COURSE GUIDE	2026/27		
Faculty	215 - Faculty of Chemistry	**Cycle**	.
Degree	GQUIMI20 - Bachelor's Degree in Chemistry	**Year**	Third year

COURSE

26123 - Physical Chemistry II	**Credits, ECTS:**	9

COURSE DESCRIPTION

The main objective of the subject is to study chemical-physical systems from a microscopic point of view, in such a way that the macroscopic properties of the systems developed in the subject Physical Chemistry I can be related to the individual properties of the atomic-molecular systems that constitute the matter. For this, Quantum Chemistry is presented and applied in the study of atoms and molecules, whose properties obtained by theoretical calculations are confronted with experimental data obtained from the different spectroscopic techniques. Besides, atomic and molecular spectroscopies are deeply studied, in order to analyze the physical basics of different spectroscopy types. Using Statistical Thermodynamics, physicochemical magnitudes of macroscopic systems are determined from microscopic properties. The possibility of performing quantum mechanical calculations using computer programs and the need to have experimental data to confirm the theoretical calculations, recommend that the subject include a series of Computer Practices and Laboratory Practices.

COMPETENCIES/LEARNING RESULTS FOR THE SUBJECT

The subject is part of the Physical Chemistry Subject, being one of the Fundamental Modules of the Degree and, as such, shares the transversal competences assigned to this module. More specifically, this course develops the skills M02CM01 (Understanding and managing the principles of Physical Chemistry and its influence on chemical processes), M02CM08 (Capacity to select different instrumental techniques, simple or combined, for the characterization of chemical substances), M02CM09 (Be able to present ,orally and writing, in an understandable way, phenomena and processes related to Chemistry and related subjects), M02CM10 (Ability to search and select information in the field of Chemistry and other scientific fields, making use of bibliography and information and communication technologies) and M02CM11 (Being able to relate Chemistry with other disciplines, as well as understand its impact on today's society and the importance of the industrial chemical sector).

The coordination of this subject with the rest of the Module corresponds to the Coordination Commission of the Degree in Chemistry

Theoretical and Practical Contents

The course is divided into theoretical and practical contents

a) Theoretical content: It is divided into two different blocks

Block 1: Introduction to Quantum Chemistry

B1.1.- Quantum Chemistry basics: application to simple systems, Wave function and Schrödinger equation. Wave-particle duality. Eigenfunctions and eigenvalues. Average values. Begining of uncertainty. Translational movement: model of a potential box and the tunnel effect. Vibrational movement: harmonic oscillator. Angular momentum and rotational motion. Exact solutions of hydrogenoid atoms.
B1.2.- Atomic and molecular structure: Approximate methods, polyelectronic atoms, Pauli exclusion principle. Antisymmetry of the wave function. Spectral terms. Molecular orbital method, electronic configurations. Molecular terms. Computational Quantum Chemistry.

Block 2: Molecular Spectroscopy

B2.1. Radiation-matter interaction: Phenomena of absorption, emission and dispersion of light. Transition moments and selection rules. Intensity of the spectral signals.
B2.2. Rotation and vibration spectroscopies: IR and Raman Pure rotation spectra in linear molecules: microwaves and rotational Raman. Vibration spectra in diatomic molecules: rotational structure. Normal modes of vibration in polyatomic molecules. IR and Raman spectra. Group vibrations.
B2.3. Electron spectroscopies: Absorption spectra in diatomic molecules: vibrational structure. Chromophores. Charge transfer complexes. Fluorescence and phosphorescence. Quantum yield and lifetime. lasers. UV and X-ray photoelectron spectra.
B2.4. Resonance spectroscopy: NMR and RSE. Interaction of a magnetic field with matter. NMR: basics. Chemical shifts and spin-spin coupling. Electron spin resonance.
B2.5. Statistical Thermodynamics Fundamentals. Maxwell-Boltzmann statistics. Molecular partition functions. Calculation of thermodynamic magnitudes. Equilibrium constant. Potential energy surfaces. Transition state theory.

