CHEM 333

Introduction to Quantum Theory

A. General Information

- Course: CHEM 333, *Introduction to Quantum Theory*, 3 credits, Winter 2023.
- Time and place: Tuesdays, 18:00-20:45, CJ-1.121.
- 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, **CHEM 333 51 2224**.
- Office Hours: Wednesdays, 13:15-14:45, 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 Schroedinger 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 Applied 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. Exam Schedule (May be subject to change)

- Midterm Exams, during class time, tentatively February 21 and March 21, 2023.
- Final Exam, during exam period (April 20 - May 2), date TBA.

E. Course Materials

Standard textbooks (none required):

- *Physical Chemistry*, Laidler, Meiser and Sanctuary.
- *Quantum Chemistry and Spectroscopy*, Engel (advanced).

- *Physical Chemistry*, Atkins & De Paula, or *Physical Chemistry, Volume 2: Quantum Chemistry, Spectroscopy, and Statistical Thermodynamics* Atkins & De Paula. On reserve in the Library.
  Note: Selected useful chapters from the 8th edition are available electronically from the library via links on the Moodle course page.
- *Physical Chemistry: A Molecular Approach*, McQuarrie & Simon.

F. Grading / Evaluation

- The final grade is based on two midterm exams (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 can 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

All individuals participating in courses are expected to be professional and constructive throughout the course, including in their communications. Concordia students are subject to the Code of Rights and Responsibilities which applies both when students are physically and virtually engaged in any University activity, including classes, seminars, meetings, etc. Students engaged in University activities must respect this Code when engaging with any members of the Concordia community, including faculty, staff, and students, whether such interactions are verbal or in writing, face to face or online/virtual. Failing to comply with the Code may result in charges and sanctions, as outlined in the Code.

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, translating the work of another person into French or English and not citing the source is also plagiarism.

Please consult https://www.concordia.ca/conduct/academic-integrity.html for further information.

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Mandatory quiz and seminar

"CHEM 101": The Academic Code of Conduct: Ethical Use of Information Sources

As part of your CHEM course, you are **required** to i) attend a Chemistry and Biochemistry Departmental Seminar on the academic conduct code and the appropriate use of information sources and ii) pass the online quiz associated with this seminar (the passing grade for the quiz is 100%). **Note**: this quiz is graded by the Department of Chemistry and Biochemistry, and you do not have access to it until after you have attended the seminar. Therefore, any other quiz you may have taken on the academic code of conduct does not count toward the CHEM 101 requirement. The aim of this seminar and quiz is to clarify the academic conduct code in terms of which practices will be considered unacceptable with regards to work submitted for grading in your CHEM course. **You are only exempt from repeating the seminar and the quiz if you have done both in Winter 2018 or more recently**,* otherwise you are required to repeat both this term. This short seminar (1 hour) will be held at the following times (note that you will not be given credit if you join too late and/or leave too early):

Date (Winter 2023)	Time (EST)	Mode	Registration link
Jan. 24 (Tuesday)	21:00-22:00	Zoom	https://concordia-ca.zoom.us/meeting/register/tZUrcemqrj4tHNYUyp-gnOR8uREtmKGIyU9u
Jan. 26 (Thursday)	21:00-22:00	Zoom	https://concordia-ca.zoom.us/meeting/register/tZckf-GhqDkuHNA4TuWQ5yWQqBPGD_Ai27-l

As space for each of the Zoom seminars is limited, please **register early** for your preferred slot (copy the corresponding link above into your browser). You will **receive** a notice from Zoom with the link to the actual seminar. Then do not forget to **attend** that seminar slot on the date above! Attendance at the Zoom seminar will be recorded.

If you do not complete this course requirement, your final grade for the course may be lowered by one full letter grade with an incomplete (INC) notation until such time as this requirement is completed. Please refer to the undergraduate calendar (section 16.3.5) for details on removal of an incomplete notation.

* You are exempt if you can locate your ID in the pdf file on the Department web site (http://www.concordia.ca/content/dam/artsci/chemistry/docs/Compliance-list.pdf) and if there is no entry in the "quiz" column for you.

Plagiarism and other forms of academic dishonesty

The Academic Code of Conduct can be found in section 17.10 of the academic calendar (https://www.concordia.ca/academics/undergraduate/calendar/current/section-17-university-secretariat/section-17-10-academic-integrity-and-the-academic-code-of-conduct.html). Any form of unauthorized collaboration, cheating, copying or plagiarism found in this course will be reported and the appropriate sanctions applied. The mandatory seminar is 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.

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