UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: PHYSICAL-CHEMISTRY III: POLYATOMIC MOLECULES AND A
Type: CORE COURSE
Degree: 409 - CHEMISTRY
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
Year: 3
Main language: Spanish
Use of additional languages:
Web site:

Code: 57319
ECTS credits: 6
Academic year: 2022-23
Group(s): 20 23
Duration: First semester
Second language: English
English Friendly: Y
Bilingual: N

Lecturer: **BERNABE BALLESTEROS RUIZ** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie, primera planta	QUÍMICA FÍSICA	926052049	bernabe.ballesteros@uclm.es	Monday, Tuesday: 9-11h Thursday: 17-19h.

Lecturer: **MARIA DEL PILAR MARTIN PORRERO** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie, 2ª planta	QUÍMICA FÍSICA	926052614	mariapilar.martin@uclm.es	Monday 11 to 13, wednesday and thursday 16 to 18

Lecturer: **LUCIA SANTOS PEINADO** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
Edificio Marie Curie/2.05	QUÍMICA FÍSICA	926052480	lucia.santos@uclm.es	Monday, wednesday and thursday from 16 to18

2. Pre-Requisites

They have not been established, but it is advisable to have passed the subject Physical Chemistry II: Introduction to Quantum Chemistry and Spectroscopy.

3. Justification in the curriculum, relation to other subjects and to the profession

In this subject the application of Quantum Mechanics extends to the study of polyatomic molecules in order to obtain the molecular structure and properties of them. This allows to address the spectroscopy of polyatomic molecules, filling in the contents of the "Physical Chemistry II: Introduction to Quantum Chemistry and Spectroscopy". Likewise, the Statistical Thermodynamics is presented, which allows to relate the molecular properties with the macroscopic thermodynamic properties ("Physical Chemistry I: Chemical Thermodynamics").

In this subject, computational calculations are used that are currently considered an essential tool in the different branches of Chemistry.

4. Degree competences achieved in this course

Course competences

Code	Description
E07	Relate macroscopic properties with those of atoms, molecules and non-molecular chemical compounds
E08	Know the principles of quantum mechanics and their application to the structure of atoms and molecules
E15	Know how to handle the standard chemical instrumentation and be able to elaborate and manage standardized procedures of work in the laboratory and chemical industry
E16	Plan, design and develop projects and experiments
G01	Know the principles and theories of Chemistry, as well as the methodologies and applications characteristic of analytical chemistry, physical chemistry, inorganic chemistry and organic chemistry, understanding the physical and mathematical bases that require
G02	Be able to gather and interpret data, information and relevant results, obtain conclusions and issue reasoned reports on scientific, technological or other problems that require the use of chemical tools
T10	Ability to use specific software for chemistry at user level
T11	Ability to obtain bibliographic information, including Internet resources

5. Objectives or Learning Outcomes

Course learning outcomes

Description

Ability to solve chemical problems applying the proper methodologies of physical chemistry

Ability to correctly use scientific language.

Dexterity in the analysis of errors of the magnitudes measured in the laboratory and in the use of computer programs for the treatment of experimental data.

Skill in the use of computer programs for calculating properties of matter and simulation of chemical.

Ability to search, understand and use relevant bibliographic and technical information.

Ability to understand and predict the behavior and reactivity of atoms and molecules from their structural characteristics, which can be determined from spectroscopic data or quantum chemical calculations

6. Units / Contents

Unit 1: Theory of groups and molecular symmetry

Unit 2: Structure of polyatomic molecules
Unit 3: Spectroscopy of polyatomic molecules
Unit 4: Spectroscopies of resonance
Unit 5: Statistical thermodynamics.
Unit 6: Calculation of thermodynamic magnitudes
Unit 7: Intermolecular forces: real gases.
Unit 8: Condensed phases
Unit 9: Laboratory practices

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Class Attendance (theory) [ON-SITE]	Lectures	E07 E08 G01 T10 T11	0.88	22	N	-	Theory classes dedicated to explaining contents of the temary
Laboratory practice or sessions [ON-SITE]	Practical or hands-on activities	E07 E08 E15 E16 G02 T10	0.6	15	Y	Y	Carrying out practices in the laboratory for 3 days and in the computer room for 2 days
Workshops or seminars [ON-SITE]	Workshops and Seminars	E07 E08 G02 T10 T11	0.56	14	Y	N	Questions from seminars and problems previously raised and worked autonomously by the students will be resolved and clarified students. Occasionally a proposed problem will be worked individually in the classroom
Practicum and practical activities report writing or preparation [OFF-SITE]	Self-study	G02	0.32	8	Y	Y	Study of the scripts and preparation of a report with the results obtained in the laboratory practices.
Study and Exam Preparation [OFF-SITE]	Combination of methods	E07 E08 E16 G01 G02 T10 T11	3.28	82	N	-	Autonomous resolution of the problems or seminars raised and study of the theoretical contents of the program.
Mid-term test [ON-SITE]	Assessment tests	G01	0.06	1.5	Y	N	Partial written exam of the first 4 topics
Final test [ON-SITE]	Assessment tests	G01	0.1	2.5	Y	Y	Partial examination of the second part of the agenda with the possibility of recovering the first part.
Computer room practice [ON-SITE]	Practical or hands-on activities	E08 G02 T10	0.12	3	Y	Y	
Group tutoring sessions [ON-SITE]	Group Work	G02 T11	0.08	2	Y	N	
		Total:	**6**	**150**			
		Total credits of in-class work: 2.4					**Total class time hours: 60**
		Total credits of out of class work: 3.6					**Total hours of out of class work: 90**

