

Chem 3BA3 Course Outline - Fall 2008
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:

- Where does quantum mechanics fit in?
- Schroedinger equation, wave functions
- Operators
- Particle in a box
- Particles and potentials, tunneling
- Scanning tunneling microscopy
- Heisenberg uncertainty principle & wavefunction collapse
- Harmonic oscillator
- Rigid rotor
- Angular momentum
- Vibrational-rotational spectroscopy
- Hydrogen atom
- Born-Oppenheimer approximation
- Bonding in diatomic molecules
- Molecular orbital theory
- Electronic spectroscopy
- Hueckel theory
- Magnetic resonance spectroscopy

Textbook: (required)

- T. **Engel**, Quantum Chemistry and Spectroscopy, Pearson, ISBN 0-8053-3843-8. Most of the lecture material as well as a lot of background information for the four experiments.

or T. **Engel**, P. Reid, Physical Chemistry, Pearson, ISBN 0-8053-3842-X. (add 11 to all chapter numbers given here or in any course material)

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.

- 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)

Office Hours:

Dr. Kruse: Mon & Wed after class (11:20 – 12:00)

TA's: during lab hours (i.e. Mon & Wed 14:30 – 17:30) and by email

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

Evaluation:

6 Assignments	=	6 x 2%
2 Midterm exams (50 min, during lecture time)	=	2 x 15%
1 Final exam (3 hours)	=	30%
3 Lab interviews	=	3 x 4%
4 Lab reports	=	4 x 4%
Total	=	100%

- Scheduled Midterm dates: Thu, 09 Oct 2008 and Thu, 13 Nov 2008

- The tutorials will be conducted by a TA and serve to hone your problem solving skills. They are most effective if you attempt the problems by yourself. 6 assignments (sets of questions) will be posted for this purpose.

- 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.

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

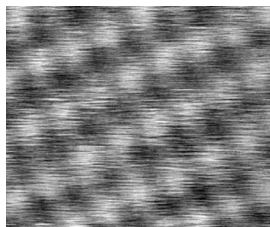
- Lab reports are due to the TA or course instructor (print version in person or electronic copy via WebCT email) at the latest 1 week (i.e. 604800.0 seconds) after conclusion of the lab part of the experiment. Late fees are 0.1% off the total course grade at the beginning of each day that a lab report 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 is available on WebCT. 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; *Engel* Ch. 5)

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 with 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/DCl (Shoemaker, #37, p. 403 in 7th ed.; **Engel** Ch. 8)

Who thought that a quantum mechanics course would require you to do synthesis? Although, the synthesis of gaseous HCl and DCl 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. 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 there 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 (Shoemaker, #39, p. 423 in 7th ed.; **Engel** Ch. 15)

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; **Engel** Ch. 18)

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 2008)

#	Date	Contents	Engel
1	Thu, 04 Sept 2008	Introduction, Double Slit Experiment	1.1-7
2	Mon, 08 Sept 2008	Lengthscales for Quantum Effects	2.1
3	Wed, 10 Sept 2008	Review of Classical Mechanics	--
4	Thu, 11 Sept 2008	Schrödinger's Wave Mechanics, Schrödinger Equation	2.2-4
5	Mon, 15 Sept 2008	Guest Lecture: X-ray Diffraction, Compton Effect (Dr. Jim Britten)	--
6	Wed, 17 Sept 2008	Operators I	2.5-8
7	Thu, 18 Sept 2008	Operators II	2.5-8
8	Mon, 22 Sept 2008	Quantum Mechanical Postulates	3.1-5
9	Wed, 24 Sept 2008	Free Particle & Particle in 1D Box with Infinite Walls	4.1-2
10	Thu, 25 Sept 2008	Particle in a 2D & 3D Box & Box with Finite Walls	4.3-4, 5.1
11	Mon, 29 Sept 2008	Particles & Potentials	5.2-4, 5.8
12	Wed, 01 Oct 2008	Tunneling, Scanning Tunneling Microscopy (STM)	5.5-7
13	Thu, 02 Oct 2008	Commuting Operators, Stern Gerlach Experiment	6.1-2
14	Mon, 06 Oct 2008	Heisenberg Unschärferelation (Uncertainty Principle), Probabilities	6.3-6
15	Wed, 08 Oct 2008	Q&A Review for Midterm	<u>1-6</u>
16	Thu, 09 Oct 2008	*** 1st Midterm ***	<u>1-6</u>
17	Wed, 15 Oct 2008	Schrödinger Equation for Diatomic Molecules	--
18	Thu, 16 Oct 2008	Harmonic Oscillator	7.1, 7.6
19	Mon, 20 Oct 2008	Rigid Rotor	7.2-5, 7.7-8
20	Wed, 22 Oct 2008	Introduction to Spectroscopy	8.1-2
21	Thu, 23 Oct 2008	Vibrational-Rotational Spectra of Diatomics	8.3-4, 8.6
22	Mon, 27 Oct 2008	Vibrational Spectra of Large Molecules (= more than 2 atoms...)	8.5
23	Wed, 29 Oct 2008	Hydrogen Atom	9.1-6
24	Thu, 30 Oct 2008	Many Electron Atoms	10.1-10
25	Mon, 03 Nov 2008	Atomic Spectroscopy	11.1-7
26	Wed, 05 Nov 2008	Chemical Bonding in Dihydrogen	12.1-7
27	Thu, 06 Nov 2008	Chemical Bonding in Diatomics	13.1-8
28	Mon, 10 Nov 2008	Electronic Spectroscopy of Molecules	15.1-11
29	Wed, 12 Nov 2008	Q&A Review for Midterm	<u>7-13, 15</u>
30	Thu, 13 Nov 2008	*** 2nd Midterm ***	<u>7-13, 15</u>
31	Mon, 17 Nov 2008	Hückel Theory I	14.1-7

#	<i>Date</i>	<i>Contents</i>	<i>Engel</i>
32	Wed, 19 Nov 2008	Hückel Theory II	14.1-7
33	Thu, 20 Nov 2008	Solid State Electronic Structure	14.8-9
34	Mon, 24 Nov 2008	NMR Introduction, Chemical Shift	18.1-6
35	Wed, 26 Nov 2008	Nuclear Spin Coupling, Solid State NMR, MRI	18.7-11
36	Thu, 27 Nov 2008	NMR, Fourier Transform & 2D	18.12-14
37	Mon, 01 Dec 2008	Q&A Review for Final Exam	<u>1-15, 18</u>

Approximate Tutorial & Assignment Schedule (Fall 2008)

#	<i>Date</i>	<i>Contents</i>
1	Tue, 09 Sep 2008	--- (no tutorial scheduled)
2	Tue, 16 Sep 2008	Differential Equations & Complex Numbers; <u>Assignment 1</u>
3	Tue, 23 Sep 2008	Operators; <u>Assignment 2</u>
4	Tue, 30 Sep 2008	Probability; <u>Assignment 3</u>
5	Tue, 07 Oct 2008	Review in preparation of Mid-term I
6	Tue, 14 Oct 2008	Results and solutions of Mid-term I
7	Tue, 21 Oct 2008	Variational Method; <u>Assignment 4</u>
8	Tue, 28 Oct 2008	Perturbation Theory; <u>Assignment 5</u>
9	Tue, 04 Nov 2008	Angular Momentum Coupling; <u>Assignment 6</u>
10	Tue, 11 Nov 2008	Review in preparation of Mid-term II
11	Tue, 18 Nov 2008	Results and solutions of Mid-term II
12	Tue, 25 Nov 2008	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.