



COURSE GUIDE

Scenarios 1, 2 & 3:

PHYSICAL CHEMISTRY I



FACULTAD DE CIENCIAS QUÍMICAS
UNIVERSIDAD COMPLUTENSE DE MADRID
ACADEMIC YEAR 2021-2022



SCENARIO: FACE-TO-FACE

I.- IDENTIFICATION

COURSE NAME:	Physical Chemistry I
NUMBER OF CREDITS (ETCS):	12
CHARACTER:	Mandatory
SUBJECT:	Physical Chemistry
MODULE:	Fundamental
DEGREE:	Degree in Chemistry
SEMESTER/FOUR-MONTH PERIOD:	Yearly (second year)
DEPARTMENT:	Physical Chemistry

RESPONSIBLE LECTURERS:

Course co-ordinator	Professor: FRANCISCO JAVIER AOIZ MOLERES Department: Química Física Office: QA-279 e-mail: aoiz@ucm.es
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Grupo A	
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<u>2nd semester</u> Theory Seminar Tutoring	Professor: FRANCISCO ORTEGA GÓMEZ Department: Química Física Office: QA-212 e-mail: fortega@ucm.es



Grupo B		
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<u>2nd semester</u> Theory Seminar Tutoring	Profesor: Department: Office: e-mail:	JOSÉ TORTAJADA PÉREZ Química Física QA-512 jtp@quim.ucm.es

Grupo C		
<u>1st semester</u> Theory Seminar Tutoring	Professor: Department: Despacho: e-mail:	MARTA MENÉNDEZ Química Física QA-244 menendez@ucm.es
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Grupo D		
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<u>2nd semester</u> Theory Seminar Tutoring	Professor: Department: Office: e-mail:	FRANCISCO JAVIER SÁNCHEZ BENITEZ Química Física QB-221 javiersbenitez@ucm.es

Grupo E (English)		
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<u>2nd semester</u> Theory Seminar Tutoring	Professor: Department: Office: e-mail:	PEDRO GÓMEZ CALZADA Química Física QA-506 pgomez@quim.ucm.es



Grupo F	
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<u>2nd semester</u> Theory Seminar Tutoring	Professor: CRISTINA DÍAZ BLANCO Department: Química Física Despacho: QA-508 e-mail: crdiaz08@ucm.es



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 fundamental to transmit to the student 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 become acquainted with 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.
- To 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 the classical rotational motion: angular momentum. Quantum mechanical case. Commutation rules of the components of angular momentum. Solution of the Schrödinger equation: Spherical harmonics. 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. Breakdown 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 -electronic 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. Vibro-rotational energy.

Lesson 16: 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: Spin 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.

Zones 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. Mechano-quantum 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:** 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:** 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:** To connect 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 autonomous learning.
- **CT12-MF1:** Recognize the current energy problem and its importance.
- **CT12-MF2:** Develop sensitivity to environmental issues.

VI. - LEARNING OUTCOMES

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. To 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. To apply and solve the Schrödinger equation to the particle in a box of one or more dimensions.
2. To explain the relationship between energy quantization and spatial confinement.
3. To 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. 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. 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 antisymmetry of the electronic wave function due to the indiscernibility of the electrons.
9. To show that a Slater determinant produces an antisymmetric electron wave function.
10. To write the Slater determinant for the helium atom.
11. Define and apply the Pauli exclusion principle.
12. Relate the energy of orbitals to their electronic configuration.

Lesson 9.



1. Define the coupling of orbital and spin angular momentum within the LS coupling scheme.
2. Distinguish between equivalent and non-equivalent electrons.
3. 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-electronic atoms.
6. To apply the selection rules to transits in atomic spectra.

