Teaching Guide				
Identifying Data				2023/24
Subject (*)	Advanced Crystallography		Code	610G04042
Study programme	Grao en Nanociencia e Nanotecnoloxía			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	2nd four-month period	Fourth	Optional	4.5
Language	SpanishGalicianEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	BioloxíaFísica e Ciencias da TerraQuímica			
Coordinador	López Vicente, Manuel	E-mail	manuel.lopez.vicente@udc.es	
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Web				
General description	"Advanced Crystallography" is an applied subject of the second quarter of the fourth year of the Degree in Nanoscience and Nanotechnology, which belongs to the Optional Training Module. This matter delves into the contents of the first year "Crystallography and Symmetry" -Basic Training character-. It is a subject where it is intended that students learn to identify and recognize spatial symmetry groups, relate physical properties to crystal symmetry, determine and explain crystalline structures by X-ray diffraction on a single crystal, and finally, the relationship of crystallography with other disciplines. This learning will provide expert knowledge and practical skills that are necessary for the characterization of crystalline nanomaterials and biological macromolecules.			

Study programme competences / results	
Code	Study programme competences / results
A3	CE3 - Reconocer y analizar problemas físicos, químicos, matemáticos, biológicos en el ámbito de la Nanociencia y Nanotecnología, así como plantear respuestas o trabajos adecuados para su resolución, incluyendo el uso de fuentes bibliográficas.
A5	CE5 - Conocer los rasgos estructurales de los nanomateriales, incluyendo las principales técnicas para su identificación y caracterización
A6	CE6 - Manipular instrumentación y material propios de laboratorios para ensayos físicos, químicos y biológicos en el estudio y análisis de fenómenos en la nanoescala.
A7	CE7 - Interpretar los datos obtenidos mediante medidas experimentales y simulaciones, incluyendo el uso de herramientas informáticas, identificar su significado y relacionarlos con las teorías químicas, físicas o biológicas apropiadas.
A8	CE8 - Aplicar las normas generales de seguridad y funcionamiento de un laboratorio y las normativas específicas para la manipulación de la instrumentación y de los productos y nanomateriales.
B3	CB3 - Que los estudiantes tengan la capacidad de reunir e interpretar datos relevantes (normalmente dentro de su área de estudio) para emitir juicios que incluyan una reflexión sobre temas relevantes de índole social, científica o ética
B4	CB4 - Que los estudiantes puedan transmitir información, ideas, problemas y soluciones a un público tanto especializado como no especializado
B6	CG1 - Aprender a aprender
B7	CG2 - Resolver problemas de forma efectiva.
B8	CG3 - Aplicar un pensamiento crítico, lógico y creativo.
B9	CG4 - Trabajar de forma autónoma con iniciativa.
B10	CG5 - Trabajar de forma colaborativa.
C3	CT3 - Utilizar las herramientas básicas de las tecnologías de la información y las comunicaciones (TIC) necesarias para el ejercicio de su profesión y para el aprendizaje a lo largo de su vida

C7	CT7 - Desarrollar la capacidad de trabajar en equipos interdisciplinares o transdisciplinares, para ofrecer propuestas que contribuyan a un desarrollo sostenible ambiental, económico, político y social.
C8	CT8 - Valorar la importancia que tiene la investigación, la innovación y el desarrollo tecnológico en el avance socioeconómico y cultural de la sociedad
C9	CT9 - Tener la capacidad de gestionar tiempos y recursos: desarrollar planes, priorizar actividades, identificar las críticas, establecer plazos y cumplirlos

Learning outcomes			
Learning outcomes	Study programme competences / results		
Identify and recognize symmetry and spatial symmetry groups.	A3 A5 A7	B3 B6 B7 B8 B9	C3 C8
Calculate the molecular structure by X-ray diffraction on crystals.	A3 A5 A6 A7 A8	B3 B4 B6 B7 B8	C3 C7 C8
Recognize the physical and optical properties of crystals.	A3 A5 A7	B3 B4 B6 B7 B8	C3 C8
Solve advanced problems of crystallography.	A3 A6 A7 A8	B4 B7 B8 B10	C3 C7 C8 C9

Contents	
Topic	Sub-topic
Topic 1. Spatial symmetry, and spatial symmetry groups.	Know the 230 spatial symmetry groups. Symmorphic and non-symorphic groups: translation operations. Chiral and enantiomeric crystals (associated with protein structures and nucleic acid molecules). Nomenclature, Diagrams, and International Tables. Space group visualizer with free software.
Topic 2. Physical and optical properties of crystals.	Relationship between symmetry and magnetic and dielectric properties and optical activity.
Topic 3. Study of crystals by X-ray diffraction.	Structural determination of biological macromolecules, organic and inorganic compounds by X-ray crystallography: Basic protein, organic and inorganic compounds crystallization techniques; Main methods to solve the phase problem: multiple isomorphic replacement, multiple anomalous diffraction and molecular replacement; Refinement and validation of the models.

