



FACULTAD DE
CIENCIAS QUÍMICAS

PHYSICAL CHEMISTRY I

COURSE GUIDE

BSc Chemistry

Academic Year 2023-2024



UNIVERSIDAD
COMPLUTENSE
MADRID



I.- IDENTIFICACIÓN

NOMBRE DE LA ASIGNATURA:	Physical Chemistry I
NÚMERO DE CRTÉDITOS:	12
CARÁCTER:	Mandatory
MATERIA:	Physical Chemistry
MÓDULO:	Fundamental
TITULACIÓN:	Degree in Chemistry
SEMESTRE/CUATRIMESTRE:	Annual (second year)
DEPARTAMENTO/S:	Physical Chemistry

PROFESOR/ES RESPONSABLE/S:

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Theory Grupo E (English)

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II.- OBJETIVES

▪ GENERAL OBJECTIVE

This course is intended to convey to the students the fundamental concepts of quantum chemistry and spectroscopy required for a chemistry graduate. The quantum-mechanical concepts and tools necessary to study atoms and molecules in a quantitative way will be introduced. The study of the basic concepts of the basic molecular spectroscopies and their practical application to obtain molecular information, determination of molecular structures, etc. will be approached.

A general objective, of vital importance, is to instil in the student a quantitative conception of Chemistry. In this sense, it is paramount to transmit the role that Physical Chemistry plays in Chemistry, not only as a set of concepts, theories and experimental and calculation tools, capable of explaining the objects and phenomena that concern Chemistry, but also as a driving force of chemical science and technology.

▪ SPECIFIC OBJECTIVES

- To know the fundamental concepts of quantum mechanics and its origins.
- To enable the student to explain quantitatively the atomic structure and spectroscopy, as well as the electronic configurations and the construction of the periodic table of the elements.
- To understand chemical bonding and molecular structure, and how it is possible to describe it quantitatively, both in diatomic and polyatomic molecules.
- To introduce the student to the approximate methods used in molecular modelling.
- To teach the basic concepts and tools of group and symmetry theory and its application in chemical bonding.
- To let the students know the fundamental concepts of molecular spectroscopies (rotation, vibration, Raman and electronic) and their application in chemistry.
- To know the fundamental concepts of magnetic resonance spectroscopies (nuclear and electronic) and their application in chemistry.
- To use molecular modelling software to optimize geometries and to obtain molecular properties and vibrational, electronic and nuclear magnetic resonance spectra.
- Learn to use group and symmetry theory to explain aspects of molecular spectroscopy.



- Use the combined information from the different spectroscopies and molecular modelling for the determination of molecular structures.

III.- PREVIOUS KNOWLEDGE AND RECOMMENDATIONS

▪ RECOMMENDATIONS:

It is recommended to have passed the basic subjects General Physics, Mathematics, General Chemistry, Computer Science Applied to Chemistry and Basic Laboratory Operations.

IV.- CONTENTS

▪ BRIEF DESCRIPTION OF THE CONTENTS:

Origins of quantum theory. Schrödinger's equation. Application to simple systems. Atomic structure. Molecular structure and chemical bonding. Diatomic molecules. Polyatomic molecules. Molecular modelling. Group theory and symmetry. Matter-radiation interaction. Spectroscopy fundamentals. Microwave, infrared, Raman and visible-ultraviolet spectroscopy. Fluorescence and phosphorescence. Magnetic resonance spectroscopies (NMR and ESR).

▪ PROGRAM:

TOPIC I. Fundamentals

Lesson 1: Quantum behavior of matter.

Wave phenomena and radiation energy. Quantization of energy. Photoelectric spectrum. Wave character of matter: De Broglie's hypothesis.

Lesson 2: Wave mechanics.

Schrödinger equation: dependent and independent of time. Stationary states. Concept of wave function for a particle: Born interpretation.

Lesson 3: Formalism of Quantum Mechanics.

Concept of operator and observables. Eigenvalue equation: eigenfunctions and eigenvalues. The Hamiltonian operator. Expected values. Compatible and incompatible observables. The Heisenberg uncertainty relation.

Lesson 4: Translational motion of a particle.

Energy of a particle confined in a one-dimensional box. Quantization of the energy. The free particle as a limiting case when the length tends to infinity. Particle in a 3D potential box: degeneracy.

Lesson 5: Two-particle system I: vibrational motion.

The harmonic oscillator as a model of vibration of a molecule. Review of the classical oscillator. Solution of the Schrödinger equation: energy levels. Properties of wave functions. Virial theorem.

Lesson 6: Two-particle system II: rotational motion.



Review of classical rotational motion: angular momentum. Quantum mechanical approach. Commutation of the components of angular momentum. Solution of the Schrödinger equation: Spherical harmonics. Representation of spherical harmonics. The rigid rotor as a model of molecular rotation.

TOPIC II. Atomic Structure

Lesson 7: The hydrogen atom.

Statement of the Schrödinger equation. Central potential. Decomposition of the equation in radial part and angular part. Centrifugal barrier and effective potential. Quantum numbers. Radial functions and energy eigenvalues: atomic orbitals. Degeneracy of energy levels. Magnetic momentum: Stern-Gerlach experiment. Spin angular momentum Total angular momentum. Spectrum of the hydrogen atom.

