Quantum Chemistry - Chemistry 262

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In this course I hope to introduce you to the fundamentals of quantum mechanics and chemical spectroscopy. We will learn the basics of how to use Dirac notation and solve the important problems in introductory quantum theory (particle in a box, harmonic oscillator, rigid rotor). These theoretical models will be used to interpret basic experiments in the real world. As well you will learn about the fundamentals behind molecular structure (molecular orbits) and how these interact to give the multitude of compounds you learned about in organic and biochemistry. Also you will be introduced to fundamental ideas in statistical mechanics, which has in many ways served as an alternate though equivalent view of thermodynamics. In preparing for this course, it is worthwhile to go back and review mathematical tools such as derivatives, integrals and basic algebra as well as reviewing you freshman chemistry textbook for introductory quantum mechanics information. The primary text we will use is a very comprehensive and mathematically rigorous physical chemistry textbook (Levine, *Physical Chemistry*) as well as a supplemental applied mathematics text (Barrante, *Applied Mathematics for Physical Chemistry*). You probably should spend some time early on in the course reading and reviewing the Barrante text, as your mathematics skills are critical for success in this course. We meet on Monday, Wednesday and Friday in Room 306 at 11:00 AM. I will hold 7 office hours where I will guarantee normally to be available in my office unless otherwise posted. These will be Monday from 9-10, Wednesday from 9-10, Friday 9-10, Tuesday from 9-11 and 1-2, and Thursday from 9-11. Any other times that my door is open I am available for questions or comments.

The grading policy will be based on the following tentative schedule. You will be required to hand in 5 homework problem sets which will account for 25 points each and due after we finish each chapter. There will be 5 laboratory assignments worth 25 points each. The first will consist of a 20 minute oral review of a paper selected from a chemistry journal in the field of quantum mechanics or statistical mechanics. For the second laboratory experiment you will turn in a 5-8 page formal laboratory report. The remaining laboratories will be graded based on evaluation of your laboratory notebook and a second oral presentation to the class on the laboratory of your choice. There will be two one hour long tests each worth 175 points with problems taken primarily from the text. *The tentative test days will be Friday, October 9th and Friday, November 13th*. There will be a final exam worth 200 points on Wednesday, December 16th at 10 a.m.

Assignment	Points each	Total Points
Homework (5)	25	125
Laboratory Write-ups (5)	25	125
Midterm Exams (2)	175	350
Final Exam	200	200
Grand Total		800

The final will be a cumulative standardized exam while the tests will cover only current material. This means there will be a total of about 800 points. The grading will be such that 90% is an A (720 points),

75% is a B (600 points), 60% is a C (480 points), 50% is a D (400 points). For each midterm exam you will be allowed a single sheet (double sided) with any information on it you like.

The attendance policy shall be that all labs must be completed, including laboratory write-ups and oral exams. Also, it is expected that the student attend all lectures. Up to two days may be missed without excuse, any subsequent absences will lead to a 15 point deduction from your total score for each additional missed day. Absence shall not be an excuse for failure to learn information covered in the course examinations. In cases involving extended absences for a good reason (i.e. hospitalization, emergency at home, etc.) a special arrangement will be made between myself and the student as to how to make up the missed material or exams.

SCHEDULE OF CLASSES/HOMEWORK/READING

Chapter 18 - Quantum Mechanics (read Barrante chapter 5, 6, 10)		
Homework due 9/21		Levine problems 6,10,18,19,23,29,45,52 Barrante problems 5.1, 5.5, 5.11
Lecture 1	Blackbody & Photoelectric Effects	Section 18.1, 18.2
Lecture 2, 3	Bohr, DeBroglie, Heisenberg, Wavefunctions	18.3, 18.4, 18.5, 18.6
Lecture 4	Schrödinger Equation, Boxes	18.7, 18.8
Lecture 5	3D Boxes, Operators	18.9, 18.10, 18.11
Lecture 6	Harmonic Oscillator	18.12
Lecture 7	Two Particle, Rigid Rotor, Approximations	18.13, 18.14, 18.15
Chapter 19 - Atomic Structure (read Barrante chapter 9)		
Homework due 10/9		Levine problems 9,16,17,30,44,57 Barrante problems 6.1, 6.4
Lecture 8, 9	Background, Hydrogen	19.1, 19.2, 19.3
Lecture 10, 11	Electron Spin, Helium, Pauli	19.4, 19.5
Lecture 12	Many Electron Atoms	19.6
Lecture 13, 14	Hartree-Fock & CI Wavefunctions	19.7
Examination 1		Friday, October 9th
Chapter 20 - Molecular Structure		
Homework due 10/30		Levine problems 11,20,24,33,40 Barrante problems 10.1, 10.4, 10.6, 10.10
Lecture 16	Bonds and Born-Oppenheimer	20.1, 20.2
Lecture 17	Hydrogen Molecule, Diatomic MOs	20.3, 20.4
Lecture 18	SCF, HF & CI Wavefunctions, Polyatomic Molecules	20.5, 20.6
Lecture 19	Molecular Properties	20.7
Lecture 20	Accurate Wavefunctions, Semiempirical Methods	20.8, 20.9
Lecture 21	Molecular Mechanics, VB Method, VSEPR	20.10, 20.11, 20.12
Chapter 21 - Spectroscopy		
Homework due 11/16		Levine problems 5,9,12,19,28,33,46,57,70,80 Barrante problems 9.1, 9.4, 9.9
Lecture 22	Light, Spectroscopy, and Lasers	21.1, 21.2
Lecture 23	Rotation and Vibration	21.3, 21.4
Lecture 24	Molecular Symmetry	21.5
Lecture 25	Polyatomic Rotation/Vibration	21.7, 21.8
Lecture 26	IR/Raman/Electronic Spectroscopy	21.9, 21.10, 21.11