Planning				
Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A3 A5 A6 B3 B6 B8 C3 C7 C8 C9	16.5	39.6	56.1

Laboratory practice	A3 A6 A8 B4 B7 B9 B10 C3 C9	10	20	30
Workshop	A7 B4 B6 B8 B9 B10 C3	7	15.4	22.4
Mixed objective/subjective test	A3 A6 B3 B7	2	0	2
Introductory activities	B3 C7	1	0	1
Personalized attention		1	0	1
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	**Description**
Guest lecture / keynote speech	In-person master classes lasting 50 minutes aimed at teaching the theoretical contents of the subject with the help of audiovisual material and online resources.
Laboratory practice	Practical classes in which the 230 spatial symmetry groups will be identified with specific software, the relationship between symmetry and magnetic, dielectric and optical activity properties will be observed with practical cases; crystallization techniques will be used to crystallize a biological macromolecule and a simulation will be carried out to determine the structure of a protein by means of X-ray crystallography. Organic and inorganic compounds will also be crystallized and their structure will be determined.
Workshop	These sessions will be dedicated to the resolution of problems and questions by the students, with the guidance of the teaching staff. These problems will be provided in a sequence in time according to the contents covered in the master sessions. The work will be carried out individually or in groups under the direction of the teaching staff.
Mixed objective/subjective test	This activity will aim to assess the knowledge acquired by the student through a writing test.
Introductory activities	Introductory session to develop on the first day of class, in which the program of the subject, the methodology, the evaluation criteria, as well as a calendar of each of the planned activities will be explained.

Personalized attention	
Methodologies	**Description**
Workshop Guest lecture / keynote speech Laboratory practice Introductory activities	Personalized attention will be provided through tutorials and personal interviews on designated dates. In addition, this personalized attention can also be carried out electronically, through email, the virtual campus, and the Microsoft Teams platform. Special attention will be paid to those students who, due to their special characteristics, may have greater learning problems and to those with part-time dedication.

Assessment			
Methodologies	**Competencies / Results**	**Description**	**Qualification**
Workshop	A7 B4 B6 B8 B9 B10 C3	Both the responses of the students and their individual or group participation in the corresponding face-to-face activities will be graded. Occasionally, and at the teacher's request, students must present problem sets that can also be evaluated.	15
Laboratory practice	A3 A6 A8 B4 B7 B9 B10 C3 C9	The following aspects of work in the laboratory will be evaluated: - Organization of work and safety. - Attitude, scientific curiosity and degree of involvement in the work. - Quality in the interpretation of the results. - Quality of the final report (laboratory notebook).	30

Mixed objective/subjective test	A3 A6 B3 B7	It will consist of a test on theoretical content. It will consist of both development questions and multiple choice questions and problems that will be similar to those presented throughout the course. The minimum score required to pass this test is 5 points out of 10.	55

