

Chem 3BA3 Course Outline - Fall 2006
Quantum Mechanics and Spectroscopy I
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Welcome to Introductory Quantum Mechanics! This course outline will summarize the most important information about this course. Please also keep yourself current using the WebCT course website. As the instructor of this course, I strive to provide you with all the necessary resources to start understanding quantum mechanics and its applications.

Course Content:

- Classical Mechanics (Equations of Motion, Harmonic Oscillator, Multiple Degrees of Freedom, Many Particle Systems)
- Schroedinger equation, wave functions
- Operators, Hermitian Operators
- Quantum-Mechanical Harmonic Oscillator
- Particles and Potentials, Tunneling
- Scanning Tunneling Microscopy
- Variation Theory
- Perturbation Theory
- Rigid Rotor/ Angular Momentum
- Vibrational-Rotational Spectroscopy
- Atomic Force Microscopy
- Hydrogen atom
- Born-Oppenheimer Approximation
- Molecular Orbital Theory
- Electronic Spectroscopy
- Hueckel Theory
- Magnetic Resonance Spectroscopy

Textbook: (required)

- C. E. **Dykstra**, Introduction to Quantum Chemistry, Prentice Hall, ISBN 0-13-701293-4. Most of the lecture material as well as a lot of background information for the four experiments.

Recommended Additional Reading:

- C. W. **Garland**, J. W. **Nibler**, D. P. **Shoemaker**, Experiments in Physical Chemistry, 7th edition, McGraw Hill, ISBN 0-07-231821-X (in particular, experiments 37, 39) This is a very useful book containing information related to two of the labs as well as general information about experimental techniques and data processing.
- I. N. **Levine**, Quantum Chemistry, 5th edition, Prentice Hall, ISBN 0-13-685512-1. This book is for those of you thirsting for more math. Same as textbook for *Chem 4Q03*.
- J. M. **Hollas**, Modern Spectroscopy, 4th edition, Wiley, ISBN 0-470-84416-7. This book is for those of you thirsting for more spectroscopy. (sorry, no NMR) Same as textbook for *Chem 4B03*.

Office Hours:

Dr. Kruse: to be announced in class

TA's: during lab hours and by email

Email contacts:

Instructor and TA's can be reached under their email accounts *on the Chem 3BA3 WebCT site.*

Evaluation:

Weekly pre-lecture WebCT quizzes	=	12 x 0.5%
2 Midterm exams (50 min, during tutorial time)	=	2 x 12%
1 Final exam (3 hours)	=	30%
4 Lab experiments	=	4 x 10%
Total	=	100%

- Scheduled Midterm dates: Tutorial times of week 5 and week 9

- Weekly pre-lecture quizzes will consist of five multiple choice questions that should be easy to answer by flipping through the book, plus one feedback question. Each multiple choice question weighs in with 0.1% of your final grade, for a total of 6% if you answer all questions correctly. The main benefit of these quizzes is that they encourage you to read through the textbook ahead of each week of lectures.

- There are no assignments or homework. However, you will have plenty of opportunities to practice for both mid-terms and the final exam. (pre-lecture quizzes, tutorial questions)

- No course component is compulsory for passing the course. However, if you skip or do not complete any exam or lab experiment, you will be assigned a grade of ZERO for that component.

Laboratory Evaluation:

- Lab grades for each experiment are divided into

4% lab interview,

2% lab performance,

2% calculations (submitted as part of the report),

2% report

- ***all*** parts have to be completed & ***passed by either the instructor or a TA*** in order to get any credit for the experiment

- Lab reports have to be handed in in person to the appropriate TA. Sloppy or incomplete reports may be refused. Alternatively, reports may be submitted in electronic form to the appropriate TA by email within the Chem 3BA3 WebCT site.

- The final decision over all lab grades rests with the instructor, usually following the recommendation given by the TA.

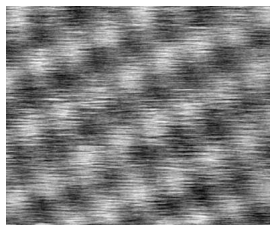
- ***Lab reports are due to the TA or course instructor (print version in person or electronic copy via WebCT email) at the latest 1 week (i.e. 604800.0 seconds) after conclusion of the lab part of the experiment. Late fees are 0.1% off the total course grade at the beginning of each day that a lab report is late, up to the last day of class. No lab report will be accepted after the end of the last lecture of the course. Experiments without lab report will be counted overall as 0%.***

Laboratory Experiments:

The experiments in this course were carefully selected to closely relate to the lecture material, help you understand quantum mechanics and expose you to a selection of modern research tools and techniques in physical chemistry. They are done in groups of two to four students and typically take two lab periods of 3 hours each. A manual for each experiment in .pdf format will be available on WebCT. You must have hard cover bound lab notebook to take notes, record data and collect TA or instructor signatures. Don't forget to also bring a 3.5" floppy or USB key to each lab to record your data! The safety bulletin must be filled out before starting actual lab work. It is available on the website. A \$30 (max) breakage fee applies to all broken equipment.