Lesson 8: Many-Electron atoms I

Electronic repulsion. Indiscernibility of identical particles: antisymmetry of the electron wave function. Zero-order functions for the ground state of the He atom: antisymmetric product of one-electron functions. Pauli's principle. Slater determinants. Variational method. Effective nuclear charges.

Method of linear variation of coefficients. Refinements in the calculation of the energy and wave function in He: electronic configurations are an approximation. Self-Consistent Field (SCF) method. Expressions of the Hartree-Fock method. Energy of orbitals and electronic configurations. Periodic properties.

Lesson 9: Many-Electron Atoms II

Angular momentum coupling. LS coupling scheme. Electronic terms. Non-equivalent and equivalent electrons. Hund's rule: the energy of a state depends on the orbital angular momentum and electronic spin. Total angular momentum. Spin-orbit interaction. Selection rules in atomic spectroscopy.

THEME III. Molecular Structure and Chemical Bonding

Lesson 10: The simplest molecule.

Born-Oppenheimer separation and electronic Hamiltonian. Molecular orbitals. Linear combination of molecular orbitals (CLOA) method. Example of the variational method. Energies of the simplest molecular orbitals for H_2^+ . Charge densities and bonding or anti-bonding character of the wave function.

Lesson 11: Diatomic molecules.

The Hamiltonian for the H_2 molecule. The electronic repulsion term. Molecular orbitals as CLOA. Molecular electronic configurations. Diatomic molecules of the first and second periods: bond order, dissociation energies and physical properties. Molecular electronic terms. The CLOA method does not work in the dissociation limit: electronic correlation. Interaction of configurations. Heteronuclear molecules of similar atoms. Heteronuclear molecules of very different atoms: cases of HF and LiH. The limit of ionic bonding.

Lesson 12: Simple polyatomic molecules.

Molecular geometry and electronic structure. Linear triatomic molecules: BeH_2 . Symmetry molecular orbitals. Localized molecular orbitals. Hybrid orbitals. Non-linear triatomic molecules: H_2O . Symmetry molecular orbitals. Walsh diagrams. Hybridization in polyatomic molecules. π -electron approximation: Hückel's method.

**Lesson 13: Molecular modelling**

Introduction to molecular modelling methods. Molecular mechanics methods. Ab initio and semiempirical methods. Molecular orbitals as development in basis functions. Description of the most common bases used: STOs, GTOs. Introduction to the Hartree-Fock method. Most used semiempirical methods. Energy of the molecular orbitals and of the electronic state of the molecule. Charge distribution analysis. Molecular geometry and molecular vibrations. Transition states. Electronic correlation. Beyond Hartree-Fock.

Laboratory 1: Group theory and symmetry I
Laboratory 2: Group theory and symmetry II
Laboratory 3: Group theory and symmetry III

TOPIC IV. Spectroscopy**Lesson 14: Introduction to Molecular Spectroscopy**

Electromagnetic spectrum: types of spectroscopy. Black body radiation: Planck's law. Matter-radiation interaction: absorption, spontaneous emission and stimulated emission. Einstein coefficients and half-lives. Transition moments and electric dipole selection rules. Intensity of a spectral transition. Transmittance, absorbance, integrated intensity and oscillator strength. Lambert-Beer law. Width of spectral lines. Types of broadening: natural width, collisional broadening and Doppler broadening. Fundamentals of laser radiation and types of lasers.

Lesson 15: Born-Oppenheimer approximation.

Separation of electronic and nuclear motions: Born-Oppenheimer approximation. Potential energy curves and surfaces. Dissociation energies and minimum energy molecular geometry. Separation of vibrational and rotational motions: harmonic oscillator and rigid rotor equations. Rovibrational energy.

Lesson 16: Nuclear Magnetic Resonance Spectroscopy.

Spin angular momentum and magnetic momentum. Spin states. Spin-magnetic field interaction. NMR spectroscopy: chemical shift and shielding. Measurement of chemical shift: scale. Signal intensity. Spin-spin coupling: first-order analysis of fine structure. Relaxation phenomena. Experimental methods. Applications of NMR spectroscopy. CSR spectroscopy.

Lesson 17: Rotational Spectroscopy.

Microwave and far-infrared spectroscopy: pure rotational spectra. Diatomic molecules: rigid and elastic rotor models. Energy levels. Selection rules. Spectral transitions Intensity distribution of spectral lines. Polyatomic molecules: classification by moments of inertia. Energy levels. Selection rules. Spectral transitions. Isotopic substitution Stark effect. Experimental methods. Applications of rotation spectroscopy.

Lesson 18: Vibrational spectroscopy.



Regions of the infrared region: near-IR, mid-IR and far-IR. Vibration of diatomic molecules: Harmonic oscillator. Anharmonic oscillator: anharmonicity of vibrations. Energy levels. Selection rules. Spectral transitions. Rotational vibration spectra: Energy levels. Selection rules. Spectral transitions. Influence of vibration on rotation. Vibration of polyatomic molecules: normal modes. Quantum mechanical treatment of molecular vibrations. Fundamental bands, overtones and combination bands. Parallel and perpendicular vibrations. Profiles of vibration-rotation bands. Influence of the nuclear spin on the relative intensity of the rotation lines. Experimental methods. Applications of infrared spectroscopy.

