

A. General Information

- Course: CHEM 333, *Introduction to Quantum Theory*, 3 credits, Winter 2017.
- Time and place: Tuesdays, 18:00-20:30, CC-405.
- Instructor: Dr. Gilles H. Peslherbe, Professor, Department of Chemistry & Biochemistry, Faculty of Arts & Science, Concordia University.
- Office location: SP-275.19.
- Telephone: 514-848-2424 ext. 3335.
- E-mail: Gilles.Peslherbe@Concordia.CA.
- Website: <http://moodle.concordia.ca/moodle>.
- Office Hours: Tuesdays, 13:30-14:30, or by appointment (e-mail preferred). No office hours on exam days.

B. Course Description

- The course introduces students to the concept of quantum mechanics and the electronic structure of atoms and molecules. Topics include the origins and postulates of quantum theory, the Schrödinger equation and applications to simple systems such as the harmonic oscillator, rigid rotor and the hydrogen atom. The course looks at the quantum mechanical treatment of the chemical bond and provides an introduction to spectroscopy. Lectures only.
- Prerequisites: CHEM 234, 241.
- Detailed outline:

INTRODUCTION

1. REVIEW OF CLASSICAL PHYSICS

- 1.1. Newtonian Mechanics of Particles
- 1.2. Electrostatics
- 1.3. Magnetism
- 1.4. Wave Physics
- 1.5. Electromagnetic Radiation and Classical Theory of Light

2. FAILURE OF CLASSICAL PHYSICS AND EMERGENCE OF THE "OLD" QUANTUM THEORY

- 2.1. Blackbody Radiation
- 2.2. Photoelectric Effect
- 2.3. Heat Capacities and Vibrations in Crystals
- 2.4. The Hydrogen Atom Spectrum. Rydberg formula and the Bohr model
- 2.5. De Broglie Postulate
- 2.6. Electron Diffraction Experiment
- 2.7. The Heisenberg Uncertainty Principle

3. GENERAL PRINCIPLES AND POSTULATES OF QUANTUM MECHANICS

- 3.1. The Schrodinger Equation
- 3.2. Operators, Eigenvalues and Eigenfunctions
- 3.3. Wavefunction and Probability Density
- 3.4. Postulates of Quantum Mechanics

4. APPLICATION OF QUANTUM MECHANICS TO SIMPLE SYSTEMS

- 4.1. The Particle in a Box - Translational Motion
- 4.2. The Harmonic Oscillator - Vibrational Motion
- 4.3. The Rigid Rotor - Rotational Motion
Notes on Vibrational-Rotational Spectroscopy

5. THE HYDROGENOID ATOM: ELECTRONIC STRUCTURE AND SPECTRA

- 5.1. Energy and Wavefunction
- 5.2. Electronic Structure and Orbitals
- 5.3. Quantum Numbers and Spectroscopic Selection Rules
Notes on Magnetic Resonance Spectroscopy

6. MANY-ELECTRON ATOMS: ELECTRONIC STRUCTURE AND SPECTRA

- 6.1. The Variational Principle
- 6.2. Electronic Structure
- 6.3. Spectroscopy

7. MOLECULAR STRUCTURE AND THE CHEMICAL BOND

- 7.1. Born-Oppenheimer approximation
- 7.2. Valence-Bond theory
- 7.3. Molecular Orbital theory
- 7.4. Modern Quantum Chemistry

C. Objectives

In this course, you will learn the foundations of the quantum theory, and you will be expected to 1) understand and remember its basic concepts and 2) be able to apply them to solve problems. You will also be expected to follow the major steps of the derivations given in class, but you will not be required to reproduce some of the more complex and mathematically-involved derivations.

D. Schedule (May be subject to change.)

- Midterm Exams, during class time, February 7 and April 4, 2017.
- Final Exam, during exam period (April 19 - May 2), date TBA.

E. Course Materials

- Suggested (not required) textbooks: *Physical Chemistry*, Atkins & De Paula, or *Physical Chemistry, Volume 2: Quantum Chemistry, Spectroscopy, and Statistical Thermodynamics* Atkins & De Paula. Available for purchase at the bookstore.

- Other textbooks: *Physical Chemistry*, Laidler, Meiser and Sanctuary.
Quantum Chemistry and Spectroscopy, Engel (advanced).
- On reserve in the Library: *Physical Chemistry*, Atkins & De Paula.

