COURSE GUIDE 2022/23

Faculty 215 - Faculty of Chemistry

Cycle Not Applicable

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. 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.

CONTENIDOS TEÓRICO-PRÁCTICOS

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.

2.- Atomic and molecular structure: Review of hydrogen atoms, polyelectronic atoms, Pauli exclusion principle. Antisymmetry of the wave function. Spectral terms. Molecular orbital method, electronic configurations. Molecular terms. Computational Quantum Chemistry.

3.-Radiation-matter interaction: Phenomena of absorption, emission and dispersion of light. Transition moments and selection rules. Intensity of the spectral signals.

4.-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.

5.-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.

6.- Resonance spectroscopy: NMR and RSE. Interaction of a magnetic field with matter. NMR: basics. Chemical shifts and spin-spin coupling. Electron spin resonance.

7.- Statistical Thermodynamics Fundamentals. Maxwell-Boltzmann statistics. Molecular partition functions. Calculation of thermodynamic magnitudes. Equilibrium constant. Potential energy surfaces. Transition state theory.

Computational Chemistry (Computer Practices) Application of computational methods in quantum mechanical calculations linked to the optimization of molecular geometries, determination of molecular parameters, thermodynamic functions and spectroscopic magnitudes.
Spectroscopy practices (Laboratory 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 4 modules of an eminently theoretical nature, and 2 practical modules.
The theoretical parts will be distributed in the following way:

1. Quantum Chemistry: application to simple systems
2. Atomic and molecular structure
3. Radiation-matter interaction and rotation and vibration spectroscopies: IR and Raman
4. Electron spectroscopy, resonance spectroscopy: NMR and RSE, and Statistical Thermodynamics.

Computer and laboratory sessions are mandatory.

Computer sessions related to 1 and 2 parts will take placein the first term.

Laboratory and computer sessions related to parts 3 and 4 will take place in the second term.

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

EVALUATION

. Theoretycal exam, written.
. Completion of practices (exercises, problems).
. Team work.
. Presentation of works.

Instructions:

45% of the mark will be divided into 4 partial exams (the 4 parts are descrived above), with the same % for each part. The student who passes will release the corresponding part (which will require a minimum grade of 5.0), and in the final exam he will have to complete only the part corresponding to exam 4 and the parts not passed. The first three exams will take place in around november, January and April.
Passed parts are not kept for the extraordinary call.

The other 55% of the grade is distributed as follows:

- Second Semester Laboratory practices: 25%. This will take into account a theoretical-practical test and an evaluation of the actions taken in the internship (work done, quality of results, reports, presentation, ...). Attendance at these sessions is compulsory in order to pass the subject and, in turn. The competencies to be developed are M02CM01, M02CM08, M02CM09 and M02CM10.

- Seminars: 20%. Assessment of exercises, presentation of work, teamwork, presentation, preparation of internships, etc. will be taken into account. The competencies to be developed are M02CM01, M02CM09 and M02CM10.

- First Semester Computer Labs: 10%. evaluation of reports, presentation of work, teamwork, presentation, etc. will be taken into account. Attendance at these internships will be compulsory in order to pass the subject and, in turn, will ensure that the assessment of the subject is carried out in the regular convocation. The competencies to be developed are M02CM01, M02CM09 and M02CM10.

As the subject is subject to continuous evaluation, the student will have a grade in the regular convocation (May-June). A No Show will be considered in the following cases:

a) A student who has applied to be evaluated by the single exam call (between the 1st and 18th teaching weeks), when he / she does not present himself / herself for the exam. A written request for the single test exam must be submitted in writing to the Professor.

b) A student who has not applied for a single exam call within the deadline (between weeks 1 and 18) if he / she has not presented himself / herself in all the examinations and assignments for the assessment of the subject, or if he / she withdrawas / drops the course.

It will be possible to drop/withdraw the course, even if a student has taken part in one of the activities, if he / she sends the corresponding written form, completed and signed, one month before the last teaching activity of the course.

SINGLE EXAM CALL

In both calls, the single exam will be the following: an analysis of the theoretical-practical content observed throughout the course, a practical analysis of laboratory and computer laboratory sessions, and an oral presentation of a topic covered in seminars, using multimedia resources. This single test will assess competencies M02CM01, M02CM08, M02CM09 and M02CM10.

In the case of a continuous assessment, if the weight of the final test exceeds 40% of the grade for the subject, it will be sufficient not to take the test so that the final grade is "not presented". On the other hand, if the weight of the final test is 40% or less of the subject grade, students who wish to refuse the call must apply at least one month before the end of the teaching period of the subject in question. This request must be submitted in writing to the teacher in charge of the subject.

EXTRAORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

Students with continuous assessment:

The marks of the parts passed in the regular call will be saved for the non-regular call. On the other hand, he will have to retake all the parts that he has not passed. All the evaluated activities with the same weighting as in the regular call will be considered. If the students dos not show on the exam, it will be graded as no show.

Students requesting a single exam call:

The single test will consist of an examination of the entire theoretical-practical content of the subject, a practical examination of computer and laboratory practices, and an oral presentation with the help of multimedia resources of a topic developed in the seminars. The single test will evaluate the skills M02CM01, M02CM08, M02CM09, M02CM10.

MANDATORY MATERIALS

They will be indicated in the Teaching Guide.

BIBLIOGRAFÍA

Basic bibliography

R. J. Silbey, R. A. Alberty. Kimika Fisikoa. Euskal Herriko Unibertsitatea, 2006.
I. R. Levine. Fisicoquímica, vols. 1 y 2. 5º ed. Ed. McGraw-Hill, 2004.
P. Atkins, J. de Paula. Química Física. Ed. Panamericana, 2008.
J. M. Elorza. Kimika Fisikoa. Elhuyar, 2000.

Detailed bibliography

A. Requena y J. Zúñiga. Espectroscopia. Pearson Prentice-Hall, 2004.
J. M. Hollas. Modern Spectroscopy, 4th ed. Wiley, 2003.
J. Bertran, V. Branchadell, M. Moreno y M. Sodupe. Química Cuántica. Ed. Síntesis, 2002.
E. H. Brittain, W. O. George y C. H. Well. Introduction to Molecular Spectroscopy: Theory and Experiment. Academic Press, 1970.
A. M. Halpern, G. C. McBane. Experimental Physical Chemistry. A laboratory textbook, 3rd edition. W.H. Freeman, 2006.
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

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

OBSERVATIONS