Assessment comments
The course will be divided into three parts: one focused on the study of spatial symmetry and spatial symmetry groups, another will address the physical and optical properties of crystals, and the third on the study of crystals by X-ray diffraction. Each of these parts will have a third of the percentage of each mentioned activity assigned in the final grade. To pass the subject, it is an essential requirement to obtain a minimum score of 5 points out of a maximum of 10 in the total calculation. In the case of the 'Mixed Test', the minimum score will be 5 out of 10, and in the cases of 'Laboratory Practices' and 'Workshop', it will be 4.6 out of 10. These scales are maintained for each of the three parts in which the subject is divided. Otherwise, the subject will not be passed. In the event that the average grade among all the activities is greater than 5, but any of the evaluable activities has not been passed with the previously indicated grades, the grade that will appear in the minutes will be 4. Once all the activities have been passed, the final grade will be calculated as follows: the 'Mixed Test' will account for 55% of the final grade, the 'Laboratory Practices' will account for 30% of the final grade, and the resolution of 'Workshop' problems will contribute with the remaining 15%. Attendance to workshop classes and laboratory practices, and the delivery of problems are mandatory to be evaluated. Unjustified absence from one of the laboratory sessions, or from a small group activity will mean disqualification from the course. The student will be declared NOT PRESENTED only if he does not attend any of the activities whose evaluation represents more than 10% of the final grade.Honors will only be awarded to students who have been evaluated during the course and have passed the corresponding evaluation on either of the two opportunities, until reaching the maximum number of Honors possible according to the institution's regulations.In the calls for June (first opportunity) and July (second opportunity) it will be evaluated in the same way (percentages). Students with recognition of part-time dedication will not have the obligation to attend theoretical classes or activities in small groups, although their attendance at practices will be mandatory. The percentage of the qualification corresponding to the small group activities will be assimilated to the qualification of the mixed test both in the first and in the second opportunity.During the test, on either occasion, except as otherwise indicated, the use of any device with Internet access is prohibited. If, during the practical test, there is evidence of the unauthorized use of these devices, the student will be expelled from the classroom, and the procedure will be followed according to Law 3/2022, of February 24, on university coexistence and disciplinary regulations of the UDC student body. Fraudulent performance of tests or evaluation activities, once verified, will directly imply a failing grade in the call in which it is committed: the student will be graded with "fail" (numerical grade 0) in the corresponding call for the course academic, whether the commission of the offense occurs on the first opportunity or on the second. For this, their qualification will be modified in the first opportunity record, if necessary.In the extraordinary call for December, the evaluation criteria of the teaching guide for the 2022-23 academic year will be applied.

Sources of information	
Basic	- Sands, Donald E. (1974). Introducción a la cristalografía. Barcelona, Reverté.- Kettle, Sidney F.A. (2007). Symmetry and structure readable group theory for chemists. Hoboken: John Wiley.- Borchardt-Ott, Walter (2011). Crystallography : an introduction . Berlin, Springer.- Dept. de Cristalografía y Biol. Estruc. , CSIC (2020). Crystalografía.- Hargittai, István (1995). Symmetry through the eyes of a chemist. New York : Plenum Press.- Hammond, C (2009). The Basics of crystallography and diffraction. Oxford University Press.- Klein, C; Hurlbut, C.S. Jr. (1996-1997). Manual de mineralogía basado en la obra de J.D. Dana. Vol. 1.. Barcelona, Reverté.- Bloss, F.D. (1994). Crystallography and crystal chemistry: an introduction. Washington, Mineralogical Society of America.- Tilley, Richard J.D. (2020). Crystals and Crystal Structures, 2nd Edition. Editorial Willey. ISBN: 978-1-119-54859-1.- Bergfors. T.M. (2022). Protein Crystallization, 3th Edition. International University Line. - Rodes, G. (2010). Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models. 3th Edition. Academic Press.
Complementary	- Müller, Ulrich (2013). Relaciones de simetría entre estructuras cristalinas : aplicaciones de la teoría de grupos cristalográficos en cristaloquímica. Madrid- DAVID J. WILLOCK (2009). Molecular Symmetry. Willey- Giacovazzo, C (2011). Fundamentals of crystallography. Oxford ; New York : Oxford University Press- Amorós, J.L. (1990). El Cristal : morfología, estructura y propiedades físicas. Madrid, Ed. Atlas- Nesse, W.D. (2009). Introduction to optical mineralogy. New York : Oxford University Press- Amigo, J.M. et al. (1981). Cristalografía. Madrid, Rueda.

Recommendations
Subjects that it is recommended to have taken before
Crystallography and Symmetry/610G04006
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Other comments
'Green Campus' College of Science Program To contribute to achieving an immediate sustainable environment and comply with point 6 of the "Environmental Declaration of the Faculty of Sciences (2020)", the documentary works carried out in this matter: a) They will be requested mostly in virtual format and computer support. b) If done on paper: - No plastics will be used. - Double-sided prints will be made. - Recycled paper will be used. - Drafts will be avoided. Incorporation of the gender perspective- As stated in the different applicable regulations for university teaching, the gender perspective must be incorporated in this matter (non-sexist language will be used, bibliography of authors of both sexes will be used, intervention in class of students will be encouraged and students...). - Work will be done to identify and modify prejudices and sexist attitudes and the environment will be influenced to modify them and promote values ??of respect and equality. - Situations of discrimination based on gender must be detected and actions and measures to correct them will be proposed.