Lesson 19: Raman spectroscopy.

Raman effect: classical and quantum theories. Molecular polarizability. Pure rotational Raman spectra of diatomic and polyatomic molecules. Selection rules. Spectral transitions. Raman spectra of vibration-rotation of diatomic and polyatomic molecules. Selection rules. Spectral transitions. Polarization of Raman lines. Experimental methods. Applications of Raman spectroscopy.

Lesson 20: Electronic spectroscopy.

Molecular electronic states: pure electronic transitions. Diatomic molecules: notation of states. Selection rules. Vibrational structure of an electronic band: Frank-Condon principle. Polyatomic molecules: types of electronic transitions. Pathways of deactivation of excited electronic states: fluorescence and phosphorescence. Photodissociation and predissociation. Experimental methods. Photoelectron spectroscopy. Applications of electronic spectroscopy.

Laboratory 4:	<i>Molecular Modelling I</i>
Laboratory 5:	<i>Molecular Modelling II</i>
Laboratory 6:	<i>Lambert-Beer law. Einstein coefficients</i>
Laboratory 7:	<i>Group theory and symmetry applied to spectroscopy I</i>
Laboratory 8:	<i>Group theory and symmetry applied to spectroscopy II</i>
Laboratory 9:	<i>Infrared Spectroscopy I</i>
Laboratory 10:	<i>Infrared Spectroscopy II</i>
Laboratory 11:	<i>UV-VIS Spectroscopy</i>
Laboratory 12:	<i>Photochemistry</i>
Laboratory 13:	<i>Simulation and modelling of NMR spectra</i>

V.- COMPETENCES

▪ GENERAL:

The general competences of the degree, CG1, CG2, CG3, CG5, CG6, CG7, CG8, CG9, CG10, CG11, CG12 and CG13, developed in the fundamental module, CG-MF, and which are applicable in this subject are the following:

- **CG1-MF1:** Recognize chemical processes in daily life.
- **GC2-MF1:** Relate Chemistry with other disciplines.
- **GC3-MF1:** To continue their studies in multidisciplinary areas.



- **GC5-MF1:** Demonstrate knowledge and understanding of the essential facts, concepts, principles and theories related to the areas of Chemistry.
- **GC6-MF1:** Analyse and solve qualitative and quantitative problems.
- **GC7-MF1:** Recognize and analyse new problems and plan strategies to solve them.
- **GC8-MF1:** Consult and use scientific and technical information effectively.
- **GC9-MF1:** To demonstrate knowledge of laboratory materials and practical skills.
- **GC10-MF1:** Safely handle chemical materials.
- **GC10-MF2:** Recognize and assess the hazards in the use of chemicals and laboratory procedures.
- **GC11-MF1:** Handle standard chemical instrumentation.
- **GC11-MF2:** Develop the ability to apply techniques to characterize chemical species.
- **GC12-MF1:** Interpret data from observations and measurements in the laboratory.
- **GC13-MF1:** To recognize and implement good scientific practices of measurement and experimentation.

▪ **SPECIFIC:**

The specific competences of the Subject Physical Chemistry that are applicable in this subject are the following:

- **CE11-MFQF2:** To use the main spectroscopic instrumental techniques used in chemistry and to be able to determine through experimental work the molecular structure and structural properties of molecules.
- **CE11-MFQF3:** Relate macroscopic properties and properties of individual atoms and molecules, including macromolecules, polymers, colloids and other materials.
- **CE12-MFQF1:** To describe the principles of Quantum Mechanics and apply them to the description of the properties of atoms, molecules and solids.
- **CE12-MFQF2:** To explain the origin of spectroscopic phenomena and the quantum basis of the different techniques for the determination of the different molecular structural parameters.
- **CE13-MFQF3:** To manage computer programs for the calculation of microscopic properties of matter and simulation programs.

▪ **TRANSVERSAL:**

The transversal competences of the degree, CT1, CT2, CT3, CT5, CT6, CT7, CT11 and CT12, developed in the fundamental module, CT-MF, and which are applicable in this course, are the following:

- **CT1-MF1:** Prepare and write scientific and technical reports.



- **CT2-MF1:** Cooperate with other students through teamwork.
- **CT3-MF1:** Apply critical and self-critical reasoning.
- **CT5-MF1:** Use chemical information, bibliographies and specialized databases.
- **CT6-MF1:** Identify the importance of chemistry in the industrial, environmental and social context.
- **CT7-MF1:** Use tools and computer programs for the treatment of experimental results.
- **CT11-MF1:** Developing self-learning.
- **CT12-MF1:** Recognize the current energy problem and its importance.
- **CT12-MF2:** Develop sensitivity to environmental issues.

VI. - LEARNING RESULTS

Once this course has been passed, in relation to the teachings included in the theoretical and practical program, the student should be able to:

TOPIC I.

Lesson 1.

1. To know the origins of quantum theory.
2. To apply the photoelectric effect equations.
3. To explain the wave character of matter.
4. To apply the De Broglie equation.

Lesson 2.

1. Describe and explain the Schrödinger equation.
2. Use the concept of steady states.
3. Explain the concept of wave function and probabilistic interpretation.

