# NATIONAL UNIVERSITY OF ENGINEERING
## COLLEGE OF SCIENCES
## CHEMISTRY PROGRAM

# CQ362 – QUANTUM CHEMISTRY

## I. GENERAL INFORMATION

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|---|---|
| **CODE** | : CQ362 – Quantum Chemistry |
| **SEMESTER** | : 5 |
| **CREDITS** | : 04 |
| **HOURS PER WEEK** | : 06 (Theory – Practices – Laboratory) |
| **PREREQUISITES** | : Physical-chemistry II<br>Mathematics for chemists |
| **CONDITION** | : Mandatory |

## II. COURSE DESCRIPTION

The course is part of the professional specialization area, is of a theoretical nature and is aimed at training the student in the fundamental aspects on which modern Atomic Theory and the atomic - molecular structure are based, from a chemical approach, which allows the student to explain and solve specific situations applied to problems inherent to Chemistry.
Its content is organized into four thematic units of learning: **I.** Introduction: Introduction and origin of Quantum Theory. **II.** Fundamentals of Quantum Mechanics. **III.** Hydrogen atom and quantum numbers. **IV.** Fundamentals of Spectroscopy and Molecular Structure.

## III. COURSE OUTCOMES

a) Generic Outcomes

By the end this course the student will have the:

- Capacity for abstraction, analysis and synthesis.
- Ability to apply knowledge and relate them to different areas of Chemistry.
- Ability to organize and plan time.
- Oral and written communication skills.
- Skills in the use of ICTs.
- Skills to search, process and analyze information from different sources.
- Ability to identify, formulate and solve problems.
- Capacity for teamwork.

b) Specific Outcomes

By the end this course the student will:

- Interpret the fundamental postulates of Quantum Mechanics and apply differential and integral calculus to be able to deduce and / or formulate mathematical models that allow it to solve complex situations related to the atomic and molecular structure.

- Review the fundamental aspects of modern physics and on these, analyze the aspects that gave rise to the quantum theory.

- Develop the Schrodinger equation and interpret the wave function applying the postulates of Quantum Mechanics, formulated for hydrogen atoms and construct simple models such as particle in a box and circle of potential by applying the Schrodinger equation.

- Explain the general behavior of hydrogen atoms by optimizing the appropriate wave function, interpreting the meaning of quantum numbers from a chemical approach.

- Interpret the basic concepts of photochemistry and spectroscopy, to select useful information about the atomic and / or molecular structure.

- Recognize the dual behavior of matter and accept the modifications that the old atomic theory undergoes to build the basis of modern quantum theory.

- Justify the importance of the Schrodinger equation for the formulation of multiple mathematical models and physical systems applied to the description of the atom.

- Accept the modern atomic conception and, on it, adopt an analytical and objective posture of the behavior of matter.

## IV. LEARNING UNITS

1. **INTRODUCTION AND ORIGIN OF THE QUANTUM THEORY / 12 HOURS**
   Relationship between energy and relativistic mass / Blackbody radiation and photoelectric effect / Photon moment, particle nature of light / Young experiment / Compton effect / Pilot waves of Louis' De Broglie / The Bohr atomic model for the atom hydrogen.

2. **CHAPTER 2. FUNDAMENTALS OF QUANTUM MECHANICS / 16 HOURS**
   Electron diffraction / Electron microscope / Uncertainty principle / Independent and time-dependent Schrodinger equation / Operators and postulates of Quantum Mechanics / Normalization condition and orthogonality of the wave function / Particle in one-dimensional box / Color of simple organic molecules / Particle in three-dimensional box / Color of simple aromatic organic molecules. Potential circle model / Molecular stability / Frontier orbitals / Fuckui's molecular orbital theory / Hückel's rule / Fermi energy and metal bond / Band theory. Tunnel effect and probability of quantum tunneling / Tunneling microscope.

3. **CHAPTER 3. HYDROGEN ATOM AND QUANTUM NUMBERS / 12 HOURS**
   The Schrodinger equation in polar coordinates / Quantum numbers and radial and angular function / Probability density / Radial probability distribution / Atomic orbitals / Angular momentum / Electronic spin moment / Pauli exclusion principle / Polyelectronic atoms / Determination of the functions of radial and angular wave through the Schrodinger equation.

4. **CHAPTER 4. FOUNDATIONS OF SPECTROSCOPY AND MOLECULAR STRUCTURE / 12 HOURS**
   Quantum harmonic oscillator and infrared spectroscopy / Potential energy well / Vibrational levels. Rigid linear rotor, rotational levels and pure rotational spectroscopy / Rotational constant and moment of inertia of linear diatomic molecules / Nuclear magnetic resonance spectroscopy / Lambert- Beer 's law / Electronic transitions / Jablonsky diagrams / Approximate

methods of quantum mechanics: Approximation of the central field, screen effect and ionization energies with effective nuclear charge. Slater rules.

## V. LABORATORIES AND PRACTICAL EXPERIENCES

1. Laboratory 1: General Relativity and Blackbody Radiation.
2. Laboratory 2: Photoelectric Effect and Compton Effect.
3. Laboratory 3: Bohr model for the Hydrogen atom.
4. Laboratory 4: Mechanical quantum operators and Shrodinger equation
5. Laboratory 5: Particle in one, two and three-dimensional boxes.
6. Laboratory 6: Metallic Bond and Tunnel Effect.
7. Laboratory 7: Hydrogen atom and wave functions.
8. Laboratory 8: Pure vibrational and rotational spectroscopy.

## VI. METHODOLOGY

Teaching:

- Exposition and debate, encouraging the constant participation of the student.
- Work in pairs for the electron properties exposition.
- Oral demonstrations of proposed exercises.

Learning

- Search and collection of bibliographic information about the types of spectroscopy.
- Expositions in pairs of the entrusted works.
- Workshops with proposed exercises to develop as a group in class.

## VII. EVALUATION FORMULA

Calculation of the final grade (FG):

$$FG = \frac{1 * PE + 2 * FE + 1 * PA}{4}$$

PE: Partial Exam (Weight 1)
FE: Final Exam. (Weight 2
PA: Practices Average (Weight 1)

The PRACTICE AVERAGE (PA) is obtained as follows: Two (02) laboratory practices with the lowest grades are eliminated, by regulation, and the AVERAGE OF LABORATORY PRACTICES (ALP) of the six (06) remaining laboratory practices is obtained. The qualified practice with the lowest grade is also eliminated and the AVERAGE OF QUALIFIED PRACTICES (AQP) of the three (03) remaining qualified practices is obtained.

$$PA = \frac{1 * ALP + 1 * AQP}{2}$$

## VIII. BIBLIOGRAPHY


- **Levine, Ira.** Química Cuántica. España: Pearson Educación, S.A.. 5ta ed.; 2001.
- **Hanna, Melvin.** Mecánica Cuántica para Químicos. México D.F.: Fondo Educativo Interamericano S.A. de C.V. (Universidad de Colorado); 1985.
- **Cruz, Garritz, Chamizo.** Estructura Atómica, un Enfoque Químico. U.S.A.: Editorial Addison-Wesley Iberoamericana, S.A. Fondo Educativo Interamericano; 1991.


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