THEME 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. Schematically 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 electronic repulsion term.
2. 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 -electronic 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 for the prediction of molecular structures.
2. Describe the energy terms used in molecular mechanics methods.
3. Describe the molecular electronic Hamiltonian terms and reason 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) in terms of 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. Perform molecular electronic energy calculations using standard available modelling programs.
10. 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. Describe the electromagnetic spectrum and locate in the spectrum the areas corresponding to the different molecular spectroscopy techniques.
2. Explain Planck's law and black body radiation.
3. Explain the matter-radiation interaction and perform simple calculations with the Einstein coefficients and related quantities.
4. Describe the basic operation of a laser and the requirements necessary for a given system to produce laser radiation.
5. Explain the different types of lasers, their operation and differences.
6. Define the transition moment and the relationship to the intensities of spectroscopic transitions and the selection rules.
7. Perform calculations with the Lambert-Beer law to extract information from spectral bands.
8. Describe the various contributions to spectral line broadening.
9. 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. Describe potential energy surfaces.
4. Separate internal vibrational and rotational motions.
5. Calculate vibro-rotational energy using the harmonic oscillator and rigid rotor models.

Lesson 16.

1. Define the spin angular momentum (nucleus and electron) and magnetic dipole momentum. 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. Describe in general terms the experimental techniques of NMR.
7. State some of the most important applications of NMR.
8. Describe electron spin spectroscopy and its main applications.

Lesson 17.

1. Describe the pure spin spectrum: Microwave and Far-Infrared spectroscopies defining the corresponding spectral ranges.
2. 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. 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. 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. Describe the model of the anharmonic oscillator. Calculate the energy levels and apply the selection rules.
4. Predict vibration-rotation spectra of diatomic molecules.
5. Explain the influence of vibration on rotation.
6. 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. Explain the influence of nuclear spin on the relative intensity of the rotation lines.
10. Describe the experimental methods and applications of infrared spectroscopy.

Lesson 19.

1. 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. 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. Explain the vibrational structure of an electronic band making use of the Frank-Condon principle.
4. To describe the types of electronic transitions in polyatomic molecules.
5. Explain the phenomena of deactivation of excited electronic states: fluorescence and phosphorescence.
6. To study the photodissociation and predissociation processes.
7. Describe the experimental methods and applications of electronic spectroscopy.

VII. – WORKING HOURS AND DISTRIBUTION BY ACTIVITY

Activity	Presential (hours)	Autonomous work (hours)	Credits
Theoretical classes	56	56,5	4,5
Seminars	20	17,5	1,5
Tutorials / Directed work	8	12	0,8
Laboratory practices	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:

Face-to-face theory lectures will be given to the whole group and in them 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 lectures, the necessary teaching material will be provided, either in photocopies or in the Virtual Campus.

In the **face-to-face 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

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- 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.
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X.- ASSESMENT AND GRADING RULES

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 this call for midterm exams it will be necessary:

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

Students who pass this exam by midterm, that is to say, who meet the above conditions, 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, final and final exams of the ordinary exam will consist of questions and problems on the contents of the course, both theoretical classes 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 exam, 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.

In any case, the minimum grade of the final exam required to pass the subject, both in the ordinary and extraordinary exams, is 4 out of 10. In both the ordinary and extraordinary exams, for those 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, CT11-MF1.

▪ **HOMEWORK:**

15%

The evaluation of the individual learning 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 in the face-to-face 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, CT12-MF2.

▪ **LABORATORY:**

20%

The students will develop in reduced groups throughout the course a series of laboratory practices 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 valued.

During the development 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.

Each student will obligatorily deliver at the end of the laboratory, within the deadlines indicated, a report containing the treatment of the data of the practices carried out in the laboratory established by the coordinators. 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 have not reached 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 kept in the extraordinary call.

