COURSE DESCRIPTION

COURSE DETAILS

Title (of the course): **FUNDAMENTOS DE ESPECTROSCOPÍA**
Code: 100529
Degree/Master: **GRADO DE FÍSICA** Year: 4
Field: OPTATIVA 4
Character: OPTATIVA Duration: SECOND TERM
ECTS Credits: 6.0 Classroom hours: 60
Face-to-face classroom percentage: 40.0% Study hours: 90
Online platform:

LECTURER INFORMATION

Name: MADUEÑO JIMÉNEZ, RAFAEL
Department: QUÍMICA FÍSICA Y TERMODINÁMICA APLICADA
Area: QUÍMICA FÍSICA
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PREREQUISITES AND RECOMMENDATIONS

Prerequisites established in the study plan

None

Recommendations

None specified

INTENDED LEARNING OUTCOMES

CB1	the skills to analyse and summise
CB3	written and oral communication
CB5	Problem solving
CB6	Team work
CB7	Critical thinking
CB8	Independent Study
CE1	knowledge and understanding of the most important phenomenons and physics theories
CE4	The ability to measure, interpret and design experiences both in and out of the laboratory

OBJECTIVES

Fundamental knowlegde of molecular spectroscopy concepts and the application of experimental methods to the study of molecular structure by obtaining molecular parameters of interest in the field of Physical Chemistry.

COURSE DESCRIPTION

CONTENT

1. Theory contents

1.- SPECTROSCOPY AND QUANTUM MECHANICS. Introduction. The atomic model and quantum mechanics solutions. The Born-Oppenheimer approximation and Spectroscopy. Molecular Model. Rigid rotor and harmonic oscillator.

2.-THE INTERACTION OF THE ELECTROMAGNETIC RADIATION WITH MATTER Introduction. Absorption and emision of radiation. Spectral line broadening. Experimental methods.

3.- ROTATIONAL SPECTROSCOPY. Introduction. Classification of molecules by symmetry. Rotational spectra. Diatomic and linear polyatomic molecules. Centrifugal distorsion. Symmetric rotor. Stark effect. Asymmetric rotor. Spherical rotor. Rotational Raman Spectrocopy. Nuclear spin statistical weights.

4.- VIBRATIONAL SPECTROSCOPY. Introduction. Diatomic molecules. Infrared (IR) and Raman spectra. Anharmonicity. Vibration–rotation spectroscopy. Polyatomic molecules. Applications of vibrational spectroscopy.

5.-MOLECULAR SYMMETRY AND ELECTRONIC SPECTROSCOPY. Molecular symmetry. Elements of symmetry: Generation. Point groups of symmetry. Character Tables. Degenerate and non-degenerate point groups. Diatomic molecules. Molecular orbitals. Electronic configuration and classification of electronic states. Selection rules. Ground and excited electronic states. Potential energy curve. Vibrational structure in electronic spectra. The Franck-Condon principle. Fluorescence and phosphorescence.

6.- OTHER SPECTROSCOPIES. Resonance Spectroscopy. Mössbauer Spectroscopy. Auger Spectroscopy. Photoelectron Spectroscopy.

2. Practical contents

The lab practices proposed as possible are the following ones:

Practice 1. Beer-Lambert Law.

Practice 2. IR Spectra of diatomic molecules in air. Determination of molecular parameters

Practice 3. Energy of hydrogen bonding formation determined by UV-visible spectroscopy.

METHODOLOGY

Methodological adaptations for part-time students and students with disabilities and special educational needs

Part-time students will be governed by the same rules as full-time students. The teacher will meet with students affected by disabilities and special educational needs to establish the most

Face-to-face activities

Activity	Large group	Medium group	Total
Assessment activities	3	-	3
Debates	17	-	17
Group presentation	6	-	6
Group work (cooperative)	7	-	7
Lab practice	-	7	7
Seminar	-	20	20
Total hours:	***33***	***27***	***60***

COURSE DESCRIPTION

Off-site activities

Activity	Total
Exercises	10
Information search	40
Reference search	30
Self-study	10
Total hours	***90***

WORK MATERIALS FOR STUDENTS

Case studies
Dossier
Lessons summary
References

EVALUATION

Intended learnig	Oral Presentation	Placement reports	Project
CB1	X	X	X
CB3	X	X	
CB5		X	
CB6	X		
CB7		X	X
CB8		X	
CE1	X	X	X
CE4		X	
Total (100%)	***40%***	***20%***	***40%***
Minimum grade	***0***	***0***	***0***

(*)Minimum grade necessary to pass the course

COURSE DESCRIPTION

Method of assessment of attendance:

15% included in the corresponding evaluation instruments

General clarifications on instruments for evaluation:

The instruments included allow for proper evaluation of the requirements and skills (Competencies) to be developed in this subject. All instruments are for continuous evaluation

A minimum mark is not necessary in any evaluation instrument to make the average.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs:

Part-time students are governed by the same rules as full-time students. For students with special educational needs, the agreements of the initial meeting will apply.

