SAGRADO
Universidad del Sagrado Corazón

SCHOOL OF HEALTH AND SCIENCES

SYLLABUS

TITLE:	Physical Chemistry I
CODE:	QUI 401
PREREQUISITE:	QUI 202 and FIS 203
CORREQUISITES:	QUI 401L
CREDITS:	4 credits | 45 contact hours | 45 lab hours | 1 term

DESCRIPTION

Course developed in a theoretical and experimental way where the active learning methodology is used so that Chemistry students acquire knowledge related to quantum mechanics and simple problem solving. It discusses topics such as particle in the box, simple harmonic oscillator, rigid rotor, and hydrogen atom as well as approximation methods, variation theorem and perturbation theory, polyelectronic atom systems and single molecules, principles of molecular and atomic spectroscopy, gas kinetic theory, and fundamental principles of the kinetics of chemical reactions.

JUSTIFICATION

In introductory and intermediate Chemistry courses, students learn and use a number of properties that are a product of Chemistry laws. The Physical Chemistry course offers the physical and mathematical foundation of these laws and how the properties of matter that explain and predict its behavior are derived from them. Only knowledge at this level allows for the conscious transformation of matter for the benefit of human beings. In the final analysis, this is the purpose of scientific knowledge. This course allows Chemistry students to apply this knowledge in their professional development, whether in the chemical industry or in scientific research.

COMPETENCES

The course develops the following competences in students:

- **Critical questioning**
- **Research and exploration**

OBJECTIVES

After completion of the course, students will be able to:

1. Explain the state functions of the particle in the box, the harmonic oscillator, the rigid rotor, and the hydrogen atom by applying the Schrödinger equation.
2. Apply the variation method and the perturbation theory.
3. Approximate wavefunctions of higher atoms using the Slater determinant.
4. Use atomic orbitals to generate molecular orbitals of simple molecules.
5. Know the fundamentals of spectroscopy of diatomic molecules.
6. Explain the kinetic theory of gases.
7. Apply the integrated forms of reactions with rate laws of various orders.
8. Derive rate laws from reaction mechanisms using the slow-step and steady-state approximations.

CONTENTS

I. Quantum Mechanics
   A. Historical development
   B. Fundamentals of quantum mechanics
      1. Schrödinger equation
      2. Postulates of quantum mechanics
   C. Simple applications
      1. Free particle
      2. Particle in a box
      3. Simple harmonic oscillator
      4. Rigid rotor
   D. Angular momentum
   E. Hydrogen atom
   F. Approximation methods
      1. Variation method
      2. Perturbation theory
   G. Polyelectronic atoms
      1. Spin functions and the Pauli exclusion principle
      2. Slater's determinants
   H. Diatomic molecules

I. H_2^+ and H_2
J. Linear combinations of atomic orbitals (LCAO)

II. Atomic and Molecular Spectroscopy
   A. Electronic states and selection rules
   B. Vibrational and rotational spectroscopy

III. Chemical Kinetics
   A. Kinetic theory of gases
   B. Kinetics of gas-phase reactions
      1. Integrated Rate Law
      2. Mechanisms
      3. Temperature dependency
   C. Kinetics of reactions in solution
   D. Heterogeneous catalysis

LAB EXPERIENCES

A. Bohr's Theory
B. Particle in a potential box
C. Harmonic oscillator
D. Rigid rotor
E. Atomic and molecular orbitals
F. Molecular spectroscopy
G. Kinetic data analysis
H. Dependence of temperature on velocity constants

METHODOLOGY

The following strategies from the active learning methodology are recommended:

- Solution of a problem posed
- Literature research
- Lecture
- Phenomenon-based learning: observation, discussion, and analysis of processes, problems, or phenomena
- Collaborative learning and teamwork
- Demonstration & hands-on exercises

EVALUATION

Participation	15%
Partial assignments	30%
Compositions	15%
Final exam	20%
Immersion experience	20%
Total	**100%**

LEARNING ASSESSMENT

The institutional assessment rubric is applied to the course's core activity.

BIBLIOGRAPHY

TEXTBOOK

Atkins, P., De Paula, J., & Keeler, J. (2018). *Physical Chemistry* (11th ed.). Oxford University Press.

REFERENCES

Carey, F. (2019). *Organic Chemistry* (11th ed.). McGraw Hill Higher Education.

Engel, T. (2019). *Physical Chemistry: Quantum Chemistry and Spectroscopy* (4th ed.). Pearson.

Tinoco, I., Sauer, K., Wang, J., Puglisi, J., Harbison, G., & Rovnyak, D. (2014). *Physical Chemistry: Principles and Applications in Biological Sciences* (5th ed.). Pearson.

ELECTRONIC RESOURCES

American Chemical Society. (n.d.). *ACS Chemistry for Life*. https://www.acs.org/content/acs/en.html

Massachusetts Institute of Technology (2020). MITOPENCOURSEWARE. https://ocw.mit.edu/courses/chemistry/5-60-thermodynamics-kinetics-spring-

2008/lecture-notes/

Scientific Research an Academic Publisher (2011-2020). Open Journal of Physical Chemistry. https://www.scirp.org/journal/ojpc/

For more information resources related to the course's topics, access the library's webpage http://biblioteca.sagrado.edu/

REASONABLE ACCOMMODATION

For detailed information on the process and required documentation you should visit the corresponding office. To ensure equal conditions, in compliance with the ADA Act (1990) and the Rehabilitation Act (1973), as amended, any student in need of reasonable accommodation or special assistance must complete the process established by the Vice Presidency for Academic Affairs.

ACADEMIC INTEGRITY

This policy applies to all students enrolled at Universidad del Sagrado Corazón to take courses with or without academic credit. A lack of academic integrity is any act or omission that does not demonstrate the honesty, transparency, and responsibility that should characterize all academic activity. Any student who fails to comply with the Honesty, Fraud, and Plagiarism Policy is exposed to the following sanctions: receive a grade of zero in the evaluation and / or repetition of the assignment in the seminar, a grade of F (*) in the seminar, suspension, or expulsion as established in the Academic Integrity Policy effective in November 2022.