

# Quantum Chemistry - Chemistry 362

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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 your freshman chemistry textbook for introductory quantum mechanics information. The primary text we will use is a very comprehensive and mathematically rigorous physical chemistry textbook (Atkins, *Physical Chemistry*, 6<sup>th</sup> edition) as well as an optional 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 (if you choose to purchase it), 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 9 office hours where I will normally be available in my office for drop-in visitation/questions unless otherwise posted. These will be Monday from 9-10 & 3-4, Tuesday 9-11 & 1-2, Wednesday 9-10, and Thursday 9-11 & 1-2. 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 8 homework problem sets which will account for 10 points each and due after we finish each chapter. There will be 6 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 three one hour long tests

| Assignment               | Points each | Total Points |
|--------------------------|-------------|--------------|
| Homework (8)             | 10          | 80           |
| Laboratory Write-ups (6) | 25          | 150          |
| Midterm Exams (3)        | 150         | 450          |
| Final Exam               | 320         | 320          |
| Grand Total              |             | 1000         |

each worth 150 points with problems taken primarily from the text. *The tentative test days will be Friday, September 22<sup>nd</sup>, Friday, October 27<sup>th</sup> and Monday, November 27<sup>th</sup>.* There will be a final exam worth 320 points on Monday, December 11<sup>th</sup> at 10 a.m. 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 1000 points. The grading will be such that 92% is an A (920 points), 80% is a B (800 points), 60% is a C (600 points), 50% is a D (500 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. Failure to complete all labs will result in failure of the course. 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

|  |  |  |
|--|--|--|
| September 1 <sup>st</sup>                          | Go Over Syllabus (Dr. Baltisberger will be absent) |  |
| <b>Chapter 11 - Quantum Theory</b>                 |  |  |
|  | Homework due 9/15                                  | Exercise 1a, 6b, 11a, 17b<br>Problems 2, 9, 15, 22 |
| September 4 <sup>th</sup>                          | Origins of Quantum Mechanics                       | Section 11.1 – 11.3                                |
| September 6 <sup>th</sup>                          | Principles of Quantum Mechanics                    | 11.4 – 11.6  |
| September 8 <sup>th</sup>                          | Problem solving                                    |  |
| <b>Chapter 12 – Techniques &amp; Applications</b>  |  |  |
|  | Homework due 9/20                                  | Exercise 3b, 4a, 8a, 15b<br>Problems 3, 5, 10, 22  |
| September 11 <sup>th</sup>                         | Spectroscopy & Rotation                            | Section 12.1 – 12.4                                |
| September 13 <sup>th</sup>                         | Vibration  | 12.5 – 12.8  |
| September 15 <sup>th</sup>                         | Problem solving                                    |  |
| September 18 <sup>th</sup>                         | Problem solving, 1 <sup>st</sup> Laboratory due    |  |
| <b>Chapter 13 – Atomic Spectra &amp; Structure</b> |  |  |
|  | Homework due 10/9                                  | Exercise 2a, 9b, 12b, 19a<br>Problems 5, 15, 20    |
| September 20 <sup>th</sup>                         | Hydrogen and Many Electron Atoms                   | Section 13.1 – 13.5                                |
| September 22 <sup>nd</sup>                         | Problem Solving                                    |  |
| September 25 <sup>th</sup>                         | Hydrogen and Many Electron Atoms                   | Section 13.1 – 13.5                                |
| September 27 <sup>th</sup>                         | Problem Solving                                    |  |
| <b>Examination 1 (Chapter 11 - 12)</b>             |  | <b>Friday, September 29<sup>th</sup></b>           |
| October 2 <sup>nd</sup>                            | Complex Atoms, 2 <sup>nd</sup> Laboratory due      | 13.6 – 13.10                                       |
| <b>Chapter 14 – Molecular Structure</b>            |  |  |
|  | Homework due 10/16                                 | Exercise 2b, 5a, 9b, 12a<br>Problems 2, 7, 14      |
| October 4 <sup>th</sup>                            | Climb a Mountain (Mt. Day)                         |  |
| October 6 <sup>th</sup>                            | Problem Solving (Dr. Baltisberger will be absent)  |  |
| October 9 <sup>th</sup>                            | Born-Oppenheimer and MO Theory                     | Section 14.1 – 14.5                                |
| October 11 <sup>th</sup>                           | Polyatomic Molecules                               | 14.6 – 14.10                                       |
| October 13 <sup>th</sup>                           | Problem Solving (Dr. Baltisberger will be absent)  |  |
| <b>Chapter 15 – Molecular Symmetry</b>             |  |  |
|  | Homework due 10/25                                 | Exercise 1b, 5a, 7a, 13b<br>Problems 7, 13         |
| October 16 <sup>th</sup>                           | Mid Term Reading Period                            |  |
| October 18 <sup>th</sup>                           | Symmetry Elements, 3 <sup>rd</sup> Laboratory due  | Section 15.1 – 15.3                                |
| October 20 <sup>th</sup>                           | Problem solving (Dr. Baltisberger will be absent)  |  |