Lesson 3.

1. Know and handle the concept of operator.
2. To use eigenvalue equations.
3. To use the Hamiltonian operator and to calculate expected values.
4. To know the commutation rules and the compatibility of observables.
5. To deduce the uncertainty relation.

Lesson 4.

1. Apply and solve the Schrödinger equation to the particle in a box of one or more dimensions.
2. Explain the relationship between energy quantization and spatial confinement.
3. Explain the concept of degeneracy and its relation to symmetry.

Lesson 5.

1. To use the harmonic oscillator as a model for the vibration of a molecule.
2. To apply and solve Schrödinger's equation to a harmonic oscillator.
3. To calculate the energy levels and study the properties of the wave functions of the harmonic oscillator.
4. To apply the virial theorem.



5. To solve harmonic oscillator problems.

Lesson 6.

1. To use the rigid rotor as a model for the rotation of a molecule.
2. To solve the Schrödinger equation for a rigid rotor and learn the basic concepts of the quantum theory of angular momentum.
3. To use the angular momentum operators and their switching properties.
4. To describe spherical harmonics and their representations.
5. To solve rigid rotor problems.

TOPIC II.**Lesson 7.**

1. To write the Schrödinger equation for the hydrogen atom.
2. To decompose the equation into radial and angular part and schematize the solution of the Schrödinger equation.
3. To describe the possible values of the quantum numbers.
4. To analyse the dependence of the radial part of the wave function on distance.
5. To analyse the dependence of the angular part on the Euler angles.
6. To calculate the number of maxima and minima of the radial and angular wave functions as a function of quantum numbers.
7. Write the energy of the orbitals as a function of the principal quantum number n .
8. To relate the total angular momentum and its projection on the z -axis to the quantum numbers l and m .
9. To describe and interpret the Stern-Gerlach experiment.
10. To justify the existence of a spin angular momentum.
11. To calculate the total angular momentum of the hydrogen atom.
12. To interpret the spectrum of the hydrogen atom.

Lesson 8.

1. To write the Schrödinger equation for the helium atom.
2. To show the effect of electronic repulsion on the possible solution of the Schrödinger equation for the helium atom.
3. To write an approximate solution for the equation.
4. To formulate the variational principle.
5. To explain the shielding phenomenon and analyse the dependence of the energy on the effective charge.
6. To write the expression of the Hartree-Fock method.
7. Describe the Self Consistent Field method.
8. To justify the antisymmetric electronic wave function due to the electron indistinguishability.
9. To show that a Slater determinant produces an antisymmetric electron wave function.
10. To write the Slater determinant for the helium atom.
11. To define and apply the Pauli Exclusion Principle.



12. Relate the energy of orbitals to their electronic configuration.

Lesson 9.

1. Defining the coupling of orbital and spin angular momentum within the LS coupling scheme.
2. Distinguishing between equivalent and non-equivalent electrons.
3. To determine the electronic terms resulting from an angular momentum coupling.
4. Order the electronic terms in terms of their total spin and orbital angular momenta using Hund's rules.
5. Obtain the total angular momentum of many-electron atom.
6. To apply the selection rules to transitions in atomic spectra.

TOPIC III.**Lesson 10.**

1. Apply the variational method in the resolution of the electronic Schrödinger equation using CLOA molecular orbitals for the H_2^+ molecule.
2. Energetically order the CLOA-OMs obtained for the H_2^+ molecule.
3. To draw the electronic charge density for bonding and anti-bonding orbitals.

Lesson 11.

1. Define the Hamiltonian of the H_2 molecule and explain the role of the electronic repulsion term.
2. To present and explain the approximations used to solve the electronic Schrödinger equation for the H_2 molecule.
3. Explain the molecular electronic configurations for homonuclear diatomic molecules of the first and second periods.
4. Define, analyse and justify the bond order, dissociation energy and physical properties of homonuclear diatomic molecules of the first and second periods.
5. Explain the molecular electronic terms of diatomic molecules of the first and second periods.
6. Define and explain electronic correlation and configuration integral.
7. Present and discuss the molecular electronic configurations for simple heteronuclear diatomic molecules of similar atoms and of very different atoms.
8. Define and estimate the ionic character of a bond.

Lesson 12.

1. Contrast the molecular geometry with the electronic structure of simple polyatomic molecules.
2. Introduce and explain localized and delocalized molecular orbitals.
3. To introduce the concept of hybrid orbitals.
4. To apply the delocalized and localized molecular orbitals to polyatomic molecules of linear (BeH_2), trigonal planar (BH_3) and tetrahedral (CH_4) geometry.
5. Explain and analyse the geometry of nonlinear triatomic molecules (H_2O). Present and discuss Walsh correlation diagrams.



6. Present the π -electron approximation in conjugated and aromatic hydrocarbons: ethene, butadiene and benzene.
7. Apply the approximate Hückel method to obtain the molecular wave functions and some properties of simple molecules with delocalized bonds.

Lesson 13.

