

Inter-American University of Puerto Rico
_____ *Campus*
Department of _____
Chemistry Program

Syllabus

I. General Information

Course Title:	Quantum and Kinetics
Code and Number:	CHEM 3920
Credits:	4 credits
Requirements:	PHYS 3002, MATH 2252, CHEM 2222, 3320 and 3330
Academic Term:	
Professor:	
Office Hours:	
Office Phone:	
Email:	

II. Course Description:

Theoretical and experimental study of the fundamental physical principles that govern the properties and behavior of chemical systems, with emphasis on the microscopic aspect. It includes quantum mechanics and its application to atomic and molecular structure, spectroscopy, and chemical kinetics. It requires 45 hours of conference and 45 hours of face-to-face laboratory.

III. Objectives

1. Course Goals

Upon successful completion of the CHEM 3920 course, the student will have acquired the following knowledge and developed the corresponding skills:

- 1.1. Apply the postulates of quantum mechanics to the particle in the box, harmonic oscillator, and rigid rotor.
- 1.2. Description of simple atoms (H, He⁺, Li²⁺, He) and simple molecules (H⁺₂, H₂) according to the principles of quantum mechanics. Knowledge of the LCAO method for simple molecules.
- 1.3. Application of the principles of quantum mechanics to matter-light interaction: spectra of rotation and vibration of diatomic molecules; electronic spectra of atoms and molecules; magnetic spectroscopy; Raman spectroscopy.

- 1.4. Differential and integrated kinetic expressions for single-step and multi-step reactions, with emphasis on zero-order, first-order, and second-order reactions. Relaxation processes; speed laws and mechanisms. Steady-state approximation; enzymatic catalysis and activated complex.

2. Enabling Objectives:

The following objectives enable the student to achieve the terminal objectives of the course.

2.1. Historical Development and Experimental Basis of Quantum Mechanics

- 2.1.1 Discuss blackbody radiation and Planck's explanation in terms of its importance to quantum theory.
- 2.1.2. Discuss the photoelectric effect and Einstein's explanation in terms of its importance to quantum theory.
- 2.1.3. Discuss the spectrum of the hydrogen atom and Bohr's explanation in terms of its importance to quantum theory.
- 2.1.4. Identify the expression for the de Broglie wavelength and the explanation and importance of its meaning.
- 2.1.5. Enunciate Heisenberg's uncertainty principle and explain its importance and meaning.

2.2. Postulates of Quantum Mechanics

- 2.2.1. Discuss how a system is defined according to Quantum Mechanics.
- 2.2.2. Identify the time-dependent Schrödinger equation and explain its meaning.
- 2.2.3. Describe the meaning of $|\Psi|^2$ and $|\Psi|^2 dx dy dz$. Identify the normalization condition of Ψ (the wave function).
- 2.2.4. Identify the time-independent Schrödinger equation and explain its meaning.
- 2.2.5. Establish the mathematical conditions that a wave function must meet to be an acceptable solution of the Schrödinger equation.

2.3. Applications of Quantum Mechanics

- 2.3.1. Solve the Schrödinger equation for a particle of mass "m" in a one-dimensional box. Identify the expression for Ψ .
- 2.3.2. Identify the expression for the energy of a particle in a one-dimensional box.
- 2.3.3. Graphically represent Ψ as a function of x and $|\Psi|^2$ as a function of x for a particle in a one-dimensional box for different values of n . Discuss their importance in terms of probability.
- 2.3.4. Generalize to two and three dimensions the results of the particle in a one-dimensional box. Identify the expressions for Ψ (n_x, n_y, n_z) and E (n_x, n_y, n_z).
- 2.3.5. Define and illustrate with examples the concept of degeneration for an energy level.
- 2.3.6. Define and illustrate with examples the concept of a quantum mechanical operator. Apply operator algebra.
- 2.3.7. Identify and define the most common operators in Quantum Mechanics. Write operators' expressions for properties such as momentum, kinetic energy, and potential energy.
- 2.3.8. Write the Hamiltonian operator for a system of "n" interacting particles in three dimensions.
- 2.3.9. Write the time-independent Schrödinger equations in terms of the Hamiltonian operator.
- 2.3.10. Identify the expression for the average value (or expectation value) of a physical property M , $\langle M \rangle$.
- 2.3.11. Write the Schrödinger equation for a simple harmonic oscillator and identify the expression of the oscillator energy.
- 2.3.12. Write the Schrödinger equation for the rigid rotor and identify the expression for the rotational energy. Explain the degeneration of rotational energy levels.
- 2.3.13. Discuss the variational method for obtaining approximate values of energy.

