CHEMISTRY 331 / F09
Quantum and Statistical Mechanics

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Office Hours: W 2:00-3:00 CSB , R 1:30-3:30 WSC (or by appointment)

> *"During recent years it has come to be more widely recognized in our Universities and Colleges that the course of study for students of Chemistry, no matter what special branch of the subject they may intend to devote themselves later, cannot be regarded as complete or satisfactory unless it include both systematic and practical Physical Chemistry."*[1]

CHM 331 is the first course in a two-semester sequence which introduces the application of physical and mathematical methods to the investigation of chemical systems. CHM 331 will introduce students to the theoretical and experimental foundations of quantum theory as it applies to atomic structure, molecular electronic structure, symmetry, and spectroscopy. Students in CHM 331 will also be exposed to the theoretical and experimental bases of statistical mechanics and their relevance to chemical systems. Throughout the semester students will be introduced to topics from advanced mathematics necessary to solve problems in physical chemistry. Students are expected to already have a foundation in chemistry (CHM 111/112), single variable differential and integral calculus (MAT 191/192), as well as classical dynamics, electromagnetism, and wave phenomena (PHY 161/162). Upon completion of this course, a student will demonstrate competence in each of the following areas:

- utilizing physical reasoning to derive and solve mathematical representations of chemical phenomena,
- utilizing available resources and tools to understand and solve physical chemistry problems,
- understanding chemical concepts from the lecture by successfully applying these concepts on homework and tests.

Class Meeting Times and Locations
Lecture: MWF 11:00-11:50 a.m., WSC Room 322

Course Materials
Physical Chemistry, Alberty and Silbey, 4th ed.,
The Chemistry Maths Book, Steiner, 2nd ed.
Scientific Calculator

Course Structure

Seven chapters of the text will be covered during the semester in the order listed on the class schedule. Additional material will be provided by the instructor. The lecture time will be used to expound on and augment the text and also discuss problem solving strategies. Students are responsible for all material covered in class as well as the material from the textual sections listed in the class schedule and materials indicated by the instructor. Exams will consist of two evening tests and the final. There will be regularly assigned homework.

[1] Alex Findlay. *Practical Physical Chemistry*, 1906

Grading

Evening Exams (2 @ 250 pts)	500 pts
Homework/Capsules (11 @ 25 pts)	275 pts
Final Exam	225 pts
Total Possible	1000 pts

The following grading scale is assured but *may* be *slightly* lowered based on test results.

A $\geq$880 pts
B $\geq$760 pts
C $\geq$640 pts
D $\geq$520 pts
F $<$520 pts

General Information

Honor Code: All students in CHEM 331 are expected to adhere to the Mercer University Honor Code. Any suspected violations will be reported to the Honor Council for further investigation.

Attendance: Except for the first day of the semester, attendance will not be taken. Students are expected to be in class and are accountable for all material covered in class as well as any announcements made during the lecture period. If you think that you might have the H1N1 virus, please contact me via e-mail and then contact Student Health Services and the associate Dean of CLA via phone.

Missed Exams: Anyone missing an exam for *any* reason (personal illness, death in the immediate family, or other emergency) must notify Dr. Pounds in advance. The absence will be considered unexcused otherwise. Make-up exams will be individually scheduled.

Partial Credit: Partial credit will not be awarded on any exam or homework unless individuals show their work and clearly delineate how they arrived at their answers.

Re-grading Policy: If a student suspects that an error was made in the grading of a submitted work, they may return the paper for re-grading with the understanding that the entire work will be re-graded and not only the portion in question.

Evening Exams: Two evening exams will be given. These will be open-resource exams where "resource" refers to any available non-living item in the Willet Science Center which meets the approval of the instructor. The exam dates are listed in the schedule. The exam period will start at 6:00 pm and conclude at 10:00 pm. THERE WILL BE NO CLASS ON THE DAY OF THE EVENING EXAM.

Mathematical Tools Capsule: You will quickly need to become adept at using several pieces of mathematical software. Primary among these are *MuPAD*, *Mathematica*, and *Excel*. This capsule will introduce and enhance your knowledge of these software tools. It will be due on September 21$^{\text{st}}$.

Group Theory Capsule: Sections from chapter twelve of the text (Symmetry) will be completed outside of class as independent study. Homework from this capsule will be due on October 5$^{\text{th}}$

Computational Chemistry Capsule: A group of computational chemistry modules from the *SHODOR* Computational Science website will be completed to enhance you knowlege of this specific field of chemistry. In addition you will be asked to complete a small calculation on a molecule. Homework from this capsule will be due on November 9$^{\text{th}}$.

