CHEM 161 - Quantum Chemistry
(quantum mechanics and chemical applications)
Fall 2012, MWF 9:35 - 10:25 AM, Angell B-203

Prof. W.R. Leenstra

Introduction

Chem 161 is one-half of the year-long course in physical chemistry and covers quantum mechanics and its applications to chemistry, as well as some statistical mechanics if time allows. (The companion course, Chem 162, covers thermodynamics and kinetics.) In this course, the general objective is to understand the underlying theory of many of the facts and rules you have learned in previous chemistry courses. This essentially entails math/physics material, rather than considering chemistry in the form of molecules and their reactions. For example, it is a fact that atomic orbitals are the basis of bonding, but do you know why a p-orbital has a "dumbbell" shape? [This was not plucked out of thin air.] It is also a fact that bonding is the basis for chemical reactions, but do you know why two hydrogen atoms would rather get together to form a molecule than exist apart? [Saying that two orbitals "overlap" is fuzzy, and is not a real answer.] It is the goal of this course to help you to understand how this discipline provides clear answers to the above questions, and in the process, demystify quantum mechanics for you.

Prerequisites

The prerequisites for the course are second-semester Physics (either 12, or 42, or 152), and concurrent enrollment in Math 121 or the special math prep course, Chem 167, which is a scaled-down version of Math 121 with just the pertinent topics presented. Regarding the latter, Chem 167 will prepare you better for this Quantum Chemistry course than will Math 121, so if you have a choice, I'd recommend that. But to reiterate, you must have under your belt one year of physics and one-plus years of calculus. Although your conceptual understanding of the subject matter is more important to me than being able to crank out mathematical calculations, the two cannot be separated. If you don't have a good grasp of the math or physics underneath the subject material, you may have serious difficulties. If you do have the appropriate background, being a little foggy on the details can certainly be remedied by reviewing your earlier class material, or by stopping by my office to see me.

Minor in Chemistry

If you are enrolled in this course to satisfy the Chemistry minor you must, of course, satisfy the prerequisites. If you do but you feel apprehensive about your math/physics background, I strongly urge you to consider one of the less mathematically challenging courses such as, for example Quantitative Analysis (Chem 121), which is offered this semester, MWF 12:50-1:40, or Chem 131 (Inorganic Chemistry) next semester.

Topics

The topics, in order of discussion, are as follows. Lecture numbers are very approximate.

- Background and the Schrodinger Equation — Lectures 2-6
- Particle in the Box — Lectures 7-10
- Harmonic Oscillator and Rigid Rotor — Lectures 11-15
- Hydrogen Atom — Lectures 16-20
- Multi-Electron Atoms — Lectures 21-25
- Molecular Bonding — Lectures 26-32
- Spectroscopy — Lectures 33-40

Textbook

Our textbook this year will again be "Physical Chemistry" by David Ball (1st edition). We will cover chapters 9-14, some completely and some more sporadically. While this textbook closely approximates my pedagogic approach, you should understand that for most upper level courses the textbook is an aid, not the "bible". Depending on the material/chapter, various sub-topics will not be covered in class (or the reverse). The rule of thumb to use in this course is that if a concept is not discussed in lecture, you don't need to know the corresponding passage of a chapter unless I assign some reading on your own. Conversely you are responsible for all material discussed in class. Also, be aware that much of the content may be presented by me differently from the way the author has done a given topic. Having said all this, I want to emphasize that trying to learn the subtleties of quantum mechanics just from attending lectures and reviewing my notes is probably not going to cut it. There is real value to reading a textbook with wording that is different from the way the instructor presents it – and it is a good book to reference for any future chemistry topic.The UVM Bookstore sells this book for ~$137 in the form of a high-quality used copy. On the other hand, I have seen copies for sale on the internet (e.g., Amazon.com) for less than that.

Also, there exists a Student Solutions Manual which shows the worked-out solution to every odd-numbered problem in the back of each chapter. This book is not required because I will xerox, and make available, every problem that I assign. But if you do want your own copy, it can be found on the internet as well.

Responsibilities

Attendance. From the above, it should be very clear that missing a lecture (or spacing out on one) can be extremely detrimental to your continued understanding of the material. Thus, I expect perfect attendance. If you have a valid, serious reason to be absent, you must call me beforehand. It will be up to you to get all the information presented at the missed class.

Preparation. Secondly, I expect you to come prepared for each lecture by having read ahead in the textbook. The lectures won't seem so mysterious if you know what is coming. If I find that the class, in general, is not keeping up with the outside reading, I may "pop" a quiz on you.

