energy curve for H_2^+	11/13
11/13	(10) Vibrational levels of H_2^+	11/27
11/20	No labs – Thanksgiving	
11/27	(11) Ammonia inversion	12/11 all sections

First lab

Lab sessions begin the week of September 4. Students should arrive at Morehead 213 on their scheduled day with their laptop, internet cable, CD drive, prepared to complete Lab Module #1 – Introduction to Virtual Substance.

Honor Code

Policy adopted by the faculty of the Department of Chemistry on September 9, 1977:

“Since all graded work (including homework to be collected, quizzes, papers, mid-term examinations, final examinations, research proposals, laboratory results and reports, etc.) may be used in the determination of academic progress, no collaboration on this work is permitted unless the instructor explicitly indicates that some specific degree of collaboration is allowed. This statement is not intended to discourage students from studying together or working together on assignments which are not to be collected.”

When you sit down to type up the weekly write-ups, you must do your own work. The exercises required for this class are intended so that your understanding at the end of the course will be proportional to the effort you put into it.

Unless explicitly stated in the lab procedure, students MAY NOT share data.

Acknowledgements

The authors of the individual Mathcad documents are indicated on those units. As lab modules for this course continue to evolve, specific faculty authors are listed where appropriate.