In those cases, in which a student fails the course, but has passed the **laboratory with a grade higher than or equal to 5**, the grade of the classroom activity and reports will be maintained for a maximum of two consecutive academic years with the condition that he/she attends the sessions of the laboratory with obligatory character. Group Theory and Symmetry, of which the student will be evaluated every year. The grade obtained in the evaluation of these sessions in each academic year will be prorated with the grade obtained and saved from the rest of the practices. In addition, the student **will have to take the exam of the laboratory contents** in the ordinary or extraordinary call 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 face-to-face activities is **mandatory**. Except in exceptional circumstances, attendance to 70% of the face-to-face activities will be required in order 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 Lecture	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.	Calificación de las respuestas realizadas a preguntas relacionadas con los conceptos teóricos.	56	56,5	112,5	15%
Face-to-face seminars		Application of the theory to solving numerical exercises and problems. Raising new questions.	Solving the numerical exercises, problems and questions.	Qualification of the answers (approach and result) made to solve numerical exercises and problems.	20	17.5	37,5	
Tutorials		Direction and supervision of the study and student activities. Raising questions. Doubts resolution.	Consult 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 evaluable.				
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, of the analysis carried out and the oral presentation of the analysis.	8	12	20	
Laboratory	CG6-MF1, CG7-MF1, CG8-MF1,	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
	CG9-MF1, CG10-MF1, CG10-MF2, CG11-MF1, CG11-MF2, CG12-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. Obtaining 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	Proposal, proctoring and correction of the exam. Student's grading.	Preparation and implementation	Correction and evaluation of exams.	6	24	30	65%
P : Face-to-face; NP: non face-to-face (autonomous work); C: Mark								

SCENARIO 2. MIXED LEARNING

VIII.- METHODOLOGY

- **Theory lectures and seminars** given by the professor in the usual regime, as in Scenario 1, and with the same content. In accordance with the principle of maximum attendance approved by the UCM, the session will be followed by the students in the classroom, up to full capacity considering social distance. Students located in classrooms equipped with cameras, and who do not fit in the classroom, will follow the session virtually, either from home or in public areas enabled by the Faculty for this purpose, which will be duly advertised in the CV. For classrooms that do not have a camera, a rotating shift of students in the classroom will be established, according to the numbering of the ID card. This procedure may be modified by the professor throughout the course, as he/she deems appropriate, to adjust the capacity of the classroom with the students attending his/her class.
 - The teaching material used will be the class presentations enabled in the Virtual Campus UCM also used in Scenario 1, as well as videos related to the subject and other types of materials that the professors of the course consider relevant and interesting. All the material will be available in advance to the students through the Virtual Campus for their use.
 - The online means used for students without classroom attendance to follow the sessions virtually will be the following platforms: Microsoft Teams available in the CV or Google Meet. The professor will keep open a session of this type to maintain a direct and fluid relationship with the students attending virtually, being able to simultaneously project the .ppt presentation and follow the traditional explanations given on the blackboard.
- **Laboratory practices** are foreseen with an overall minimum attendance of 60% in order to comply with the necessary social distance. Depending on the particularities of each practice, if possible, in some cases the attendance may be slightly modified. The experimental teaching organization is based on the following aspects:
 - The resolution of a test before the beginning of each session is foreseen.
 - The teaching of each practical session is structured in three parts: theoretical-practical introduction, experimental procedure and treatment of results.
 - The experimental procedure will be carried out in person. In cases where this is not feasible, the use of recorded material or commercial videos is foreseen.
 - The other two parts will be taught according to one of these situations, or combinations of them:
 - (a) Face-to-face in a classroom, thus maintaining greater social distance.
 - (b) Virtual in synchronous sessions.
 - (c) Virtual in asynchronous sessions.
 - The teaching material used will be the same as that used in Scenario 1, in addition to written material in the form of manuals, numerical and graphical results and/or PowerPoint presentations accompanied by explanations.
 - All the material will be made available to the students in advance through the Virtual Campus.

- **Individual tutorials**

They will be conducted by video conference and/or e-mail.

- **Follow-up of students**

In the face-to-face teaching part of the course, the same techniques used in the traditional way will be followed.

In the virtual teaching part of the course, monitoring will be carried out using different techniques, as the teacher considers: using the activity registration tool of each session (Microsoft Teams), the name of the attendees (Google Meet), signature sheet enabled in the CV as a questionnaire, analysis of downloads made by the students in the CV, etc.

X.- GRADING AND STUDENT'S ASSESMENT

Face-to-face examinations will be conducted using the procedure described in Scenario 1.