2.4. Atomic Structure

- 2.4.1. Write the Hamiltonian operator for hydrogen-like atoms (H, He⁺, Li²⁺, Be³⁺, ...).
- 2.4.2. Write the Schrödinger equation for hydrogen-like atoms and explain its meaning.
- 2.4.3. Express the wave function for hydrogen atoms in terms of the radial function and angular functions.
- 2.4.4. Identify and define the quantum numbers associated with the wave function of hydrogen atoms. Establish their possible values.
- 2.4.5. Identify the expression for the energy of hydrogen-like atoms in terms of the principal quantum number (n).
- 2.4.6. Define the concept of orbital angular momentum of the electron and discuss its quantization.
- 2.4.7. Discuss the real wave functions for hydrogen-like atoms.
- 2.4.8. Define the concepts of orbital and its shape. Draw the shapes of the orbitals s, p and d.
- 2.4.9. Define the concept of intrinsic angular momentum of the electron in hydrogen atoms and discuss their quantization.
- 2.4.10. Write the Hamiltonian operator for atoms with two electrons (He, Li⁺, Be²⁺...) and explain the meaning of each term in the expression.
- 2.4.11. Write the wave function for two-electron atoms and explain its meaning.
- 2.4.12. Discuss spin functions for two-electron atoms; write the possible combinations of spin functions and identify their symmetric or antisymmetric character.
- 2.4.13. Enunciate the Pauli Principle and explain its importance.
- 2.4.14. Discuss, through He's excited states, the concepts of "atomic term" and "multiplicity".
- 2.4.15. Enunciate Hund's rule and explain its importance.

2.5. Molecular Structure

- 2.5.1. Write the general expression of the Hamiltonian operator for a molecule and explain its meaning.
- 2.5.2. Discuss the Born-Oppenheimer approach. Write the Schrödinger equations for the motion of electrons and nuclei.
- 2.5.3. Write the Expression of the Hamiltonian Operator for H_2^+ and explain its meaning.
- 2.5.4. Discuss LCAO theory and define the concept of molecular orbital (MO).
- 2.5.5. Discuss the concepts of bonding and anti-bonding molecular orbital; "gerade" (g) and "ungerade" (u).
- 2.5.6. Define the concept of σ , π y δ . molecular orbital.
- 2.5.7. Draw the following linear combinations of atomic orbitals:
- $$1s_A + 1s_B \quad y \quad 1s_A - 1s_B \qquad 2p_{z,A} + 2p_{z,B} \quad y \quad 2p_{z,A} - 2p_{z,B}$$
- $$2p_{x,A} + 2p_{x,B} \quad y \quad 2p_{x,A} - 2p_{x,B} \qquad 2p_{y,A} + 2p_{y,B} \quad y \quad 2p_{y,A} - 2p_{y,B}$$
- Identify in the resulting molecular orbital: the type of orbital (σ, π), its symmetry (g ó u) and its bonding or anti-bonding character.
- 2.5.8. Represent the energy level diagram for molecular orbitals of homonuclear diatomic molecules. Write the electron configuration of these molecules and determine the bond order.
- 2.5.9. Write the expression of the Hamiltonian operator for the molecule of H_2 and explain its meaning.
- 2.5.10. Identify the approximate wave function for the H_2 molecule (MO).
- 2.5.11. Represent an energy level diagram for valence molecular orbitals of heteronuclear diatomic molecules. Write the electron configuration of these molecules and determine the bond order.
- 2.5.12. Discuss a simple triatomic molecule according to the theory of molecular orbitals.
- 2.5.13. Write the approximate wave function of $BeHe_2$ according to Slater's determinant and explain its meaning.
- 2.5.14. Define the concept of hybrid orbitals and illustrate with examples.