Homework: Students are encouraged to work together on homework assignments. Each person, however, must turn in their own assignments in their own words. Submitted work must be turned in **USING ONLY THE FRONT SIDE OF THE PAPER** with problems in the order that they appear on the assignment sheet. In some cases students will be asked to submit items electronically. *Homework Grading Policy:* Homework problems

will typically be divided into two sections: book problems and special problems from me. Individual problems from the book will be graded on a three point scale and the composite score from all problems on a given assignment converted to a 15 point scale. Points will be awarded as follows: 3 (essentially correct), 2 (minor errors or omissions), 1 (major errors or omissions), 0 (no effort). The point breakdown for problems from me will be indicated on the homework handouts and the composite score converted to a 10 point scale. Each homework assignment is worth a total of 25 points. Homework will be considered late if it is not turned in by 5:00 p.m. on the date due. Late homework will be penalized 33% per day.

Seminar Attendance: Througout the semester there will be a few seminars that will contain information specifically designed for your class. The time and place of these seminars will be arranged in accordance with your schedules and attendance is mandatory.

American Disability Act: "Students with a documented disability should inform the instructor at the close of the first class meeting or as soon as possible. If you are not registered with Disability Services, the instructor will refer you to the Student Support Services office for consultation regarding documentation of your disability and eligibility for accommodations under the ADA/504. In order to receive accommodations, eligible students must provide each instructor with a Faculty Accommodation Form from Disability Services. Students must return the completed and signed form to the Disability Services office on the 3rd floor of the Connell Student Center. Students with a documented disability who do not wish to use accommodations are strongly encouraged to register with Disability Services and complete a Faculty Accommodation Form each semester. For further information please contact Disability Services at 301-2778 or visit the website at `http://www.mercer.edu/stu_support/swd.htm`."

Electronic Submission of Materials: "Students bear sole responsibility for ensuring that papers or assignments submitted electronically to a professor are received in a timely manner and in the electronic format(s) specified by the professor. Students are therefore obliged to have their e-mail client issue a receipt verifying that the document has been received. Students are also strongly advised to retain a copy of the dated submission on a separate disk. Faculty members are encouraged, but not required, to acknowledge receipt of the assignment."

Cell Phones and Pagers: "Out of courtesy for all those participating in the learning experience, all cell phones and pagers must be turned off, or placed on vibrate, before entering any classroom, lab, or formal academic or performance event."

E-mail Listserve: I communicate heavily with the class (and encourage you to do the same) via an e-mail listserve which I maintain myself. Please subscribe to the listserve by going to

`http://theochem.mercer.edu/mailman/listinfo/chm331`

and filling out the required fields. Once subscribed, you may send e-mail to the class by using the e-mail address `chm331@theochem.mercer.edu` I personally moderate all requests to limit e-mail spam.

Tentative Class Schedule[2]

Week Starting	Chapter Sections	Lecture and Problem Solving Topics
August 23rd	9.1, Handouts	Mathematical Preliminaries, Computational Tools Quantum Theory
August 30th	9.2–9.5	Schrödinger Equation Operators and Expectation Values
September 6th	9.10–9.15	**Labor Day – 9/7/08** Model Potentials Angular Momentum The Postulates
September 13th	10.1–10.9	Atomic Structure Orbital Angular Momentum Electron Spin Variation Method
September 20th	10.10–10.15, 11.1	**Math Tools Capsule Due (Sept. 21)** The Hartree-Fock Method Molecular Electronic Structure
September 27th	11.2–11.8	**EXAM #1, 9/28/09** Born-Oppenheimer Approximation
October 4th	11.9–11.10	Molecular Orbital Theory **Group Theory Capsule Due (Oct. 5)**
October 11th	13.1 – 13.6	Selection Rules Rotational Spectroscopy **FALL BREAK**
October 18th	13.7-13.8	Vibrational Spectroscopy Rotational-Vibrational Spectroscopy Raman Spectra
October 25th	13.9, 14.1–14.3	Electronic Spectroscopy **Withdrawal Deadline 10/29/09**
November 1st	14.4–14.10	Spectrophotometers and LASERS Photoelectron Spectroscopy
November 8th	16.1	**Computational Chemistry Capsule Due (Nov. 9)** Review of Probability Introduction to Statistical Mechanics
November 15th	16.2 – 16.4	**EXAM #2, 11/16/09** The Boltzmann Distribution Independent Particle Approximiation
November 22nd	16.5 – 16.10	Partition Functions **THANKSGIVING**
November 29th	16.10	Ideal Gases Direct Calculation of Thermodynamic Quantities
December 6th	16.10 – 16.13	Direct Calculation of Equilibrium Constants Equipartition Statistical Ensembles REVIEW FOR FINAL
December 13th	16.11 – 16.13	**FINAL EXAM, 12/17/09, 9 a.m.** (Thursday)

[2]I reserve the right to modify this schedule as situations warrant.