Participation. Finally, I expect you to participate in class by being alert and ready to answer questions. I find it personally insulting to see you spacing out, looking off into space, or exhibiting a case of "sleepy eyes". This expectation falls in the rubric of common courtesy or mutual respect. Please make a determined effort to absorb all the information from each lecture.

Grading

Exams. We will have three semester exams at approximately equal intervals. From experience, I know that students appreciate not having the one-hour time constraint for their exams. Instead, I will design exams that could be finished in just over an hour but give you two hours, and have them outside of lecture's class times. I have tentatively scheduled them on Tuesday evenings from 7 PM till 9 PM. What you are responsible for does not include the previous Monday's lecture material. The three exams are spread out as evenly as possible on the following schedule:

Exam 1 — September 25 (covering Lecture #1 through Lecture #11)
Exam 2 — October 23 (covering Lecture #12 through Lecture #23)
Exam 3 — November 27 (covering Lecture #24 through Lecture #35)

If your schedule does not fit with this, I will allow some flexibility in your exam start time on those days. Exams count as 100 points each, for a total of 300 points. In general terms, on exams will appear calculational problems, short-answer questions, longer-answer explanations, and multiple choice questions. Two related issues to keep in mind are that I will not discuss exam material on the day of the exam, and that my standing policy is that no make-up exams will be given.

Homework. The content in this course is pretty challenging, and can not be mastered without blood, sweat, and tears as you review the material and do the homework problems. I will assign homework problems topically when we start a new topic (trying to use even-numbered problems). Then every Friday I will designate a few (1-3) to be turned in by the start of class on the following Monday. These will be graded as follows:

A: Perfect in content and presentation, i.e., could be used as the key (4 points)
B: Imperfect content or presentation (3 points)
C: Imperfect content and presentation (2 points)
D: Incomplete work (1 point)
F: Did not turn in work (0 points)

I will collect 12 HW sets, with the first one to be assigned Friday, September 7. With a base of 2 points you will be able to garner 50 points for the homework category (i.e., the weight of half an exam).

Answers will be posted on Blackboard. It goes without saying, however, that actually doing the problems on your own firms up the knowledge that is in your head.

Final. Our final exam is scheduled for Friday, December 14, at 1:30 PM. It is cumulative (comprehensive) in nature, and multiple-choice in format, worth 200 points. Please get your travel plans in order right away with this date in mind.

Grade. Your grade for the course will be based on the total number of points you accumulate out of 550, relative to the class average. Thus, there is no meaningful letter grade that can be assigned to any one exam. I can only indicate approximate ranges based on a "curve". Although I cannot at this time predict the difficulty of the exams and the overall strength of the class, I can say that the average score for the course has usually been around 65%. In a large statistical sample, for this course the average performance falls on the B-/B border. But please note that the average could also be a little lower or higher, depending on the overall performance of the class. This grading scheme is based on the assumption that attendance is perfect, and that students come prepared and are engaged.

Office Hours and Outside Help

My office is Cook A-119. I will be available in my office Monday, Wednesday, and Friday, 10:30-11:30 AM. You are welcome to just stop by my office during these times, but it would be even more efficient if you let me know that you will be coming in, and what I can help you with. If these times are not suitable for you, we can also set up an appointment at another, mutually convenient time. I encourage you very strongly to use me to clear up difficulties the material as soon as possible. Obviously, the next lecture will be that much easier to follow. The only time I will not answer questions is on the day of the exam because I want to discourage "cramming" at the last moments. Also, in addition to the above, you can call me at 656-0273, or use e-mail (*willem.leenstra@uvm.edu*) for quick consultations. You will find that I am exceedingly available. Review sessions may be scheduled if student demand warrants it. Organize it yourselves, and contact me.

Class Notes

My own experience tells me that it is hard to follow the thread of a discussion if you are furiously copying from the blackboard. Instead, I will have available on the web, via Blackboard, copies of my notes after each lecture. This allows you to just listen (or take skeleton notes) and possibly stay engaged easier. If, however, you are the type of student who learns better by taking your own notes, you should of course do so, and then use my notes as a backup.

Math Preparation

As mentioned previously, the math-preparation companion course to Chem 161 is Chem 167, Physical Chemistry Preparation. This class nominally meets MW at 4:05-5:20 PM in Angell B-104, starting on Wednesday, September 7. (Time may be changed if a better schedule can be found.) Unless you have already taken this course (or Math 121), everyone is expected to participate in this class or be enrolled in Math 121. If you feel weak in math, you should audit Chem 167. Even if not, this mini-course will be a boon to your understanding of Chem 161.