1. Differentiate the classical and quantum mechanical methods to predict molecular structures.
2. Describe the energy terms used in molecular mechanics methods.
3. Describe the molecular electronic Hamiltonian terms and discuss the necessity of resorting to approximate methods to solve the molecular electronic wave equation.
4. Justify the use of determinant functions (Slater determinants) as approximate wave functions and describe the self-consistent process of solving the electronic Schrödinger equation for a molecular system.
5. State the advantages and disadvantages of developing one-electron functions (molecular orbitals) as a set of known basis functions.
6. Specify the most common basis functions.
7. Describe the strategy of semiempirical methods: numerical approximations and parametrization.
8. Summarize the concept of electronic correlation and the schemes of correlation methods.
9. To perform molecular electronic energy calculations using standard available modelling programs.
10. To analyse the information provided by the program concerning molecular energy, equilibrium geometry, energy and description of molecular orbitals, charge distribution and normal modes of vibration.

TOPIC IV.**Lesson 14.**

1. To describe the electromagnetic spectrum and locate in the spectrum the areas corresponding to the different molecular spectroscopy techniques.
2. To explain Planck's law and black body radiation.
3. To explain the matter-radiation interaction and perform simple calculations with the Einstein coefficients and related quantities.
4. Describing the basic operation of a laser and the requirements necessary for a given system to produce laser radiation.
5. To explain the different types of lasers, their operation and differences.
6. To define the transition moment and the relationship to the intensities of spectroscopic transitions and the selection rules.
7. To perform calculations with the Lambert-Beer law to extract information from spectral bands.
8. To describe the various contributions to spectral line broadening.
9. To explain the fundamentals of laser radiation and the major types of lasers.

Lesson 15.



1. Apply the Born-Oppenheimer approximation to separate nuclear and electron motion.
2. Draw potential energy curves and specify the dissociation energy and minimum energy molecular geometry.
3. To describe potential energy surfaces.
4. Separate internal vibrational and rotational motions.
5. To calculate rovibrational energies using the harmonic oscillator and rigid rotor models.

Lesson 16.

1. To define the spin angular momentum (nucleus and electron) and magnetic dipole momentum. To determine the number of nuclear states from the nuclear spin.
2. Calculate and plot the energy of the nuclear spin states in the presence of a given magnetic field. Calculate the resonance frequency of an unshielded nucleus.
3. Justify the influence of the temperature and the applied magnetic field on the intensity of NMR signals.
4. To explain the shielding phenomenon. Define the chemical shift and the scales to measure it. Perform simple chemical shift calculations.
5. Explain spin-spin coupling. Predict the appearance of spectra of simple organic molecules using the first-order approximation.
6. To describe in general terms the experimental techniques of NMR.
7. State some of the most important applications of NMR.
8. To describe electron spin spectroscopy and its main applications.

Lesson 17.

1. To describe the pure spin spectrum: Microwave and Far-Infrared spectroscopies and define the corresponding spectral ranges.
2. To explain the states or energy levels, selection rules and spectral transitions that provide the rotational spectra in diatomic molecules according to the rigid rotor and elastic rotor models.
3. To calculate the line intensity distribution in pure rotation spectra of diatomic molecules according to the Boltzmann distribution law.
4. Establish the classification of polyatomic molecules by the moments of inertia in different types of rotors.
5. Explain the effect of isotopic substitution in molecules (isotopomers) to determine molecular constants.
6. Describe the first-order Stark effect in pure rotation spectra.
7. State some of the most important applications of microwave spectroscopy.

Lesson 18.

1. To distinguish the zones of the infrared region: IR-near, IR-mid, and IR-far.
2. Apply the harmonic oscillator model to study the vibration of diatomic molecules.
3. Describing the model of the anharmonic oscillator. Calculate the energy levels and apply the selection rules.
4. To Predict rovibrational spectra of diatomic molecules.



5. To explain the influence of vibration on rotation.
6. To describe the normal modes of vibration.
7. Explain the fundamental bands, overtones and combination bands.
8. Distinguish parallel and perpendicular vibrations and predict vibration-rotation band profiles.
9. To explain the influence of nuclear spin on the relative intensity of the rotation lines.
10. To describe the experimental methods and applications of infrared spectroscopy.

Lesson 19.

1. To describe the mechanism of matter-radiation interaction by induced dipole effect and the concept of molecular polarizability.
2. Develop the classical and quantum theories that justify the Raman effect.
3. Describe the pure rotational and vibration-rotational Raman spectra of diatomic and polyatomic molecules and the selection rules for the different spectral transitions.
4. Perform calculations on the position of the different vibrational bands and rotation lines of Raman spectra of simple molecules.
5. Relate the Raman and IR activity of different vibrations in polyatomic molecules.
6. To use the degree of polarization of vibrations, relate it to their symmetry, and determine molecular symmetry.

Lesson 20.

1. Describe molecular electronic states and pure electronic transitions.
2. Use the notation of electronic states in diatomic molecules and selection rules.
3. Explaining the vibrational structure of an electronic band by means of the Frank-Condon principle.
4. To describe the types of electronic transitions in polyatomic molecules.
5. Explaining the phenomena of deactivation of excited electronic states: fluorescence and phosphorescence.
6. To study the processes of photodissociation and predissociation.
7. Describe the experimental methods and applications of electronic spectroscopy.