- 2.5.15. Identify bonds of the type σ , π y δ in a molecule.
- 2.6. Spectroscopy (Basic Concepts, some topics are discussed in the laboratory)
- 2.6.1. Discuss Maxwell's theory of electromagnetic radiation
- 2.6.2. Define the concepts of wavelength, frequency and wave number applied to electromagnetic radiation. Establish the relationships between those quantities and the units in which they are represented.
- 2.6.3. Identify the different regions of the electromagnetic spectrum.
- 2.6.4. Discuss the quantum theory of electromagnetic radiation.
- 2.6.5. Describe the results of the quantum mechanical treatment of the interaction between matter and electromagnetic radiation. Explain what absorption, spontaneous emission and stimulated emission is.
- 2.6.6. Write the expression that determines the probability of a transition between the states "m" and "n" and explain its meaning.
- 2.6.7. Write the selection rules for transitions in the systems: particle in the box, simple harmonic oscillator, and rigid rotor.
- 2.6.8. Discuss the Beer-Lambert law concerning absorption. Define the concepts of absorption, transmittance, and molar absorptivity.
- 2.7. Rotational and Vibrational Spectra of Diatomic Molecules in Gas Phase (Discussed in the laboratory)
- 2.7.1. Write the expressions for the rotational and vibrational energy of diatomic molecules and explain their meaning.
- 2.7.2. Identify the expression for the internal energy of a diatomic molecule that includes corrections due to anharmonicity, vibration-rotation interaction and centrifugal distortion, explain its meaning.
- 2.7.3. Discuss the separation between molecular internal energy levels (translational, rotational, vibrational, and electronic) and the relative populations of these levels in terms of Boltzmann's law of distribution.

- 2.7.4. Write the selection rules for transitions between vibration-rotation levels within the same electronic level, in diatomic molecules and explain their meaning.
- 2.7.5. Identify the expressions for the frequency and wavenumber of the pure rotational transitions, for diatomic molecules and explain their meaning.
- 2.7.6. Describe the information that can be obtained from the analysis of a pure rotational spectra of a diatomic.
- 2.7.7. Establish the position of the origin of the bands in the vibration-rotation (IR) absorption spectrum of diatomic molecules. Identify the fundamental band and the overtones, indicating the transitions that give rise to these bands.
- 2.7.8. Identify wavenumber expressions for the R and P branches of the absorption band of the vibration-rotation absorption spectrum of diatomic molecules. Draw the corresponding transitions on the vibration-rotation energy level diagram.
- 2.7.9. Describe the information that can be obtained from the analysis of the vibration-rotation spectra of diatomic molecules.

2.8. Electronic Spectra

- 2.8.1. Write the expression for the wavenumber for the electronic spectrum of the hydrogen atom and explain its meaning. Identify the different hydrogen emission lines and the transitions that originate them.
- 2.8.2. Write the expression for the frequency corresponding to molecular electronic transitions and explain its meaning.
- 2.8.3. Identify the most important selection rule for molecular electronic transitions.
- 2.8.4. Describe the bands in the electronic spectra of molecules and identify the information they provide.

2.9. NMR Spectroscopy

- 2.9.1. Define the concepts of magnetic induction and magnetic dipole moment.

- 2.9.2. Write the energy expression for a magnetic dipole exposed to an external magnetic field and explain its meaning.
- 2.9.3. Define the concept of spin angular momentum and establish its quantization.
- 2.9.4. Identify the expression for the magnetic dipole moment of a nucleus.
- 2.9.5. Identify the selection rule for transitions between nuclear spin energy levels and expression for the corresponding absorption frequency.
- 2.9.6. Define the concept of a shielding constant of a nucleus and explain its meaning. Write the expression for the NMR absorption frequency in terms of that constant.

2.10. Chemical Kinetics

- 2.10.1 Define the concepts of reaction rate, rate law, partial and total order of a reaction, rate constant, half-life and reaction mechanism.
- 2.10.2. Discuss the most common experimental methods for determining the rate of a reaction.
- 2.10.3. Integrate the differential equation for a first-order, zero-order, and second-order rate law. Discuss the graphical method for determining the rate constant. Identify the expressions for the half-life.
- 2.10.4. Present the differential equation corresponding to a reaction of the type Reactants \rightarrow Products. Discuss the graphical method for determining the rate constant. Identify the expression for the half-life.
- 2.10.5. Discuss reversible, consecutive, and competitive reactions for first order and zero order.
- 2.10.6. Discuss the main methods for the experimental determination of the rate law.
- 2.10.7. Define the concept of elementary reaction and identify its types: unimolecular, bimolecular and trimolecular.
- 2.10.8. Establish the expression of the rate law and the equilibrium constant for elementary reactions.