1) Scanning Tunneling Microscopy (see lab manual, resources on WebCT)

During this experiment, you will get an introduction to a fairly young experimental technique (invented in 1981, Nobel prize in 1986) that has revolutionized surface science and enabled nanotechnology due to its unique ability to let us see single atoms and molecules on surfaces. You will start off by discovering nanometer scale features on supposedly flat gold surfaces. During the second part of this experiments you will be able to resolve carbon atoms on a graphite surface and measure the bond distance between them. Your TA and your course instructor (Prof. Kruse) have a lot of experience using this technique for their research and will be happy to answer all your questions and even supply you will more challenging samples in case the gold and the graphite were to easy for you...



Carbon atoms on a graphite sample

2) Vibrational-Rotational Spectra of HCl/DCI (adapted from Shoemaker, #37, p. 403 in 7th ed.)

Who thought that a quantum mechanics course would require you to do synthesis? Although, the synthesis of gaseous HCl and DCI from sodium chloride and sulfuric acid is maybe a bit different from your organic labs. All the same, you will stick the final product into a modern Bruker FT-IR spectrometer. However, since this time you are looking at a gas phase IR spectrum, you will be able to resolve features due to the free rotation of the molecule and extract quantitative information about the molecular structure. As part of this experiment, you will explore some challenges in gas phase spectroscopy, such as pressure broadening and understand the important differences to the more familiar solution (or solid) phase spectra. This classic experiment will go a long way in illustrating the lecture material and teaching you about basic principles of spectroscopy and quantum mechanics. While here may not be too many groups anymore doing gas phase spectroscopy on small molecules as an active field of research, Canada has a very strong and rich tradition in this field (Nobel Prize in Chemistry 1971 for Gerhard Herzberg).

3) Vibronic Spectrum of Iodine (adapted from Shoemaker, #39, p. 423 in 7th ed.)

Iodine may be a simple molecule, but there is a lot it can teach you about electronic structure and electronic (UV/vis) spectra. You will take gas phase absorption spectra using a state-of-the-art

research grade UV/vis spectrometer (Varian Cary 100, 0.2nm resolution) at a resolution that allows you see more than the usual broad, washed-out peaks that you have come to associate with UV/vis spectroscopy. You will resolve the vibrational structure of the electronic transition and use this additional information to calculate important molecular properties. This classic experiment may be simple, but it will very effectively help you to understand some of the concepts discussed in lecture and help you get familiar with important principles of spectroscopy.

4) Nuclear Magnetic Resonance (see lab manual, Dykstra 7.2, 7.4)

After being discarded by physicists due to the annoyance of chemical shift, nuclear magnetic resonance has gone on to revolutionize molecular structure determination in chemistry (NMR) and imaging of tissues, organs and whole organisms in medicine (MRI). In our department, there are several physical chemistry groups using NMR as their main research tool (Profs. Bain, Goward, Melachini) in addition to the many synthetic groups making heavy use of the state-of-the-art NMR facilities at McMaster (1x 700MHz, 1x 600MHz, 2x 500 MHz, 1x 300 MHz, 2x 200 MHz, very few places in Canada can match that!). You will likely have already come across NMR in several other courses, but during this lab you will finally learn more about how it really works. Your knowledgeable TA will take an NMR probe apart for you and show you all its inside workings. During the first part of the experiment you will use the shim coils to establish a field gradient across your sample and do some simple imaging, just like in MRI. During the second part of this lab, you will explore the nature of J-coupling, which forms the basis of many modern NMR experiments. For lack of time you will only get to see a small part of the wonderful worlds of NMR and MRI, but your TA uses NMR all the time for research and will be glad to answer all your questions and to be your guide.

