COURSE DESCRIPTION

COURSE DETAILS

Title (of the course): **FUNDAMENTOS DE ESPECTROSCOPÍA**
Code: 100529
Degree/Master: **GRADO DE FÍSICA** Year: 4
Name of the module to which it belongs: OPTATIVO
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: http://moodle.uco.es/moodlemap/

LECTURER INFORMATION

Name: RODRIGUEZ AMARO, RAFAEL (Coordinator)
Department: QUÍMICA FÍSICA Y TERMODINÁMICA APLICADA
Area: QUÍMICA FÍSICA
Office location: Rabanales, C3, segunda planta
E-Mail: qf1roamr@uco.es Phone: 957218617

Name: CAÑO OCHOA, RAFAEL DEL
Department: QUÍMICA FÍSICA Y TERMODINÁMICA APLICADA
Area: QUÍMICA FÍSICA
Office location: Rabanales, C3, segunda planta
E-Mail: q92caocr@uco.es Phone: 957218647

PREREQUISITES AND RECOMMENDATIONS

Prerequisites established in the study plan

To have, at least, B1 Level in English to take this course in the bilingual group

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

COURSE DESCRIPTION

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.

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

SUSTAINABLE DEVELOPMENT GOALS RELATED TO THE CONTENT

Quality education

Industry, innovation and infrastructure

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 the affected students to establish the most appropriate adaptations for each particular case, following the indications of the report issued by the Inclusive Education Unit.

COURSE DESCRIPTION

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***

Off-site activities

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

WORK MATERIALS FOR STUDENTS

Dossier - *Moodle*
Lessons summary - *Moodle*

EVALUATION

Intended learning	Oral Presentation	Placement reports	Project
CB1	X	X	X
CB3	X	X	
CB5		X	
CB6	X		
CB7		X	X
CB8		X	

COURSE DESCRIPTION

Intended learning	Oral Presentation	Placement reports	Project
CE1	X	X	X
CE4		X	
Total (100%)	***40%***	***20%***	***40%***
Minimum grade	***0***	***0***	***0***

(*)Minimum mark (out of 10) needed for the assessment tool to be weighted in the course final mark. In any case, final mark must be 5,0 or higher to pass the course.

Method of assessment of attendance:

15% already included in each corresponding evaluation instrument

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 the instruments are of continuous evaluation and can be recovered in the different official calls, both ordinary and extraordinary, provided that the subject has not been approved in previous calls.
The marks will be valid during the current academic year and for the extraordinary call and for the extraordinary call for completion of studies.
The Project consists of an individual work on the basic principles of Spectroscopy, according to a predefined script, and the generation of a written project report.
The oral presentation consists of the elaboration of a work about a specific spectroscopic technique and its oral presentation in class.

Clarifications on the methodology 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.
For affected students, the procedure will be in accordance with the indications of the report issued by the Inclusive Education Unit.

Clarifications on the evaluation of the extraordinary call and extra-ordinary call for completion studies:

These calls will be governed by the same rules as ordinary calls.

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 (Article 80 of the Regulation).

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.
- A. Requena Rodríguez, J. Zuñiga Román, Espectroscopía: (vol.1) Fundamentos. García Maroto Eds.,2020.

COURSE DESCRIPTION

- 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.
- 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.
- N.M. Atherton, Principles of Electron Spin Resonance, 1993.
- 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

Common evaluation criteria
Tasks deadlines
Tasks performance

SCHEDULE

Period	Assessment activities	Debates	Group presentation	Group work (cooperative)	Lab practice	Seminar
1# Week	0,0	2,0	0,0	0,0	0,0	2,0
2# Week	0,0	3,0	0,0	0,0	0,0	1,0

COURSE DESCRIPTION

Period	Assessment activities	Debates	Group presentation	Group work (cooperative)	Lab practice	Seminar
3# Week	0,0	3,0	0,0	0,0	0,0	1,0
4# Week	0,0	1,0	0,0	0,0	0,0	3,0
5# Week	0,0	3,0	0,0	1,0	0,0	0,0
6# Week	0,0	1,0	0,0	0,0	0,0	3,0
7# Week	0,0	2,0	0,0	0,0	0,0	2,0
8# Week	0,0	0,0	0,0	1,0	0,0	3,0
9# Week	0,0	2,0	0,0	0,0	0,0	3,0
10# Week	0,0	0,0	3,0	0,0	0,0	2,0
11# Week	0,0	0,0	0,0	1,0	3,0	0,0
12# Week	0,0	0,0	0,0	1,0	3,0	0,0
13# Week	0,0	0,0	0,0	3,0	1,0	0,0
14# Week	0,0	0,0	3,0	0,0	0,0	0,0
15# 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***

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.