

# CHEM 2010 — Symmetry, Electronic Structure and Bonding

## Winter 2010

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Course web site: go to [www.yorku.ca/renef](http://www.yorku.ca/renef) and follow the CHEM 2010 link.

Required Text: *Physical Chemistry* (PC), Thomas Engel and Philip Reid (Pearson Prentice Hall) preferably the 2nd edition (2010); or the second half of PC, *Quantum Chemistry and Spectroscopy* (QCS) 2nd edition (1st edition is OK too), Thomas Engel (Pearson, 2010).

**Note:** the first chapter of QCS corresponds to chapter 12 in PC.

Lectures: Stedman F, Mon/Wed/Fri 10:30–11:20

Tutorial: Stedman A, Friday: 14:30–15:20

Office hours: Petrie 303, Wednesday 13:30–14:30, or by appointment.

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Topics covered: Quantum Theory, Atomic Structure, Molecular Electronic Structure and Bonding, Symmetry, Applications of Symmetry to Bonding and Vibrations.

### Evaluation

Two tests: 50% (25 marks each)

Final exam: 50% (or 75%, or 100%, whichever works to your advantage, see below).

The **tests** will be 50 minutes long and worth 25 marks each. They will be held during class time on **Friday February 5** and **Wednesday March 10**.

The **final exam** will consist of four parts worth 25 marks each: (1) the 1st part will cover the same things as test #1 (roughly the first 4 weeks of lecture material); (2) the 2nd part will cover the same things as test #2 (roughly weeks 5, 6, 7 and 8); (3) the 3rd part will cover material seen in class after test #2 (roughly the last 4 weeks of lecture); (4) the 4th part will cover all of the material. Questions in parts (1), (2), (3) will be in the format of “multiple choice”, or “short answer”, or will require a simple calculation that makes direct use of a formula. Part (4) will have tougher questions: problem solving, open-ended questions, etc.

**The final numerical grade in the course** will be calculated by adding four marks:

- ★ your mark in test #1 **or, if is better**, your mark in the 1st part of the final, out of 25;
- ★ your mark in test #2 **or, if is better**, your mark in the 2nd part of the final, out of 25;
- ★ your mark in the 3rd part of the final exam, out of 25;
- ★ your mark in the 4th part of the final exam, out of 25.

If you miss a test, you will have zero on that test. I will not look at excuses or notes from doctors or others. If you miss both tests, you get zero on both: it means that your final exam will be worth 100%. I strongly advise that you write both tests. This gives you two chances to show that you know the material — on the test, and in the final exam (part 1 or 2).

## Organization of the course

It is *essential* that you read the material to be covered in class *ahead of time*. Please refer to the *reading assignments schedule* below. I will spend very little time on definitions, notation, and derivations in class. You should become familiar with these things by reading Engel & Reid ahead of lectures. Problem solving is important but we will spend very little time on that in class: it is something you must practice by yourself throughout the term. I will assign problems from the book from time to time. *So what will we do in class?*

- I will explain the most important concepts and try to do it differently than in the book. I will not cover all of the assigned reading material, but all of it is testable material.
- I will give analogies, examples, and calculations to put things in context.
- I will sometimes go over topics in mathematics that you need for the course.
- I will go over a few additional applications of symmetry.

You may want to take some notes during class. But bear in mind that your lecture notes can only be a supplement to the book, they can not be a substitute for the book.

The *tutorials*, on Friday afternoon, will be for review (or overview) of topics in mathematics needed for the course, and for help with the assigned problems. I will give mini-lectures on topics in math that may not be familiar to you but are essential for this course. At the same time, teaching assistants will go around and help with the assigned problems on an individual basis.

## Week-by-week Reading Assignments Schedule

Chapter and page numbers differ between *Physical Chemistry* and *Quantum Chemistry and Spectroscopy*, and between the 1st and 2nd editions, so I am only giving chapter titles. The material presented in lectures in a week will *roughly* correspond to what is assigned “*prior to Monday*” of that week. I want to emphasize that *everything in the assigned reading material can be tested* on the quizzes and final exam, even if it is not discussed in class. Some of the material covered in class will not be explicitly in the book (for ex., some math, some applications of symmetry), but if it is covered in class, it is “testable material”.

Read *prior to Monday, January 11*: the chapters *From Classical to Quantum Mechanics* and *The Schrödinger Equation*

Read *prior to Monday, January 18*: *The Quantum Mechanical Postulates* and first two sections of *Using Quantum Mechanics on Simple Systems*

Read *prior to Monday, January 25*: rest of *Using Quantum Mechanics on Simple Systems* and first three sections of *The Particle in a Box and the Real World*.

Read *prior to Monday, February 1*: Sections 4, 5, and 6 of *The Particle in a Box and the Real World*, and sections 1 and 6 of *A Quantum Mechanical Model for the Vibration and Rotation of Molecules* (the two sections about the Harmonic Oscillator).

Read *prior to Monday, February 8*: *The Hydrogen Atom*.

Read *prior to Monday, February 22*: *Many-Electron Atoms*.

Read *prior to Monday, March 1*: *The Chemical Bond in Diatomic Molecules*.

Read *prior to Monday, March 8*: sections 1, 5, 7, 8 and 9 of *Molecular Structure and Energy Levels for Polyatomic Molecules*

Read *prior to Monday, March 15*: first three sections of *Molecular Symmetry*

Read *prior to Monday, March 22*: remainder of *Molecular Symmetry*