

CHEMISTRY 331 / S17

Quantum and Statistical Mechanics

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“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 9:00-9:50 a.m., WSC Room 109 or 336

Course Materials

Physical Chemistry, Engel and Reid, 3rd ed.,
The Chemistry Maths Book, Steiner, 2nd ed.,
Mastering Chemistry online key
Scientific Calculator

Course Structure

Portions from 20 chapters of the text will be covered during the semester. Supporting mathematical material will also be used from the ancillary text. Additional material will be provided by the instructor as applicable. The lecture time will be used to expound on and augment the texts, discuss problem solving strategies, and to learn how to effectively utilize the provided computational tools. Students are responsible for all material covered in class, material from the textual sections denoted by the instructor and other materials as indicated by the instructor. Exams will consist of two evening tests and the final. There will be regularly assigned homework, online graded homework, and three self-guided capsules.

¹Alex Findlay. *Practical Physical Chemistry*, 1906

Grading

Evening Exams	50%
Online Homework	5%
Homework	10%
Capsules	15%
Final Exam	20%

Total Possible 100%

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

A	≥88%
B	≥76%
C	≥64%
D	≥52%
F	<52%

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: Attendance will be taken the first 10 class periods. Attendance will not be taken after that point. 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 know that you are going to miss class, please send me a text or e-mail to let me know about your absence.

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 will be coordinated with all students and a two week notice will be given before the exam date is set. The exam period will start at 6:00 pm and conclude at 10:00 pm. These exams are tentatively scheduled for **February 20th** and **April 10th** THERE WILL BE NO CLASS ON THE DAY OF THE EVENING EXAM.

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 the problems IN THE ORDER THAT THEY APPEAR ON THE ASSIGNMENT SHEET**. Students submitting work not adhering to this formatting will be asked to resubmit the work and incur any late penalties assessed. In some cases students will be asked to submit items electronically.

Capsules: There will be three independent study Capsules submitted for grading. These capsules will deal with

1. using computational tools for mathematics (selections from Appendix A and Steiner),
2. molecular symmetry, point groups and relevant group theory (portions of Chapter 27 and Steiner)
3. computational chemistry (portions of Chapter 26 and notes from Dr. Pounds)

The dates for each of the capsules will be determined when they are assigned but tentative due dates are 1/30/2017 for Computational Mathematics, 2/20/2017 for Molecular Symmetry, and 4/1/2017 for Computational Chemistry.

Online Homework: Several problems from each chapter will be assigned in the *Mastering Chemistry* online homework system. Students will be electronically notified of the due date for each of these assignments.

Written Homework Grading Policy: Homework problems will typically be divided into two sections: book problems and special problems from me. Selected problems will be graded on a three point scale as follows: 3 (essentially correct), 2 (minor errors or omissions), 1 (major errors or omissions), 0 (no effort). The composite score will then be converted to a percentage. 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.

American Disability Act: "Students requiring accommodations for a disability should inform the instructor at the close of the first class meeting or as soon as possible. The instructor will refer you to the ACCESS and Accommodation Office to document your disability, determine eligibility for accommodations under the ADA/Section 504 and to request a Faculty Accommodation Form. Disability accommodations or status will not be indicated on academic transcripts. In order to receive accommodations in a class, students with sensory, learning, psychological, physical or medical disabilities must provide their instructor with a Faculty Accommodation Form to sign. Students must return the signed form to the ACCESS Coordinator. A new form must be requested each semester. Students with a history of a disability, perceived as having a disability or with a current disability who do not wish to use academic accommodations are also strongly encouraged to register with the ACCESS and Accommodation Office and request a Faculty Accommodation Form each semester. For further information, please contact Carole Burrowbridge, Director and ADA/504 Coordinator, at 301-2778 or visit the ACCESS and Accommodation Office website at <http://www.mercer.edu/disabilityservices>"

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 listserv which I maintain myself. Please subscribe to the listserv 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.

Course Evaluations: In an ongoing effort to improve the quality of instruction, each student enrolled in this course is required to complete an end-of-semester course evaluation. Details about the evaluation process will be provided at the end of the term.

Final Exam: The final exam is scheduled for Monday, May 1st at 9 a.m.

Tentative Class Schedule¹

Week Starting	Chapter Sections	Lecture and Problem Solving Topics
January 8 th	Chapter 12 Chapter 13	From Classical to Quantum Mechanics The Schrödinger Equation Complex Numbers and Differential Equations
January 15 th	Chapter 14	MLK Holiday (Monday) The Postulates Observables and Expectation Values Superpositions of Eigenstates
January 22 nd	Chapter 15	Quantum Mechanics on Simple Systems Particles in 1D, 2D, and 3D Boxes
January 29 th	Chapter 16	PIB applied to Real World Scenarios Finite Well Potentials, Conjugated Molecules, Tunneling
February 5 th	Chapter 17	Commuting and Noncommuting Operators Heisenberg Uncertainty Principle
February 12 th	Chapter 18	EXAM ONE, 2/12/17, 6 p.m. Quantum Models for Vibration and Rotation The Harmonic Oscillator and Rigid Rotor Spherical-Polar Coordinates and Spherical Harmonics
February 19 th	Chapter 19	Vibrational and Rotational Spectroscopy Selection Rules and Normal Modes
February 26 th	Chapter 20	The Hydrogen Atom Solving the Schrödinger Equation for Hydrogen, Radial and Angular Components
March 5 th		SPRING BREAK
March 12 th	Chapter 21 Chapter 22	Many Electron Atoms Electron Spin Approximation Method 1 - Variational Method Antisymmetry / Matrix Eigenvalue Problems / Hartree-Fock Theory Atomic Spectroscopy
March 19 th	Chapter 23	The Chemical Bond in Diatomic Molecules Approximation Method 2 – Born-Oppenheimer Approximation Wavefunctions for Simple Systems Homonuclear and Heteronuclear Diatomics Bond Order, Bond Energy, Bond Length LAST DAY FOR COURSE WITHDRAWAL 3/23/17
March 27 th	Chapter 24	Molecular Structure and Energy Levels for Polyatomic Molecules Lewis and VSEPR Models Constructing Hybrid Orbitals Approximation Method 3 - Hückel MO Theory
April 3 rd	Chapter 25	Electronic Spectroscopy Molecular Term Symbols, Transitions Fluorescence, Phosphorescence, and Intersystem Crossing BEAR DAY (4/7/17)
April 9 th	Chapter 29	EXAM TWO, 4/10/17, 6 p.m. Probability, Discrete and Continuous Probability Distribution Functions Approximation Method 4 - Stirling's Approximation
April 16 th	Chapter 30 Chapter 31	The Boltzmann Distribution Ensembles and Molecular Partition Functions
April 23 rd	Chapter 32	Statistical Thermodynamics and Chemical Equilibrium Heat Capacity, Entropy, Enthalpy, Free Energy
April 30 th		FINAL EXAM, 5/1/17, 9 a.m., (Monday)

¹ I reserve the right to modify this schedule as situations warrant.