|                          |                  |             |
|--------------------------|------------------|-------------|
| October 23 <sup>rd</sup> | Character Tables | 15.4 – 15.6 |
| October 25 <sup>th</sup> | Problem solving  |             |

**Examination 2 (Chapter 13 - 15)**

**Friday, October 27<sup>th</sup>**

Chapter 16 – Spectroscopy – Rotation & Vibration

|                    |  |  |
|--------------------|--|--|
| Homework due 11/10 |  | Exercise 1b, 5b, 7a, 12b, 16b, 23b<br>Problems 1, 10, 14, 20 |
|--------------------|--|--|

|                          |   |                     |
|--------------------------|---|---------------------|
| October 30 <sup>th</sup> | Go Over Test, 4 <sup>th</sup> Laboratory due      |                     |
| November 1 <sup>st</sup> | Rotation  | Section 16.1 – 16.8 |
| November 3 <sup>rd</sup> | Problem Solving (Dr. Baltisberger will be absent) |                     |
| November 6 <sup>th</sup> | Vibration   | 16.9 – 16.16        |

Chapter 17 – Spectroscopy – Electronic

|                    |  |   |
|--------------------|--|---|
| Homework due 11/20 |  | Exercise 2a, 4b, 7a, 10b<br>Problems 2, 6, 11, 18 |
|--------------------|--|---|

|                           |  |                   |
|---------------------------|--|-------------------|
| November 8 <sup>th</sup>  | Electronic Transitions and Lasers                                      | Section 17.1-17.5 |
| November 10 <sup>th</sup> | Problem Solving (Dr. Baltisberger will be absent)                      |                   |
| November 13 <sup>th</sup> | Lasers and Photo Electron Spectroscopy, 5 <sup>th</sup> Laboratory due | 17.6 – 17.10      |

Chapter 18 – Spectroscopy – NMR

|                   |  |   |
|-------------------|--|---|
| Homework due 12/4 |  | Exercise 3b, 12a, 22a<br>Problems 2, 5, 9 |
|-------------------|--|---|

|                           |   |                   |
|---------------------------|---|-------------------|
| November 15 <sup>th</sup> | Intro to NMR                                      | Section 18.1-18.4 |
| November 17 <sup>th</sup> | Problem Solving (Dr. Baltisberger will be absent) |                   |
| November 20 <sup>th</sup> | Advanced topics in NMR                            | 18.5 – 18.11      |
| November 22 <sup>nd</sup> | Problem solving                                   |                   |

**Examination 3 (Chapter 16 - 18)**

**Monday, November 27<sup>th</sup>**

Chapter 21 – Diffraction Techniques

|                           |  |                   |
|---------------------------|--|-------------------|
| November 29 <sup>th</sup> | Go Over Test, 6 <sup>th</sup> Laboratory due |                   |
| December 1 <sup>st</sup>  | Crystal Structure & Bragg's Law              | Section 21.1-21.5 |
| December 4 <sup>th</sup>  | X-Ray, Neutron and Electron Analysis         | 21.6 – 21.10      |
| December 6 <sup>th</sup>  | Problem Solving                              |                   |

**Final Exam ACS Standardized**

**Monday, December 11<sup>th</sup> at 10 a.m.**

Suggested Problems from Barrante (I am happy to help you with these at any time)

1.2, 1.4, 1.6, 1.9, 2.1, 2.6, 2.8, 3.2, 3.5, 4.2, 4.3  
 5.1, 5.5, 5.11, 6.1, 6.2, 6.4, 6.6, 7.2, 7.4, 9.1, 9.4  
 9.9, 10.1, 10.4, 10.6, 10.10, 11.6, 12.5

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.