SCENARIO 3. TOTALLY VIRTUAL**VIII.- METHODOLOGY**

- Online lectures for each group will be carried out by publishing in the Campus files with the theoretical content of the subject and Power Point presentations provided with notes and/or audios by the professor where the necessary explanations are included as if it were a face-to-face class, as well as videos related to the subject and other types of materials that the professors of the subject consider of relevance and interest. The teaching material used will be the class presentations enabled in the UCM Virtual Campus also used in Scenarios 1 and 2. As in the previous scenarios, all the material will be available in advance to students through the Virtual Campus for their use.
- Likewise, some online lectures will be taught using platforms such as Microsoft Teams or Google Meet that allow student participation and interaction between students and the teacher.
- The online means used will be the platforms already mentioned in Scenario 2: Microsoft Teams available in the CV or Google Meet.
- Virtual (online) seminars will consist of the complete and detailed development of a set of selected problems, whose statements have already been distributed for the student to try to solve them on their own once the topic has been taught. The solutions of these problems will be provided to the students perfectly explained through the Virtual Campus.
- Virtual tutorials for the resolution of doubts will be programmed and carried out individually or in small groups that can be carried out in different hours of the established class schedule using different platforms such as Microsoft Teams, Skype or through the chat of the Virtual Campus or by e-mail addressed directly to the teacher.
- Laboratory practices will be replaced by virtual synchronous sessions supported by explanatory presentations.
- The following material is used and is available in the CV of each practice subgroup:
 - Origin application tutorial.
 - Practice script.
 - Explanatory presentation in the form of an exercise.
 - Experimental spectra.
 - Preparation by the students of the practice prior to the synchronous session.
 - 1 synchronous session with Google Meet/Microsoft Teams.
 - Recording of the synchronous session
- Follow-up of the students
It will be carried out as described in Scenario 2 for virtual teaching.

X.-GRADING**DESCRIPTION OF THE EVALUATION PROTOCOL**

- **Student identification:**

In the minutes prior to the start of the exam, students must submit a handwritten and digitalized commitment document in PDF format, accepting the rules for taking the test. The text of the document, prepared by the Department, will be available in the subject area of the Virtual Campus. The document must include: name and surname, signature, place and copy of the ID card. The identification of the students taking the exam will be carried out through: (i) entry to the Virtual Campus to be able to visualize the statements of the exam, (ii) video image through Google Meet or Microsoft Teams (from the computer or mobile camera), (iii) commitment document, and (iv) possible telematic verification throughout the exam by the professor.

- **- Type of exam:**

Particularize for the subject (Assignments or quizzes).

The exam will be designed in the Virtual Campus (Moodle) through the Assignments tool, so that different students can access different exams.

The exam will be divided into two blocks. The first block, of one and a half hour duration, will be unique and analogous for all students of the course (questions corresponding to the subject taught in the second term). In the second block, of one and a half hour duration, the students will have to choose between the final exam modality (questions corresponding to the subject taught in the first term) or the partial-final exam modality (remaining questions corresponding to the subject taught in the second term). The requirements set forth in the first addendum are still valid to opt for the partial-final exam modality.

- **- Monitoring of students during the test:**

While taking the test, students must have a camera connected (from the computer or cell phone) that makes possible the verification by the professor of the fulfillment of the commitment signed by the student to take the exam individually and with the indicated means.

- **- Revision of exams:**

Students who wish to review will contact the teachers of their group by email and the individual review schedule will be established using Microsoft Teams/Google Meet. The student will keep a copy of the PDF files submitted in response to the exam to facilitate the review. On the other hand, the professor may require the student to review and interactively discuss his/her exam within the deadline established for the review of the exams that will be notified in the CV.

- **- Mechanism used for the documentation/recording of the evaluation tests for later visualization and evidence:**

The professor will keep the files (in the electronic format specified) of the exam exercise sent by the student, with the partial grades that he/she deems appropriate. In addition, if deemed appropriate, the recording of the examination session may be made, with the limitations established by UCM, for later review if necessary. Such recording, if made, will be stored

with the necessary security measures in UCM equipment and will be deleted after the review time.