Qualifying criteria for obtaining honors:

Students with an overall grade higher than 9/10 may reach an honor degree. (And in accordance with the current administrative conditions approved by the university governing council)

BIBLIOGRAPHY

1. Basic Bibliography

- I.N. Levine, Fisicoquímica 5ª Ed. (vol. 2), 2004–Physical Chemistry 6th ed., 2008
- P.W. Atkins, Química Física 8ª Ed., 2008 - Physical Chemistry 9th ed. 2010
- J. Bertran Rusca, J. Nuñez Delgado, Química Física (vols. 1-2), 2002
- M. Gil Criado, J.L. Núñez Barriocanal, Ed. Garceta, 2018
- G.W. Castellan, Fisicoquímica 3ª Ed., 1998
- K.J. Laidler, J.H. Meiser, Fisicoquímica, Ed. CECSA, 1998- Physical Chemistry 4ed., 2002
- D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, 1997
- M. Diaz Peña y A. Roig Muntaner, Química Física, 2ª Ed. (2 Vols.), 1989

2. Further reading

- C.N. Bandwell, Fundamentos de espectroscopia molecular, 2ª Ed., 1977
- Fundamentals of Molecular Spectroscopy, 4th ed., 1994
- J.Michael Hollas, Modern Spectroscopy 4th ed., 2004
- A. Requena, J. Zuñíga, Espectroscopia, 2004
- W. Schmidt, Optical Spectroscopy in Chemistry (Wiley-VCH), 2005
- I.N. Levine, Química Cuántica 5ed., 2001-Quantum Chemistry 6th ed., 2008
- G. Aruldhas, Molecular Structure and Spectroscopy 2ed., 2008
- W. Gordy, R.L. Cook, Microwave Molecular Spectra, 1974
- N.B. Coulthup, L.M. Daly, S.E. Wiberley, Introduction to Infrarred and Raman Spectroscopy, 3th ed., 1990
- W.G. Richards, P.R. Scott, Structure and Spectra of Molecules, 1985
- J.R. Lakowicz, Principles of Fluorescence Spectroscopy, 3th ed., 1986
- D. Rendel, Fluorescence and Phosphorescence Spectroscopy, 1987
- H. Günter, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chem., 2nd ed. 1995
- R.J. Abraham, J. Fisher, P. Lofhuts, Introduction to NMR Spectroscopy, 1991
- J.K.M. Sanders, B.K. Hunter, Modern NMR Spectroscopy, 1993
- E.D. Becker, High Resolution NMR, 3th ed., 2000
- D.C. Harris, Nuclear Magnetic Resonance Spectroscopy: A Physicochemical View, 2nd ed., 1987
- J.R. Bolton, J.E. Wertz, Electron Spin Resonance: Elementary Theory and applications, 1972

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- N.M. Atherton, Principles of Electron Spin Resonance, 1993
- P.K. Ghosh, Introduction to Photoelectron Spectroscopy, 1983
- T.L: Barr, Modern ESCA: The Principles and Practice of X-Ray Photoelectron Spectroscopy, 1994
- J.W. Rabalais, Principles of Ultraviolet Photoelectron Spectroscopy, 1977
- D.P.E. Dickson, F.J. Berry (Eds.), Mossbauer Spectroscopy, 1986
- N.N. Greenwood, T.C. Gibb, Mossbauer Spectroscopy, 1971
- D. Neuhaus, M.P. Williamson, The Nuclear Overhauser Effect, 1989

Problemas:

- P.W. Atkins, Students' Solutions Manual for Physical Chemistry, 8th ed., 2006
- I.N. Levine, Students Solutions Manual to Accompany Physical Chemistry, 8th ed., 2008
- J. Bertran Rusca, J. Nuñez Delgado, Problemas de Química Física, 2007