- 2.10.9. Discuss the rate-determining step approximation to obtain the rate law from a mechanism.
- 2.10.10. Discuss the steady-state approximation to obtain the rate law from a mechanism.
- 2.10.11. Write the Arrhenius equation for the rate constant and explain its meaning.
- 2.10.12. Discuss the graphical method for determining the activation energy from the values of the rate constant at different temperatures.
- 2.10.13. Discuss the Lindemann 's mechanism for unimolecular reactions.
- 2.10.14. Discuss experimental methods for determining the rate of rapid reactions.
- 2.10.15. Discuss the relaxation kinetics for the elementary reaction $A + B \rightleftharpoons C$ and define the concept of relaxation time.
- 2.10.16. Define the concepts of catalyst and catalysis. Identify the types of catalysis.
- 2.10.17. Write the generic expression of the rate law of a catalyzed reaction and explain its meaning.
- 2.10.18. Discuss the Michaelis-Menten mechanism for enzymatic catalysis.
- 2.10.19. Discuss the Langmuir isotherm model for heterogeneous catalysis.

UNDERGRADUATE PROFILE COMPETENCES ADDRESSED IN THIS COURSE

1. Correctly perform the most characteristic calculations of kinetics and quantum chemistry such as reaction life times, concentrations, probabilities and energies.
2. Show willingness towards the use of new technologies and scientific developments, including the integration of the computer into data analysis.
3. Analyze and interpret experimental data and scientific literature related to the course topics.
4. Awareness of ethical and cultural values in the practice of chemistry.

1. Course Content

IV.1. Quantum mechanics

- IV.1.1 Experimental observations and historical perspectives
- IV.1.2 Postulates of Quantum Mechanics
- IV.1.3 Applications of Quantum Mechanics to simple systems.
- IV.1.4 Computational methods

IV.2. Atomic Structure

- IV.2.1. Hydrogen atom and its wave functions
- IV.2.2. Electronic spin and Pauli's Exclusion Principle
- IV.2.3. Helium atom and its wave functions

IV.3. Molecular Structure

- IV.3.1. Hydrogen molecule-ion H_2^+
- IV.3.2. Hydrogen molecule H_2
- IV.3.3.3 LCAO Method

IV.4. Spectroscopy

- IV.4.1. Basic concepts
- IV.4.2. Rotational and vibrational spectra of diatomic molecules.
- IV.4.3. Electronic spectra
- IV.4.4. NMR spectra

IV.5. Chemical Kinetics

- IV.5.1. Rate Laws
- IV.5.2. Integrated rate laws
- IV.5.3. Elementary reactions
- IV.5.4. Reaction mechanisms
- IV.5.5. Approximations to establish rate laws from mechanisms.
- IV.5.6. Homogeneous and heterogeneous catalysis
- IV.5.7. Unimolecular reactions
- IV.5.8. Rapid reactions (flash photolysis; T-jump)

1. Laboratory Activities:

All students will perform the following experiments. **Each** student will submit an **individual** lab report following the guidelines in the Laboratory Manual:

1. Effect of temperature on the rate constant of a reaction
2. Alkaline hydrolysis of an ester (Using conductance measurements)
3. Balmer Series
 1. Particle in a Box
 2. IR Spectrum of a Diatomic
 3. pK_a of 2-naftol in the first singlet state
 4. Flash-Photolysis of a Rapid isomerization
 5. Computational Experiment

The laboratory manual has been prepared by Professor Colom and is available on "Blackboard".

V. Grading

1. The evaluation of the course consists of two parts:

Lecture (70%) and Laboratory (30%). The following table contains the grading details:

Evaluation Criteria	Points	Weight (%)
Partial Exam 1	100	17.5
Partial Exam 2	100	17.5
Partial Exam 3	100	17.5
Final examination	100	17.5
Total Points	400	70%

2. The lecture component consists of three partial exams and a final exam of all the material discussed in class. All exams have the same weight.

- **THERE ARE NO EXAM RETAKES. IF YOU DO NOT TAKE ONE OF THE PARTIAL EXAMS THE FINAL EXAM WILL BE COUNTED BY TWO, THIS IS AS LONG AS YOU PRESENT A VALID EXCUSE.**
 - A total of three to four quizzes of 10 pts each will be offered as a bonus. These quizzes will be available on Blackboard until the last day of class You have 2 opportunities and 20 minutes for each quiz. There is no retake for quizzes
 - The bonus points accumulated by the student are added to the total points of the lecture component.
1. **IN THIS COURSE THERE ARE NO "SPECIAL ASSSIGMENTS" TO RAISE GRADES.**

3. The Laboratory component includes 7 to 8 laboratory reports, a performance evaluation, and a final exam.

Laboratory Evaluation:

	Points	weight
7 laboratory reports	700	15%
Performance	100	5%
Final Exam	100	10 %
Total	900	30%

IF YOU ARE ABSENT FROM A LABORATORY, YOU CANNOT SUBMIT THE REPORT OF THAT EXPERIMENT.