Approximate Lecture Schedule for Chem 3BA3 (Fall 2006)

#	Date	Contents	Dykstra
1	Week 0	Introduction	1
2	Week 1	Equations of Motion, Classical Harmonic Oscillator	2.1-2
3	Week 1	Multiple Degrees of Freedom and Many Particle Problems	2.3-4
4	Week 1	Wave - Particle Duality, Schroedinger Equation	3.1-2
5	Week 2	General Introduction to Operators and Their Properties	3.3
6	Week 2	The Quantum Mechanical Harmonic Oscillator	3.4
7	Week 2	Born Interpretation of the Wave Function, Heisenberg Uncertainty Principle	3.5
8	Week 3	Particle in a Box with Infinite Walls	3.6
9	Week 3	Particles and Potentials	3.7
10	Week 3	Tunneling & Scanning Tunneling Microscopy	-
11	Week 4	Nanostructures	-
12	Week 4	Hermitian Operators	4.1
13	Week 4	Multidimensional Problems, Degeneracy	4.2-3
14	Week 5	Variation Theory	4.4

#	<i>Date</i>	<i>Contents</i>	<i>Dykstra</i>
15	Week 5	Perturbation Theory	4.5
16	Week 5	Time-Dependent Phenomena	4.6
17	Week 6	Applications of Variation and Perturbation Theory	4.7-8
18	Week 6	Angular Momentum	4.9
19	Week 6	Rigid Rotor	4.10
20	Week 7	Coupling of Angular Momenta	4.11
21	Week 7	Vibration & Rotation of Diatomics	5.1-2
22	Week 7	Anharmonicity	5.3
23	Week 8	Selection Rules	5.4
24	Week 8	Rotational Spectroscopy and Polyatomic Vibrations	5.5-7
25	Week 8	Atomic Force Microscopy	-
26	Week 9	Hydrogen Atom, Radial Functions	6.1-2
27	Week 9	Orbital & Spin Angular Momentum, Atomic Orbitals	6.3-5
28	Week 9	Many-Electron Atoms	6.6
29	Week 10	Born-Oppenheimer Approximation and Antisymmetrization	6.7-8
30	Week 10	Vibronic Spectroscopy	6.10
31	Week 10	Molecular Orbital Theory	6.9
32	Week 11	Hueckel Theory	-
33	Week 11	Hueckel Theory	-
34	Week 11	Hueckel Theory	-
35	Week 12	Nuclear Spin States	7.1
36	Week 12	Spin-Spin Coupling	7.2
37	Week 12	Brief Introduction to ESR and MRI	7.3-4

Reading Assignments for Pre-Lecture Quizzes

#	<i>Quiz Due Date</i>	<i>Contents</i>
1	Week 1	Dykstra Chapter 1, 2, 3.1-2
2	Week 2	Dykstra Chapter 3.3-5
3	Week 3	Dykstra Chapter 3.6-7, Resources about Tunneling, Scanning Tunneling Microscopy
4	Week 4	Resources about Nanostructures, Dykstra Chapter 4.1-3
5	Week 5	Dykstra Chapter 4.4-6
6	Week 6	Dykstra Chapter 4.7-10
7	Week 7	Dykstra Chapter 4.11, 5.1-3

#	<i>Quiz Due Date</i>	<i>Contents</i>
8	Week 8	Dykstra Chapter 5.4-7, Resources about Atomic Force Microscopy
9	Week 9	Dykstra Chapter 6.1-6
10	Week 10	Dykstra Chapter 6.7-10
11	Week 11	Resources about Hueckel Theory
12	Week 12	Dykstra Chapter 7

Approximate Tutorial Schedule (Fall 2006)

#	<i>Date</i>	<i>Contents</i>
1	Week 1	Math and Physics Review
2	Week 2	Introduction to Experiment 3: Vibronic spectrum of iodine
3	Week 3	Introduction to Experiment 4: NMR
4	Week 4	Review in preparation of Mid-term I
5	Week 5	Mid-term I (Dykstra Chapters 1-3, Tunneling, STM & Nanostructures)
6	Week 6	Results and solutions of Mid-term I
7	Week 7	Perturbation Theory and Variational Method
8	Week 8	Review in preparation of Mid-term II
9	Week 9	Mid-term II (Dykstra Chapters 4-5, AFM)
10	Week 10	Results and solutions of Mid-term II
11	Week 11	Matrices & Hueckel Calculations
12	Week 12	Review in preparation of Final Exam

Disclaimer: Changes to the course schedule and marking scheme may be made at the discretion of the instructor and announced to the students at any time during the course. An effort will be made to keep inconveniences from changes to a minimum.

Academic dishonesty: Academic dishonesty consists of misrepresentation by deception or by other fraudulent means and can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: "Grade of F assigned for academic dishonesty"), and/or suspension or expulsion from the university.

It is your responsibility to understand what constitutes academic dishonesty. For information on the various kinds of academic dishonesty please refer to the Academic Integrity Policy, specifically Appendix 3, located at http://www.mcmaster.ca/senate/academic/ac_integrity.htm

In particular reference to the expected student work in this course, the only aides permitted during midterms and the final are your own brain, a pen, paper and sometimes a calculator. For the lab reports, do not copy any passages from each other, the lab manuals or any other sources. You may paraphrase crucial information provided you properly reference your source.