VII. – HOURS OF WORK AND DISTRIBUTION BY ACTIVITY

Activity	Presential (hours)	Autonomous work (hours)	Credits
Theory lectures	56	56,5	4,5
Seminars	20	17,5	1,5
Tutorials / Directed work	8	12	0,8
Laboratory demonstrations	42	58	4,0



Preparation of papers and exams	6	24	1,2
Total	132	168	12

VIII.- METHODOLOGY

The contents of the course are presented to the students in face-to-face classes, divided into two types:

The so-called **face-to-face theory lectures** will be given to the whole group where the student will be introduced to the fundamental contents of the subject. At the beginning of each subject, the program and its main objectives will be clearly stated. At the end of the subject a brief summary of the most relevant concepts will be made, and new objectives will be proposed that will allow the interrelation of contents already studied with those of the rest of the subject and with other related subjects. During the exposition of contents, problems that exemplify the concepts developed or that serve as an introduction to new contents will be proposed. To facilitate the student's monitoring of the face-to-face classes, the necessary teaching material will be provided, either in photocopies or in the Virtual Campus.

In the **seminars**, exercises and questions that exemplify the contents developed in the theory lectures will be solved. Periodically the student will be provided with a list of these problems/exercises with the aim of trying to solve them before the classes, which will include in some cases the consultation of scientific information. The process of solving these problems will be carried out by means of different methods: in some cases, the student will be proposed the exposition in class of the resolution of some of these problems, discussing the procedure followed, the result obtained and its meaning. In other cases, the results of the students will be discussed in small groups and, later, they will be shared. Finally, some exercises will be collected by the teacher for evaluation. These theory and seminar classes and the work they involve develop the general competences CG6-MF1, CG7-MF1 and CG8-MF1 and the transversal competences CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1 and CT7-MF1.

During the development of the syllabus, both in theory and seminar classes, the student will acquire the necessary knowledge and experience to satisfy all the specific competences to be covered, CE11-MFQF2, CE11-MFQF3, CE12-MFQF1, CE12-MFQF2 and CE13-MFQF3 and the transversal competence CT11-MF1, during the development of the sessions, special emphasis will be placed on relating the aspects studied with other disciplines and chemical phenomena in daily life, as well as on their multidisciplinary nature, which will satisfy the general competences CG1-MF1, CG2-MF1 and CG3-MF1, and the transversal competences CT12-MF1 and CT12-MF2.

There will be directed tutorials whose fundamental mission will be the realization of exercises and the resolution of theoretical-practical questions. The exercises will be given to the students in advance so that they can solve them and will be collected in the tutorials. The students will actively participate in the public resolution and correction of the exercises. All this will allow students to put into practice their skills in obtaining information, developing skills related to the management of bibliographic information and teamwork (CT2-MF1, CT3-MF1 and CT5-MF1).



The professor may schedule **tutorials** with small groups of students on issues raised by the professor or by the students themselves. Tutorials will also be available for individual students who wish to resolve any doubts that may arise during the study. These tutorials will be held in person at the times indicated by each professor or, exceptionally, virtually.

The Virtual Campus will be used to allow a fluid communication between professors and students and as an instrument to make available to the students the material to be used in the theoretical and problem classes. It may also be used as a forum in which to present some complementary topics whose content, although important in the subject as a whole, is not considered appropriate to be presented in face-to-face classes.

A laboratory will be conducted throughout the course with topics directly related to the contents of the course. This laboratory will consist of experimental practices, where the general competences will be specifically developed (CG9-MF1, CG10-MF1, CG10-MF2, CG11-MF2, CG12-MF1 and CG13-MF1), as well as calculation practices and the use of theoretical tools in which the specific competences will be developed (CE11-MFQF2, CE11-MFQF3, CE12-MFQF1, CE12-MFQF2 and CE13-MFQF3). Some practices will be proposed using a research methodology, so that students will be presented with transversal problems for them to solve them using the theoretical knowledge acquired and the experimental and calculation tools available in the laboratory, always under the guidance and supervision of the professor. Finally, the student will present individual scientific reports of some of the practices carried out (CT1-MF1, CT2-MF2, CT3-MF3, CT5-MF1, CT7-MF1).

IX.- BIBLIOGRAPHY

■ BASIC:

- Atkins, P. W.; De Paula, J.; Keeler, J.: *Atkin's Physical Chemistry*. Oxford University Press 2023 (12th Ed).
- Engel, T., Reid, P.: *Physical Chemistry*. Pearson 3rd ed. (2013).
- Engel, T.: *Physical Chemistry: Quantum Chemistry and Spectroscopy*. Pearson 4th ed. (2019).
- Levine, I.N.: *Physical Chemistry* 6 Ed. Mc Graw Hill, India (2011).

■ ADDITIONAL:

- Jim Baggott, *The Quantum Cookbook*. Oxford 2020.
- Bertrán Rusca, J.; Núñez Delgado, J. (coord.): *Química Física*, Vol. I, Ariel Ciencia, (2002).
- Levine, I. N.: *Quantum Chemistry*, 13th Edition. Pearson, (2013).
- Berry, R. S.; Rice, S. A.; Ross, J.: *Physical Chemistry*, 2nd ed., Oxford University Press, New York, 2000.
- Maurya, R.C., Mir, J. C.; *Molecular Symmetry and Group Theory: Approaches in Spectroscopy and Chemical Reactions*. De Gruyter Textbook (2019).
- McQuarrie, D. A.; Simon, J. D.: *Physical Chemistry: A Molecular Approach*, University Science Book, (1997).
- Mc Halle, J.: *Molecular Spectroscopy* CRC Taylor and Francis 2017.



