



IDENTIFYING DATA

Physical chemistry 2

Subject	Physical chemistry 2			
Code	V11G200V01403			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	9	Mandatory	2nd	2nd
Teaching language	Spanish Galician			
Department				
Coordinator	Fernández Nóvoa, Alejandro			
Lecturers	Fernández Nóvoa, Alejandro Ferro Costas, David Hermida Ramón, José Manuel Pastoriza Santos, Isabel Peña Gallego, María de los Ángeles			
E-mail	afnovo@uvigo.es			
Web				
General description	Application of the principles and methods of Quantum Mechanics to the study of molecular structure and spectroscopy.			

Competencies

Code	
A3	(*)Demostrar coñecemento e comprensión de feitos esenciais, conceptos, principios e teorías en: principios da Mecánica Cuántica e a súa aplicación na descrición da estrutura e as propiedades de átomos e moléculas
A6	(*)Demostrar coñecemento e comprensión de feitos esenciais, conceptos, principios e teorías en: principios de Termodinámica e as súas aplicacións en Química
A8	(*)Demostrar coñecemento e comprensión de feitos esenciais, conceptos, principios e teorías en: principais técnicas de investigación estrutural, incluíndo a Espectroscopía
A19	(*)Aplicar os coñecementos e a comprensión á resolución de problemas cuantitativos e cualitativos de natureza básica
A20	(*)Avaliar, interpretar e sintetizar datos e información química
A21	(*)Recoñecer e implementar boas prácticas científicas de medida e experimentación
A22	(*)Procesar datos e realizar cálculo computacional relativo a información e datos químicos
A23	(*)Presentar material e argumentos científicos de xeito oral e escrita a unha audiencia especializada
A27	(*)Monitorizar, mediante observación e medida de propiedades físicas e químicas, acontecementos ou cambios e documentalos e rexistralos de xeito sistemático e fiable
A28	(*)Interpretar datos derivados das observacións e medicións do laboratorio en termos do seu significado e relacionalos coa teoría adecuada
A29	(*)Demostrar habilidades para os cálculos numéricos e a interpretación dos datos experimentais, con especial énfase na precisión e a exactitude
B1	(*)Comunicarse de forma oral e escrita en polo menos unha das linguas oficiais da Universidade
B3	(*)Aprender de forma autónoma
B4	(*)Procurar e administrar información procedente de distintas fontes
B5	(*)Utilizar as tecnoloxías da información e das comunicacións e manexar ferramentas informáticas básicas
B6	(*)Manexar as matemáticas, incluíndo aspectos tales como análise de erros, estimacións de ordes de magnitude, uso correcto de unidades e modos de presentación de datos
B7	(*)Aplicar os coñecementos teóricos á práctica
B8	(*)Traballar en equipo
B9	(*)Traballar de forma autónoma
B12	(*)Planificar e administrar adecuadamente o tempo
B13	(*)Tomar decisións
B14	(*) Analizar e sintetizar información e obter conclusións
B15	(*)Avaliar de modo crítico e construtivo o entorno e a si mesmo

Learning aims

Expected results from this subject

Training and Learning
Results

	A3	B1
	A19	B3
		B4
		B6
		B9
	A3	B1
	A19	B3
	A20	B4
	A22	B5
	A28	B6
	A29	B7
		B9
		B12
		B13
		B14
	A19	B1
		B3
		B4
		B6
		B7
		B9
	A3	B1
		B3
		B4
		B6
		B9
	A3	B1
	A19	B3
	A20	B4
	A22	B5
	A23	B6
	A28	B7
	A29	B9
		B12
		B13
		B14
	A8	B1
		B3
		B4
		B6
		B9
	A8	B1
		B3
		B4
		B6
		B7
		B9
	A8	B1
		B3
		B4
		B6
		B9
	A3	B1
	A8	B3
	A19	B4
	A20	B5
	A22	B6
	A23	B7
	A27	B9
	A28	B12
	A29	B13
		B14

	A3 A8	B1 B3 B4 B6 B9
	A3 A8 A19 A22	B1 B3 B4 B5 B6 B7 B9
	A8 A19	B1 B3 B4 B6 B9
	A8 A19 A22	B1 B3 B4 B6 B9
	A8	B1 B3 B4 B6 B9
	A6 A19 A20 A21 A23 A27 A28 A29	B1 B3 B4 B5 B6 B7 B8 B9 B12 B13 B14 B15