BY RULES OF THE DEPARTMENT OF NATURAL SCIENCES, IF YOU ARE ABSENT FROM THREE LABORATORIES OR MORE YOU WILL RECEIVE "F" IN THE COURSE.

1. Grading Scale used in CHEM 3920

The final grade of the course is calculated by adding the percent obtained in the lecture (of 70%) and that obtained in the laboratory (of 30%).

100-85 A 84 - 75 B 74 - 65 C 64 – 55 D 54 - 0 F

FOR YOUR INFORMATION: This course introduces and discusses topics using presentations in Blackboard Collaborate Ultra. Presentations may be shared or provided by the teacher, but it is NOT obligatory to do so. Be clear that these presentations are NOT prepared for the student to study from them. It is NOT recommended to use them as the only source of study for exams. You should use the textbook to study the topics discussed in class and practice problems. Presentations may change continuously at the discretion of the teacher. Not everything discussed in class is necessarily in these presentations.

1. SPECIAL NOTES

A. Servicios Auxiliares o Necesidades Especiales

Any student who requires auxiliary services or special assistance must request them at the beginning of the course or as soon as he acquires knowledge of the services he will need, through registration in the Oficina del Consejero Profesional, el Sr. José Rodríguez del Programa de Orientación Universitaria.

B. Honesty, Plagiarism and fraud:

It is important to be clear that the different forms of plagiarism (the use of someone else's ideas or words without due recognition) is an academic infraction with very serious consequences. Dishonesty, fraud, plagiarism and any other inappropriate behavior in relation to academic work constitute infractions sanctioned by the *General Regulations of Students of the Inter-American University* (see from page 60 onwards for examples of the types of plagiarism and the sanctions that apply). Among the sanctions is the suspension of the University for a defined period of more than one year or the permanent expulsion from the University. In this course this type of practice will be penalized **ESPECIALY IN LABORATORY REPORTS**.

C. USE OF ELECTRONIC DEVICES DURING CLASS

Cell phones and any other electronic device that could interrupt teaching and learning processes or alter the environment conducive to academic excellence will be deactivated. Emergency situations will be addressed, as appropriate. The handling of electronic devices that allow access, storage or sending data during evaluations or exams is prohibited.

D. Compliance with the provisions of Title IX

The Federal Higher Education Act, as amended, prohibits discrimination based on gender in any academic, educational, extracurricular, athletic, or any other program or employment, sponsored or controlled by an institution of higher education regardless of whether it is conducted on or off the institution's premises, if the institution receives federal funds.

In accordance with current federal regulations, our academic unit has appointed a Title IX Assistant Coordinator who will provide assistance and guidance regarding any alleged incident constituting discrimination based on gender, sexual harassment or sexual assault. You can contact the Assistant Coordinator at the telephone Mr. George Rivera, extension 2262 or 2147, or email griverar@metro.inter.edu.

The Normative Document entitled **Norms and Procedures to Address Alleged Violations of the Provisions of Title IX** is the document that contains the institutional rules to channel any complaint that is filed based on this type of allegation. This document is available on the website of the Inter-American University of Puerto Rico (www.inter.edu).

Course Text:

Levine, I.N. "Physical Chemistry", 6th Edition (2009), McGraw-Hill, Inc.: New York. ISBN 978-0-07-253862-5

Laboratory Manual CHEM 3920, (on BlackBoard) by Dr. Antonio Colom

IX: Bibliography:

1. Shoemaker et al., "Experiments in Physical Chemistry", 7th Edition, McGraw-Hill: New York, 2003.
2. Raff, L.M., "Principles of Physical Chemistry", Prentice Hall: Upper Saddle River, New Jersey, 2001.
3. Ball, D. "Physical Chemistry", Brooks/Cole-Thomas Learning: Pacific Gove, CA, 2003.
4. Laidler, K.J. et al., "Physical Chemistry", 4th Edition, Houghton Mifflin Company: Boston, MA, 2003.
5. Atkins, P. and de Paula, J. "Physical Chemistry", 7th Edition, W.H. Freeman and Company: New York, 2002.

Updated OCT 2021