As: Assessable training activity
Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Practicum and practical activities reports assessment	10.00%	10.00%	Review of results reports
Laboratory sessions	10.00%	10.00%	Continuous evaluation in the laboratory
Assessment of problem solving and/or case studies	20.00%	0.00%	Follow-up in seminar classes
Mid-term tests	30.00%	0.00%	Exam with questions and problems about the contents taught in the subject
Final test	30.00%	80.00%	Exam with questions and problems about the contents taught in the subject. It will be 60% when the test involves the evaluation of the whole syllabus of the subject
Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

1. Written exam with questions and problems about the content taught in the course (60% of the grade). This percentage can be divided into two partial exams (progress test and final test) or one final exam (final test).
2. Continuous evaluation of laboratory work (10%) including the adequate preparation of the memory of results and test questions (10%).
3. Continuous assessment of learning based on problem solving in the seminar hours (20%). The student will be asked to submit resolved exercises, solve different issues related to the subject, resolution of practical cases ...
4.To apply the continuous assessment they must have at least a 4.5 in the progress tests (written exam)

Non-continuous evaluation:

1. Written exam with questions and problems about the contents taught in the course, including questions about practices (80% of the mark). This exam will be different from the one carried out for those who follow the continuous evaluation with the aim of evaluating all the competences of the subject.
2-20% the mark of the practices (work in the laboratory, report of the work done and results of the test questionnaires).

Specifications for the resit/retake exam:

1. Exam with questions and problems about the content taught in the subject (60% of the grade).
2. Continuous evaluation of laboratory work (10%) including the adequate preparation of the results memory and test questionnaires (10%).
3. Continuous assessment of problem-based learning in seminar hours (20%). The student will be asked to submit resolved exercises, solve different issues related to the subject, resolution of practical cases ...

The laboratory grade is kept for all students. If the laboratory has NOT been done, the subject will NOT be passed in any case. If the laboratory has been suspended in the ordinary call, the extraordinary call will include practical questions / activities.

The seminar grade is kept if it is higher than 5 during the continuous assessment course. Otherwise, the extraordinary call will have additional questions of the type required in the seminars.

Specifications for the second resit / retake exam:

1. Written exam with questions and problems about the contents taught in the course, including questions about practices (80% of the mark). This exam will be different from the one carried out for those who follow the continuous evaluation with the aim of evaluating all the competences of the subject.

2-20% the mark of the practices (work in the laboratory, report of the work done and results of the test questionnaires).

The student must have passed the laboratory in a previous call.

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours	**hours**

Unit 1 (de 9): Theory of groups and molecular symmetry

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	6
Mid-term test [PRESENCIAL][Assessment tests]	.5

Unit 2 (de 9): Structure of polyatomic molecules

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	2
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	13.75
Mid-term test [PRESENCIAL][Assessment tests]	.5

Unit 3 (de 9): Spectroscopy of polyatomic molecules

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	2
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	13.75
Mid-term test [PRESENCIAL][Assessment tests]	.5

Unit 4 (de 9): Spectroscopies of resonance

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	1
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	4

Unit 5 (de 9): Statistical thermodynamics.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	2
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9.75
Final test [PRESENCIAL][Assessment tests]	.5

Unit 6 (de 9): Calculation of thermodynamic magnitudes

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	3
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9.5
Final test [PRESENCIAL][Assessment tests]	.33

Unit 7 (de 9): Intermolecular forces: real gases.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	2
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9.75
Final test [PRESENCIAL][Assessment tests]	.5

Unit 8 (de 9): Condensed phases

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	6
Final test [PRESENCIAL][Assessment tests]	.5

Unit 9 (de 9): Laboratory practices

Activities	**Hours**
Laboratory practice or sessions [PRESENCIAL][Practical or hands-on activities]	18
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	8
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9.5
Final test [PRESENCIAL][Assessment tests]	.67

Global activity	
Activities	**hours**
Laboratory practice or sessions [PRESENCIAL][Practical or hands-on activities]	18
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	14
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	8
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	82
Mid-term test [PRESENCIAL][Assessment tests]	1.5
Class Attendance (theory) [PRESENCIAL][Lectures]	24
Final test [PRESENCIAL][Assessment tests]	2.5
Total horas:	150

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
Atkins, P. W. (1940-)	Atkins química física	Medica Panamericana		978-950-06-1248-7	2008	
Atkins, P. W. (1940-)	Molecular quantum mechanics	Oxford University press		0-19-855947-X	2001	
Bertrán Rusca y J. Núñez Delgado (coord.).	Problemas de Química Física	Delta Publicaciones,		84-96477-48-7	2007	
Engel, Thomas	Química física	Pearson-Addison Wesley		84-7829-077-X	2006	
Levine, Ira N.	Fisicoquímica	McGraw Hill		84-481-4005-2	2004	
Levine, Ira N.	Problemas de fisicoquímica	McGraw Hill		84-481-9833-6	2005	
McQuarrie, Donald A. (Donald Allan)	Physical chemistry : a molecular approach	University Science Books		978-0-935702-99-6	1997	
Hollas, J. Michael	Modern spectroscopy /	John Wiley & Sons,		978-0-470-84416-8	2010	