b) Practical content: it is divided into computer practical work and laboratory practical work

P1. Computer Practices (Computational Chemistry): Application of computational methods in quantum mechanical calculations linked to the optimization of molecular geometries, determination of molecular parameters, thermodynamic functions and spectroscopic magnitudes.
P2 Laboratory Practices (Spectroscopy practices): Practices using spectroscopic techniques: IR spectroscopy, UV/Vis absorption spectroscopy, fluorescence spectroscopy, etc.

TEACHING METHODS

The syllabus of this theoretical-experimental subject has been divided into 2 blocks (each one divided into 2 modules) of an eminently theoretical nature, and 2 practical modules.

Each theoretical block will comprise a four-month period, and will be evaluated in the following controls:

Controls Block 1:

M1.1. Quantum Chemistry: application to simple systems
M1.2. Atomic and molecular structure

Controls Block 2

M2.1. Radiation-matter interaction and rotation and vibration spectroscopies: IR and Raman
M2.2. Electron spectroscopy, resonance spectroscopy: NMR and RSE, and Statistical Thermodynamics.

The Practical Modules will be divided into Computer and Laboratory sessions. Both are mandatory and will be evaluated by means of Practice Reports.

Computer sessions related to block 1 (M1.1 and M1.2) will take place in the first four-month period.

Laboratory and computer sessions related to block 2 (M2.1 and M2.2) will take place in the second four-month period.

TYPES OF TEACHING

Types of teaching	M	S	GA	GL	GO	GCL	TA	TI	GCA
Hours of face-to-face teaching	35	5	15	25	10				
Horas de Actividad No Presencial del Alumno/a	52,5	7,5	22,5	37,5	15				

Legend: M: Lecture-based; S: Seminar; GA: Applied classroom-based groups; GL: Applied laboratory-based groups; GO: Applied computer-based groups; GCL: Applied clinical-based groups; TA: Workshop; TI: Industrial workshop; GCA: Applied fieldwork groups

Evaluation methods

- Continuous evaluation
- End-of-course evaluation

Evaluation tools and percentages of final mark

- See next part 100%

ORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

In order to pass the subject through continuous assessment, you must participate in each and every one of the following evaluable activities: control exams, laboratory practices, computer practices, delivery of individual work and presentation of team works.
Note Weighting

Control Exams (50% of the final mark): To pass the subject it is necessary to pass the exams corresponding to the two blocks, B1 and B2, of the subject, which will be evaluated independently, each worth 25% of the final mark. Each one of these blocks may be approved by means of two partial exams or by means of an exam for the entire syllabus of the block.

Thus, the first control of block B1, corresponding to module M1.1. described in the Methodology, will be carried out approximately in November. In case of obtaining a mark equal to or greater than 5, in the ordinary exam in January only the control of the second module (M1.2) of block B1 will be carried out, being necessary to obtain a mark equal to or greater than 5 to pass this exam and so on. approve the entire block. If you have not obtained a 5 in the control exam corresponding to module M1.1, in the ordinary exam in January a single control of the entire block will be carried out, encompassing both modules (M1.1. and M1.2.), being necessary to obtain a minimum mark of 5 to be able to pass the entire block. In case of not obtaining a 5 in this exam, a control of the entire B1 block will be carried out again in the ordinary May-June session.

The first control of block B2 (corresponding to module M2.1. described in the Methodology), will be carried out approximately between the months of March-April, and will proceed in a similar way to block B1. In case of obtaining a mark equal to or greater than 5, in the ordinary call only the control of the second module of the block (M2.2) will be carried out, being necessary to obtain a minimum mark of 5 to pass said control. In the event of having obtained a grade lower than 5 in the control related to module M2.1., in the ordinary call, a single exam will be carried out for the entire block B2, encompassing modules M2.1 and M2.2, being necessary again a minimum note of 5 to pass the block.