- Bertrán Rusca, J.; Núñez Delgado, J. (coord.): *Problemas de Química Física*, Delta Publicaciones (2007).
- Levine, I. N.: *Molecular Spectroscopy*, Wiley (1975).

X.- EVALUATION

The student's academic performance and the final grade of the course will be weighted according to the following percentages, which will be maintained in all the exams. In general, to pass the course, it will be necessary to achieve a minimum grade of 5 out of 10 points in the total computation of all the evaluated activities.

The grades of the activities foreseen for the evaluation of the course will be communicated to the students as soon as they are available.

▪ WRITTEN EXAMS:

65%

Ordinary call: two mid-term exams and a final exam, common to all groups, will be held.

To pass the theory grading by midterm exams it is necessary:

- a) To obtain a minimum grade of 10 out of 20 in the sum of the two mid-term exams.
- b) That in none of the two mid-term exams the grade obtained is less than 4 out of 10.
- c) That the total grade weighted with the rest of the activities is at least 5 out of 10.

Students who pass who meet the above requirements, will not be obliged to take the final exam. The rest of the students will be able to take the exam of the subject of the partial not passed (partial-final) or of the totality of the subject in the final exam of the ordinary call. To be able to opt for the partial-final exam modality in the ordinary exam, the student must have obtained a minimum grade of 5 in the partial of which he/she is not examined and a grade higher than 2 out of 10 in the partial of which he/she is examined.

All midterm and final exams of the ordinary exam will consist of questions and problems on the contents of the course, both theory lectures and seminars as well as of the tutorials and laboratories. In the exam of the ordinary call, the students who take only a partial exam, because they have passed the other one, will take an exam equivalent, in number of questions and duration, to those who take the final exam.

In the extraordinary call, a single final exam like the one taken in the ordinary exam will be taken. Those who do not pass the course in the ordinary exam will have to take the entire syllabus and repeat course.

In any case, the minimum grade of the final exam required to pass the subject, in either the ordinary and extraordinary exams, is 4 out of 10. In both the ordinary and extraordinary exams covering the entire content of the course, a minimum of 1.5 out of 5 will be required in the part of the exam (syllabus of the 1st and 2nd semesters) in which the lowest score has been obtained.

The grades of the partial exams will be published within a maximum period of 20 days from the date of the exams. In any case, the minimum period of seven days between the publication of the grades and the date of the final exam of the course will be respected.



Competences assessed: CG1-MF1, CG2-MF1, CG3-MF1, CG5-MF1, CG6-MF1, CG7-MF1, CG8-MF1, CE11-MFQF2, CE12-MFQF1, CE12-MFQF2, CE13-MFQF3, CT3-MF1, CT7-MF1, and CT11-MF1.

▪ **HOMEWORK:**

15%

The evaluation of the individual work done by the student will be carried out considering the following factors:

Skills of the student in the resolution of the proposed problems and exercises, which will be collected periodically lectures.

Assessment of the work carried out during the programmed group tutorials, of obligatory attendance, and to which the students will be summoned periodically throughout the course.

Assessment of the work proposed in the programmed tutorials and carried out individually or in groups by the students.

The grade obtained by the student in the ordinary call for this concept will be maintained in the extraordinary call.

Competences evaluated: CG1-MF1, CG2-MF1, CG3-MF1, CG5-MF1, CG6-MF1, CG7-MF1, CG8-MF1, CE11-MFQF2, CE12-MFQF1, CE12-MFQF2, CE13-MFQF3, CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1, CT6-MF1, CT11-MF1, CT12-MF1, and CT12-MF2.

▪ **LABORATORY:**

20%

The students will develop in reduced groups throughout the course a series of laboratory demonstrations of experimental character, as well as of calculation and use of theoretical tools, being the attendance to these practices mandatory. The general attitude of the students in the laboratory, their work during the practical sessions, the acquisition by the student of theoretical and practical skills, as well as the skill in the use of the experimental equipment and in the handling of computer packages for data processing and molecular modelling will be considered.

During the course of the laboratory, the professors will order exercises or elaboration of data that will be delivered in the established term and will count for the evaluation of the practical session.

At the end of the laboratory each student will be required to present a report containing the treatment of the data of the demonstrations carried out in the laboratory within the deadlines established by the coordinator. The evaluation of the face-to-face activity and reports will constitute 70% of the laboratory qualification. The remaining 30% of the grade will correspond to a specific exam once the laboratory is finished, being required that **the grade in this exam is equal or higher than 4**. The minimum global grade of the laboratory necessary to compensate with the rest of the evaluations (exams, personal work) will be 4 out of 10.

Those students who did not reach the grade of 4/10 in the laboratory exam of the ordinary call, could take the exam in the extraordinary call if they have passed the classroom activities with a grade higher or equal to 4. Students who have achieved the overall laboratory grade in the ordinary call equal or higher than 4/10, will be maintained in the extraordinary call.