F. Grading / Evaluation

- The final grade is based on two midterm exam (25% each) and a final exam (50%).
- 4 Problem Sets will be given, but they will not be collected nor graded. You are strongly encouraged, however, to solve them at home in exam conditions as excellent practice for the exams. Some aspects of the Problem Sets might be discussed in class upon request.
- Grading scale:

A+	90 - 100 %
A	85 - 90 %
A-	80 - 85 %
B+	77 - 80 %
B	73 - 77 %
B-	70 - 73 %
C+	67 - 70 %
C	63 - 67 %
C-	60 - 63 %
D+	57 - 60 %
D	53 - 57 %
D-	50 - 53 %
F	0 - 50 %

G. Rights and Responsibilities

Plagiarism:

The most common offense under the Academic Code of Conduct is plagiarism which the Code defines as "**the presentation of the work of another person as one's own or without proper acknowledgement.**"

This could be material copied word for word from books, journals, internet sites, professor's course notes, etc. It could be material that is paraphrased but closely resembles the original source. It could be the work of a fellow student, for example, an answer on a quiz, data for a lab report, a paper or assignment completed by another student. It might be a paper purchased through one of the many available sources. Plagiarism does not refer to words alone - it can also refer to copying images, graphs, tables, and ideas. "Presentation" is not limited to written work. It also includes oral presentations, computer assignments and artistic works. Finally, if you translate the

work of another person into French or English and do not cite the source, this is also plagiarism.

In Simple Words:

DO NOT COPY, PARAPHRASE OR TRANSLATE ANYTHING FROM ANYWHERE WITHOUT SAYING FROM WHERE YOU OBTAINED IT!

(Source: The Academic Integrity Website: <http://provost.concordia.ca/academicintegrity/plagiarism/>)

Plagiarism and other forms of academic dishonesty:

The academic code of conduct can be found in section 17.10 of the academic calendar (<http://www.concordia.ca/academics/undergraduate/calendar/current/17-10.html>). Any form of unauthorized collaboration, cheating, copying or plagiarism found in this course will be reported and the appropriate sanctions applied. The Department of Chemistry and Biochemistry offers a seminar on the academic conduct code and the appropriate use of information sources which aims to clarify what practices will be considered unacceptable with regards to work submitted for grading in Chemistry and Biochemistry courses. Attendance at this seminar is highly recommended and represents a clear and fair opportunity to learn what our faculty regards as academic misconduct. Failure to take part in this learning opportunity and thus ignorance of these regulations is no excuse and will not result in a reduced sanction in any case where academic misconduct is observed. This short seminar (1 hour) will be held at the following times (note that late-comers will not be admitted):

Date	Time	Place
Monday, Jan. 23	16:45-17:45	HC-155
Monday, Jan. 23	20:45-21:45	HC-155
Tuesday, Jan. 24	16:45-17:45	CC-308
Wednesday, Jan. 25	16:45-17:45	HC-155
Wednesday, Jan. 25	20:45-21:45	SP-S110
Thursday, Jan. 26	16:45-17:45	HC-155
Friday, Jan. 27	16:45-17:45	CC-310

As space for each of the seminars is limited by the room size, please sign up to your preferred time. Sign up sheets are available outside SP 201.01 (Departmental office).

In the event of extraordinary circumstances beyond the University's control, the content and/or evaluation scheme in this course is subject to change.

IMPROVING STUDENTS' ACADEMIC EXPERIENCE

LIST OF AVAILABLE SERVICES

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- **Ms. Hilary Scuffell, Academic Advisor, Chemistry & Biochemistry**
 - **Concordia Counselling and Development** offers career services, psychological services, student learning services, etc.
<http://cdev.concordia.ca/>
 - **The Concordia Library Citation and Style Guides:**
<http://library.concordia.ca/>
 - **Advocacy and Support Services**
<http://supportservices.concordia.ca/>
 - **Student Transition Centre**
<http://stc.concordia.ca/>
 - **New Student Program**
<http://newstudent.concordia.ca/>
 - **Access Centre for Students with Disabilities**
<http://supportservices.concordia.ca/disabilities/>
 - **Student Success Centre**
<http://studentsuccess.concordia.ca/>
 - **The Academic Integrity Website**
<http://provost.concordia.ca/academicintegrity/>
 - **Financial Aid & Awards**
<http://web2.concordia.ca/financialaid/>
 - **Health Services**
<http://www-health.concordia.ca/>