Lecture 27	NMR Spectroscopy	21.12
Lecture 28	ESR, CD and Photoelectron Spectroscopy	21.13, 21.14, 21.15
Examination 2		Friday, November 13th
Chapter 22 - Statistical Mechanics		
Homework due 11/30		Levine problems 6,16,21,22,55
Lecture 30	Canonical Ensemble	22.1, 22.2
Lecture 31	Canonical Partition Function	22.3, 22.4
Lecture 32	Boltzmann Distribution	22.5
Lecture 33	Gases	22.6, 22.7
Lecture 34	Equilibria, Entropy and Fluids	22.8, 22.9, 22.11
Chapter 24 - Solids & Liquids		
Homework due 12/9		Levine problems 13,29,45
Lecture 35	Phases, Polymers, Solid Bonding	24.1, 24.2, 24.3
Lecture 36	Cohesive Energy, Distances	24.4, 24.5, 24.6
Lecture 37	Crystals	24.7, 24.8
Lecture 38	X-Ray Diffraction, STM, Band Theory	24.9, 24.10, 24.11
Lecture 39	Review all material covered	
Final Exam	ACS Standardized	Wednesday, December 16th at 10 a.m.

Physical Chemistry II:
Quantum Mechanics & Spectroscopy - Chemistry 262

Laboratory Sessions

Lab 1	Literature Review Lab
Lab 2	Rotational Resolved IR Spectra of HCl
Lab 3	UV/Vis Spectroscopy and ab initio calculations for Dye Molecules
Lab 4	Student Chosen Laboratory
Lab 5	Spin Saturation NMR Experiment/2D COSY of Ethyl *trans*-Crotonate

Chemistry Department Oral Communication Evaluation Form

Student's Name_____ Date _____

Venue_____ Evaluator _____

Each of the following should be rated as being at a *distinguished,* D, *proficient,* P, *apprentice,* A, or *novice,* N level. The attached form describes these ratings.

Communication Skill Assessment

A. Presence- (voice, pace, eye contact, confidence, body language) _____

B. Use of supplementary material- (chalkboards, handouts, overheads) _____

C. Clarity of talk - (outline, organization, conclusion, appropriate for audience) _____

D. Response to questions- _____

General Comments

Specific Recommendations for Communication Skill Improvement

Technical Assessment

A. Understanding of material _____

B. Explanation of material (appropriate for level of audience, educational) _____

C. Substance- (technically correct) _____

D. Response to questions _____

General Comments

Specific Recommendations for Improving Technical Content

Overall Rating of Presentation

Distinguished _____ Proficient _____ Apprentice _____ Novice _____

Explanation of Rating Scale

Distinguished- The oral communication skills of the student are near perfect. The presentation was well-rehearsed with an exceptionally clear thesis and outline. Appropriate use has been made of supplementary material- writing on the chalkboard or overheads is legible, handouts add significantly to the presentation. Voice projection, the pace of the presentation are fine. Technically, the students has taken the material beyond a mere literature review or research summary by adding additional interpretation or making comparisons not present in the original literature.

Proficient - The oral skills of the student are at an acceptable level. Appropriate use has been made of supplementary material- writing on the chalkboard or overheads is legible, handouts add significantly to the presentation. Voice projection, the pace of the presentation are fine. The only minor errors that are present, if any, could be improved through additional practice. NO technical errors are present. The student has presented the reviewed material concisely, accurately, and at an appropriate level for the audience.

Apprentice - Key features of oral communication are evident, but capable of additional development. No more than one major flaw is contained in the presentation such as lack of voice projection, poor overhead usage, inappropriate body language, poor quality of supplementary material. The thesis and outline of the talk are obvious. Technically the presentation contains few flaws, however, the material is still not quite understandable at the level of the audience. Understanding could be improved through the use of more appropriate supplementary material, simplification of diagrams and figures, or by spending more time explaining each figure. It is apparent that the student has some understanding of the material.

Novice - Essential elements of effective oral communication are not evident. Poor grammar is evident throughout the presentation as shown through poor word choice, sentence structure, and pronunciation problems. No thesis or outline is apparent. Communication aids are not used effectively and are more of a hindrance than a help. The use of a chalkboard, overheads, or other auxiliary material is very awkward. Technically, the report contains numerous scientific errors showing some misunderstanding of the project. The purpose of the research is not evident and it is not presented on a level understandable by the audience.