



IDENTIFYING DATA

(*)Simetría en Átomos, Moléculas e Sólidos e Mecánica Cuántica

Subject	(*)Simetría en Átomos, Moléculas e Sólidos e Mecánica Cuántica			
Code	V11M030V01213			
Study programme	(*)Máster Universitario en Química Teórica e Modelización Computacional. R.D. 1393/2007			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	9	Mandatory	1st	2nd
Teaching language	Spanish			
Department				
Coordinator	Estevez Valcarcel, Carlos Manuel			
Lecturers	Estevez Valcarcel, Carlos Manuel			
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Web				
General description				

Competencies

Code	
A3	(*)Aplicar los métodos teóricos y de modelización a sistemas químicos en general

Learning aims

Expected results from this subject	Typology	Training and Learning Results
To identify elements and operations of symmetry	know Know How	A3
To know the point groups of symmetry and identify the molecular symmetry	know Know How	A3
To apply molecular symmetry to the resolution of problems in Theoretical and Computational Chemistry	Know How	A3
To Identify the symmetry of solids	Know How	A3

Contents

Topic	
1. Molecular symmetry	Operations and symmetry elements. Symmetry point groups. Matrix representations. Big orthogonality theorem. Projection operators
2. Applications of symmetry in Quantum Chemistry	OM Hückel. Molecular vibration. Organometallic complexes
3. Symmetry in crystalline solids	Crystal Structures. Spatial symmetry. Isotropic and anisotropic structures. Reciprocal lattices.

Planning

	Class hours	Hours outside the classroom	Total hours
(*) Resolución de problemas e/ou exercicios	34	68	102
(*) Sesión maxistral	30	60	90
(*) Probas de resposta curta	0	1	1

(*)Resolución de problemas e/ou exercicios	0	32	32
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.			

Methodologies	
	Description
(*) Resolución de problemas e/ou exercicios	(*)Resolución polos profesores de exercicios e problemas
(*)Sesión maxistral	(*)Exposición polos profesores dos contidos teóricos esenciais

Personalized attention	
Tests	Description
Probas de resposta curta	
Resolución de problemas e/ou exercicios	

Assessment		
	Description	Qualification
(*)Probas de resposta curta	(*)Proba a través de moodle	30
(*)Resolución de problemas e/ou exercicios	(*)Entrega de exercicios e problemas	70

Other comments on the Evaluation

Sources of information
F.A. Cotton, La teoría de grupos aplicada a la Química ,
I.N. Levine, Espectroscopía molecular ,
A. Requena y J. Zúñiga, Espectroscopía ,
Dove, Structure and Dynamics ,
Hammond, The Basic of Crystallography and Diffraction ,
Chrtzman, Fundamentals of Solid State Physics ,
Ashcroft, Mermin, Solid State Physics ,
C. Kytzel, Introducción a la Física del Estado Sólido ,

Recommendations