In those cases in which a student fails the subject, but has passed **the laboratory with a grade higher or equal to 5**, the grade for the laboratory activity and reports will be maintained for a maximum of two consecutive academic years. Likewise, if, having passed the laboratory, he/she has obtained a mark of 5 or more in the evaluation of the Group Theory and Symmetry sessions, he/she will be exempted from attending these sessions, and the grade will also be maintained for a maximum of two consecutive academic years. However, if he/she has not obtained this minimum mark in the Group Theory and Symmetry sessions, **even if he/she has passed the laboratory**, he/she must attend these sessions in order to be re-evaluated. In this case, the mark obtained in the evaluation of these sessions will be prorated with the mark obtained and saved from the rest of the practical sessions. In addition, **the student will have to take the exam of the laboratory contents in the ordinary or extraordinary exam** in order to pass the course.

Competences assessed: CG6-MF1, CG7-MF1, CG8-MF1, CG9-MF1, CG10-MF1, CG10-MF2, CG11-MF1, CG11-MF2, CG12-MF1, CG13-MF1, CE11-MFQF2, CE13-MFQF3, CT1-MF1, CT2-MF1, CT3-MF1 CT5-MF1, CT7-MF1.

▪ ATTENDANCE AND ACTIVE PARTICIPATION IN CLASSES

Attendance at all in person activities is **mandatory**. Save in exceptional circumstances, attendance to 70% of the in person activities will be required to be graded in the mid-term exams. **The student's attitude and active participation** in all teaching activities will be positively valued in the final grade.



ACTIVITY PLANNING - CHRONOGRAM

TEMA	ACTIVIDAD	HORAS	GRUPOS	INICIO	FIN
I. Fundamentals	Theory Lectures	8	1	1st week	4th week
	Problem solving Lectures	2	1		
	Scheduled tutoring	1	1		
II. Atomic Structure	Theory Lecture	8	1	4th week	8th week
	Problem solving Lectures s	2	1		
	Scheduled tutoring	1	1		
III. Molecular Structure and Chemical Bond	Theory Lecture s	12	1	8th week	14th week
	Problem solving class	6	1		
	Scheduled tutoring	2	1		
	Laboratory	15	4		
IV. Spectroscopy	Theory Lecture	28	1	15th week	28th week
	Problem solving class	10	1		
	Scheduled tutoring	4	1		
	Laboratory	27	4		
PLANNINGFOR EACH CLASS GROUP					



SUMMARY OF ACTIVITIES AND TASKS

Teaching activity	Associated competences	Teacher Activity	Student Activity	Evaluation procedure	P	NP	Total	C
Theory face-to-face lectures	CG1-MF1, CG2-MF1, CG3-MF1, CG5-MF1, CG6-MF1, CG7-MF1, CG8-MF1, CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1, CT7-MF1, CT11-MF1, CT12-MF1, CT12-MF2, CE11-MFQF2, CE11-MFQF3, CE12-MFQF1, CE12-MFQF2, CE13-MFQF3	Presentation of theoretical concepts and posing of questions and new objectives.	Taking notes. Resolution of questions. Development of the new objectives. Formulation of questions and doubts.	Grading the answers to questions related to the theoretical concepts.	56	56,5	112,5	15%
Face-to-face seminars		Theory application to solving numerical exercises and problems. Raising new questions.	Solving the numerical exercises, problems and questions.	Grading the answers (approach and result) made to solve numerical exercises and problems.	20	17.5	37,5	
Tutorials		Supervision of student activities. Raising questions. Doubts resolution.	Consulting the teacher about the conceptual and methodological difficulties encountered when studying the subject. Posing of questions and answer to the proposals by the professor.	Not subject of evaluation.				
Directed tutorials		Proposal and critical evaluation of works. Exposure and proposal of new objectives	Cooperation with colleagues in the preparation of work. Critical analysis of the work of other groups. Oral presentation of the corrected work. Formulation of questions and doubts.	Assessment of the work and the analysis carried out. Evaluation of the oral presentation.	8	12	20	
Laboratory	MF1, CG7-MF1, CG8-MF1, CG9-	Application of theoretical contents to practical	Preparation and study of the proposed contents. Preparation of reports of	Assessment of the work performed and the results	42	58	100	20%



Teaching activity	Associated competences	Teacher Activity	Student Activity	Evaluation procedure	P	NP	Total	C
	CG11-MF2, CG12-MF1, CG6, MF1, CG10-MF1, CG10-MF2, CG11-MF1, CG13-MF1, CT1-MF1, CT2-MF1, CT3-MF1, CT5-MF1, CT7-MF1, CE11-MFQF2, CE11-MFQF3, CE13-MFQF3	problems. Development of experimental and numerical calculation skills. Collection and treatment of experimental data. Molecular modelling tools.	some of the practices carried out.	obtained. Assessment of the internship reports submitted. Assessment of the skills and knowledge acquired.				
Exams	Face-to-face theoretical lectures, seminars and tutorials	Proposing, proctoring and grading the exam.	Preparation and implementation	Evaluation and grading exams.	6	24	30	65%
P : Face-to-face; NP: non face-to-face (autonomous work); C: Mark								