The remaining 50% of the note is distributed as follows:

- Laboratory practices: 20%. It includes the evaluation of the activities related to the practices (work done, quality of the results, reports). Attendance at laboratory practices will be an essential condition to pass the subject and, on the other hand, it will imply the obligatory evaluation of the subject in the ordinary call. The competencies associated with this assessment are: M02CM01, M02CM08, M02CM09 and M02CM10.

- Classroom practices: 10%. It includes the evaluation of issues and problems raised in class and that must be delivered resolved individually by the channels and within the deadlines established for their evaluation and correction. Participation in the classroom will also be valued. The competencies associated with this assessment are: M02CM01, M02CM09 and M02CM10.

- Seminars: 10%. It includes the presentation of group work and the corresponding presentations in the classroom. The competencies associated with this assessment are: M02CM01, M02CM09 and M02CM10.

- Computer practices: 10%. Includes evaluation reports. Attendance at laboratory practices will be an essential condition to pass the subject and, on the other hand, it will imply the obligatory evaluation of the subject in the ordinary call. The competencies associated with this assessment are: M02CM01, M02CM09 and M02CM10.-

Given the nature of continuous evaluation, the student who fails to carry out any of the compulsory activities during the course will appear as failed in the ordinary call, regardless of the grade obtained in the rest of the activities. The qualification of NOT PRESENTED will only be obtained in the following cases:

a) In case of not carrying out any compulsory activity (controls, exercises, exhibitions, practices)
b) In the event of having requested the evaluation by means of a single test within the term (within the first 18 school weeks by means of a signed document delivered to the professor), and not appearing for it. This criterion will be applied both in the ordinary call (May-June) and in the extraordinary call (June-July).

SINGLE EXAM

In both calls, both ordinary and extraordinary, the single test will consist of the following: an exam of the theoretical content and exercises corresponding to the entire course, a practical exam corresponding to laboratory and computer practices, and the presentation of a topic developed in the seminars, using multimedia resources for it. These three different parts will be carried out in three different consecutive days. This unique test will assess the M02CM01, M02CM08, M02CM09 and M02CM10 skills.

EXTRAORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

In the case of students who carry out continuous assessment, the extraordinary call will consist of two written exams, one for each block B1 and B2. Partial positive results obtained in the ordinary call may be maintained, so that each student must recover the blocks failed in the ordinary call. In case of passing these exams, the weighting of the note will be equal to that of the Ordinary Call. In case of not taking the exam, the exam will be graded as NOT PRESENTED.

In the extraordinary call (June-July) the single test is defined the same as in the Ordinary Call.

MANDATORY MATERIALS

They will be indicated in the Teaching Guide.

BIBLIOGRAPHY

Basic bibliography

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P. Atkins, J. de Paula. Química Física. Ed. Panamericana, 2008.
J. M. Elorza. Kimika Fisikoa. Elhuyar, 2000.
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Detailed bibliography

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J. M. Hollas. Modern Spectroscopy, 4th ed. Wiley, 2003.
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E. H. Brittain, W. O. George y C. H. Well. Introduction to Molecular Spectroscopy: Theory and Experiment. Academic Press, 1970.
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O. Mo, M. Yañez. Enlace Químico y Estructura Molecular. J. M. Bosch, 2000.

Journals

Journal of Physical Chemistry
Journal of Chemical Physics
Journal of Chemical Education
European Journal of Physics

Web sites of interest

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http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi
http://webbook.nist.gov/chemistry
http://bcs.whfreeman.com/pchem8e
http://www.shu.ac.uk/schools/sci/chem/tutorials/
http://scidiv.bcc.ctc.edu/s/s.html
http://www.ch.ic.ac.uk/vchemlib/course/mo_theory/main.html#triple
http://cccbdb.nist.gov/

OBSERVATIONS