Contents

Topic	
Electronic Structure of Diatomic Molecules.	- The Born-Oppenheimer Approximation. - The Hydrogen Molecule-ion. OM Method. - The Hydrogen Molecule. OM and Valence Bond Methods. - OM Method for Homonuclear and Heteronuclear Diatomic Molecules. - The Hartree-Fock Method. Basis Sets.
Electronic Structure of Polyatomic Molecules.	- OM Method in Polyatomic Molecules. - Semiempirical Methods. The Hückel Method. - Calculation of Molecular Properties - Other Methods in Computational Chemistry.
Introduction to Molecular Spectroscopy	- Matter-Radiation Interaction. A General Approach. - Transition Dipole Moment. Selection Rules. - Intensity and Position of the Spectral Transitions..
Rotational Spectroscopy.	- Pure Rotational Spectra of Diatomic Molecules. Rigid Rotor Model and Elastic Rotor Model. - Pure Rotational Spectra of Polyatomic Molecules.
Vibrational Spectroscopy.	- Vibration Spectra of Diatomic Molecules. Harmonic Oscillator Model and Anharmonic Oscillator Model. - Vibration-Rotation Spectra of Diatomic Molecules. - Vibration-Rotation Spectra of Polyatomic Molecules. - Raman Spectroscopy.
Electronic Spectroscopy.	- Electronic Spectra of Diatomic Molecules. - Vibrational Structure. The Franck-Condon Principle. - Fine Rotational Structure. - Electronic Spectra of Polyatomic Molecules.

Magnetic Resonance Spectroscopy.	<ul style="list-style-type: none"> - Introduction to Nuclear Magnetic Resonance. - Chemical Shift. - Spin-Spin Interaction. Coupling Constant. - Electronic Spin Resonance Spectroscopy.
Practices of Chemical Thermodynamics (six sessions)	<ul style="list-style-type: none"> - Experimental determination of equilibrium constants using spectrophotometric and potentiometric methods. - Experimental determination of enthalpies of combustion, solution, neutralization, fusion or vaporization. - Colligative Properties. - Experimental determination of activity coefficients using potentiometric methods.
Practices of Quantum Chemistry and Spectroscopy (seven sessions).	<ul style="list-style-type: none"> - Theoretical study of the molecular structure of H₂ and H₂⁺ molecules. - Theoretical study of the molecular structure of other diatomic molecules. - Conformational isomerism and internal rotation in n-butane. - Prediction, theoretical interpretation and resolution of the vibration-rotation spectrum for HCl. - Electronic Spectroscopy: Spectrum of I₂ in gas phase.

Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	26	39	65
Seminars	26	39	65
Laboratory practises	45.5	4.5	50
Autonomous troubleshooting and / or exercises	0	10	10
Long answer tests and development	4	8	12
Reports / memories of practice	0	9	9
Short answer tests	2	5	7
Multiple choice tests	0	4	4
Practical tests, real task execution and / or simulated.	1	2	3

*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies

Description
Master Session
Seminars
Laboratory practises
Autonomous troubleshooting and / or exercises

Personalized attention

Methodologies	Description
Master Session	
Seminars	
Laboratory practises	
Autonomous troubleshooting and / or exercises	
Tests	Description
Long answer tests and development	
Reports / memories of practice	
Short answer tests	
Multiple choice tests	
Practical tests, real task execution and / or simulated.	

Assessment

	Description	Qualification
Laboratory practises		ata 12,0
Autonomous troubleshooting and / or exercises		ata 7,0
Long answer tests and development		ata 42
Reports / memories of practice		ata 6,0

Short answer tests	ata 14
Multiple choice tests	ata 7,0
Practical tests, real task execution and / or simulated.	ata 12,0

Other comments on the Evaluation

Sources of information

LEVINE, I. N., "Fisicoquímica" (vol. II), 5ª edición,

ENGEL, T.; REID, P., "Química Física", 1ª edición,

BERTRÁN, J.; BRACHANDELL, V.; MORENO, M.; SODUPE, M., "Química Cuántica", 2ª edición,

BERTRÁN RUSCA, J.; NÚÑEZ DELGADO, J., "Química Física" (vol. I), 1ª edición,

- ATKINS P. W., DE PAULA J., "Química Física" (8ª Edición). Editorial Médica *Panamericana. (2008).
- LEVINE I.N., "Química Cuántica" (5ª ed.), Editorial Prentice Hall (2001).
- BANWELL C.N., Mc CASH E., "Fundamentals of Molecular Spectroscopy", Editorial McGraw-Hill (1994).
- LABOWITZ L.C., ARENTS J.S., "Fisicoquímica: Problemas y Soluciones", Editorial AC (1974).
- FORESMAN J.B., FRISH A., "Exploring Chemistry with Electronic Structure Methods: a guide to using Gaussian" (2ª ed.), Gaussian Inc (1996).

Recommendations

Subjects that are recommended to be taken simultaneously

Computer and communications tools for chemistry/V11G200V01401

Numerical methods in chemistry/V11G200V01402

Inorganic chemistry 1/V11G200V01404

Subjects that it is recommended to have taken before

Mathematics: Mathematics 1/V11G200V01104

Mathematics: Mathematics 2/V11G200V01203

Physics 3/V11G200V01301

Physical chemistry 1/V11G200V01303