COORDINATION CRITERIA

Tasks deadlines
Tasks performance

SCHEDULE

Period	Assessment activities	Debates	Group presentation	Group work (cooperative)	Lab practice	Seminar
1# Week	0,0	5,0	0,0	0,0	0,0	0,0
2# Week	0,0	2,0	0,0	0,0	0,0	3,0
3# Week	0,0	3,0	0,0	0,0	0,0	2,0
4# Week	0,0	2,0	0,0	0,0	0,0	3,0
5# Week	0,0	3,0	0,0	2,0	0,0	0,0
6# Week	0,0	0,0	0,0	0,0	0,0	2,0
7# Week	0,0	0,0	0,0	2,0	0,0	3,0
8# Week	0,0	0,0	0,0	0,0	3,0	2,0
9# Week	0,0	0,0	0,0	3,0	2,0	0,0
10# Week	0,0	0,0	0,0	0,0	2,0	0,0
11# Week	0,0	2,0	0,0	0,0	0,0	3,0
12# Week	0,0	0,0	3,0	0,0	0,0	2,0
13# Week	0,0	0,0	3,0	0,0	0,0	0,0
14# Week	3,0	0,0	0,0	0,0	0,0	0,0
Total hours:	***3,0***	***17,0***	***6,0***	***7,0***	***7,0***	***20,0***

COURSE DESCRIPTION

The methodological strategies and the evaluation system contemplated in this Course Description will be adapted according to the needs presented by students with disabilities and special educational needs in the cases that are required.

CONTINGENCY PLAN: CASE SCENARIO A

Case scenario A will correspond to a diminished on-site academic activity due to social distancing measures affecting the permitted capacity of classrooms.

METHODOLOGY

General clarifications on the methodology on case scenario A

A multimodal (hybrid) teaching system will be adopted, combining both on-site and remote classes via videoconference (synchronous) that will be held in the timetable approved by the corresponding Faculty or School. The time distribution of teaching activities (both on-site and remote) will be decided by the aforementioned Faculties and Schools bearing in mind the permitted capacity of classrooms and social distancing measures as established at that time.

EVALUATION

Intended learnig	Oral Presentation	Placement reports	Project
CB1	X	X	X
CB3	X	X	
CB5		X	
CB6	X		
CB7		X	X
CB8		X	
CE1	X	X	X
CE4		X	
Total (100%)	***40%***	***20%***	***40%***
Minimum grade	***0***	***0***	***0***

(*)Minimum grade necessary to pass the course

Method of assessment of attendance (Scenario A):

15% included in the corresponding evaluation instruments

COURSE DESCRIPTION

General clarifications on instruments for evaluation (Scenario A):

The instruments included allow for proper evaluation of the requirements and skills (Competencies) to be developed in this subject. All instruments are for continuous evaluation

A minimum mark is not necessary in any evaluation instrument to make the average.

Extraordinary call for the 2020-2021 academic year for students of second enrollment or higher.

The student will be able to retrieve those continuous assessment tests not passed, as long as they have been presented to them in the school period.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs (Scenario A):

Part-time students are governed by the same rules as full-time students. For students with special educational needs, the agreements of the initial meeting will apply.

Qualifying criteria for obtaining honors (Scenario A):

Students with an overall grade higher than 9/10 may reach an honor degree. (And in accordance with the current administrative conditions approved by the university governing council)

CONTINGENCY PLAN: CASE SCENARIO B

Case scenario B will bring about a suspension of all on-site academic activities as a consequence of heath measures.

METHODOLOGY

General clarifications on the methodology on case scenario B

On-site teaching activities will be held via videoconference (synchronous) in the timetable approved by the corresponding Faculty or School. Alternative activities will be proposed for reduced groups in order to guarantee the acquisition of course competences.

COURSE DESCRIPTION

EVALUATION

Intended learnig	Oral Presentation	Placement reports	Project
CB1	X	X	X
CB3	X	X	
CB5		X	
CB6	X		
CB7		X	X
CB8		X	
CE1	X	X	X
CE4		X	
Total (100%)	***40%***	***20%***	***40%***
Minimum grade	***0***	***0***	***0***

(*)Minimum grade necessary to pass the course

Moodle Tools	Exposición oral	Informes/memorias de prácticas	Proyecto
Asistencia	X	X	X
Chat			X
Tarea		X	X
Videoconferencia	X		

Method of assessment of attendance (Scenario B):

15% included in the corresponding evaluation instruments

General clarifications on instruments for evaluation (Scenario B):

The instruments included allow for proper evaluation of the requirements and skills (Competencies) to be developed in this subject. All instruments are for continuous evaluation

A minimum mark is not necessary in any evaluation instrument to make the average.

Extraordinary call for the 2020-2021 academic year for students of second enrollment or

COURSE DESCRIPTION

higher.

The student will be able to retrieve those continuous assessment tests not passed, as long as they have been presented to them in the school period.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs (Scenario B):

Part-time students are governed by the same rules as full-time students. For students with special educational needs, the agreements of the initial meeting will apply.

Qualifying criteria for obtaining honors (Scenario B):

Students with an overall grade higher than 9/10 may reach an honor degree. (And in accordance with the current administrative conditions approved by the university governing council)