TEACHING GUIDE

DETAILS OF THE SUBJECT

Title (of the subject): **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 Classroom hours: 60
Face-to-face classroom percentage: 40% Non-contact hours: 90
Online platform: Moodle

TEACHER INFORMATION

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REQUIREMENTS AND RECOMMENDATIONS

Prerequisites established in the study plan

None.

Recommendations

Minimum English level: B1 (For the course recognition in English will be necessary the accreditation of the English title)

SKILLS

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.

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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

Goberned by the same rules as full-time students.

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Face-to-face activities

Activity	Large group	Medium group	Total
Assessment activities	3	-	3
Debates	10	-	10
Group presentation	6	-	6
Group work (cooperative)	7	-	7
Laboratory	-	7	7
Lectures	7	-	7
Seminar	-	20	20
Total hours:	33	27	60

Not on-site activities

Activity	Total
Bibliographic consultations	30
Exercises	10
Finding information	40
Self-study	10
Total hours:	**90**

WORK MATERIALS FOR STUDENTS

Practical cases and examples
Dossier
Bibliographic references
Summaries of the issues

Clarifications:

Material and information about the subject contents, bibliography and development of seminar activities will be supplied to the students in the moodle on-line platform during the semester.

EVALUATION

	Tools			
Skills	**Assignments and projects**	**Attendance sheets**	**Internship reports**	**Oral presentations**
CB1	x	x	x	
CB3	x		x	x
CB5	x			x
CB6		x		x
CB7	x		x	
CB8	x		x	
CE1	x		x	x
CE4			x	
Total (100%)	**35%**	**15%**	**15%**	**35%**
Minimum grade.(*)	**4**	**4**	**4**	**4**

(*) Minimum grade necessary to pass the subject

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.

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

They are goberned by the same rules as full-time students and their continuous assessment is divided into:

Internship reports (15%) and attendance sheets (15%) represent 30% of the overall mark. The remaining 70% of the final mark corresponds to Assignments, Projects (35%) and Oral presentations (35 %).

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)

¿Hay examenes/pruebas parciales?: No

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

- 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

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- 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

- 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

- Delivery date job
- Performing activities

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SCHEDULE

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

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