CHEM 3010: Physical Chemistry

Introduction to Quantum Chemistry,
Spectroscopy,
& Statistical Thermodynamics

Course Outline, Winter 2016

prerequisite: CHEM 2011

Instructor: René Fournier, Petrie 303, renef@yorku.ca, phone ext. 30687

Required Text: *Physical Chemistry* (PC) by Thomas Engel and Philip Reid (Pearson Prentice Hall) 3rd edition (2013), ISBN-10: 0-321-81200-X ISBN-13: 978-0-321-81200-1.
This book is also available as two separate parts: TSTK "Thermodynamics, Statistical Thermodynamics, & Kinetics" and QCS "Quantum Chemistry & Spectroscopy". In CHEM 3010, we will cover roughly chapters 12 to 23 and bits of chapters 25, 30, 31 and 32 of PC. This corresponds to chapters 1 to 10 and chapter 14 of QCS, and bits of chapters 13, 14, 15 of TSTK. TSTK (or PC) is required for CHEM 2011 and CHEM 3011. So, if you have TSTK, but not PC, you can buy the other part (QCS) and you will have everything.

Course web site: go to www.yorku.ca/renef and follow the CHEM 3010 link.

Lectures: LSB 105, MWF 10:30–11:20
Office hours: Petrie 303, MWF 13:00-14:00

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and
http://secretariat.info.yorku.ca/senate/academic-standards-curriculum-and-pedagogy-committee/

Topics covered: quantum mechanics, the particle in a box, vibrational and rotational spectroscopy of diatomic molecules, the hydrogen atom, many-electron atoms, H_2 and the chemical bond, electronic spectroscopy, the Boltzmann distribution, partition functions, statistical thermodynamics — the bridge between the microscopic and macroscopic views of matter.

Evaluation

Two tests: 50% (25% each)
Final exam: 50%

The two **tests** will be 50 minutes long and worth 25 marks each. They will be held during class time on **Friday February 5** and **Friday March 11** (dates to be confirmed). The **final exam** in April will be 3 hours long. If you miss a test your marks will be shifted to the final exam. If you miss both tests, your final exam will be worth 100%.

Organization of the course

You may wish to take notes during class. But I don't advise you to write down everything I show. It is more important to *listen* to what I say in class and try to follow "in real time" than writing down everything. My lecture notes, and yours, are only summaries and comments about the book's content, they are not a substitute for it. From time to time, I will post my notes on the Web, *after* the lectures based on those notes. Do *not* rely on notes I will post on the web:

1. the book is more complete and more accurate than my notes.
2. a set of lecture notes from the Web might give you a false sense of security and make you believe that you can safely skip classes: you can not.
3. I often make changes or additions to my lecture notes in class, especially figures. I will not be able to ensure complete consistency between the web pages and what I show in class.

I will assign problems from time to time. Those assignments will not be marked, but they are very important. They should be an essential element for you to study in preparation for the tests and exam.

As a rule, you should count roughly two hours of study and practice (e.g., assignments) for every lecture hour.

Important dates:

Monday February 15 to Friday 19 — reading week, no class
Friday March 4 — last date to drop a course without a grade
Friday March 15 — Good Friday, no class
Monday April 4 — last day of class