UAB
Universitat Autònoma de Barcelona

Crystallography

2026/2027

Code: 101059
Credits: 6

Degree programme	Type	Course
Geology	OB	1

Contact lecturer

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Teaching staff

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Group languages

You can consult this information at the end of the document.

Prerequisites

There are no formal prerequisites.

In any case, it is necessary to remember, and if necessary review, previously acquired knowledges in Mathematics, Physics and Chemistry. Namely, knowledges on the following topics would be advisable:

1.- Chemical formulation

2.- Chemical valence and bonding types

3.- Matrix calculus

4.- Vector calculus

Objectives

This is a basic course within the first year, with direct application in Mineralogy (second year) as well as in Petrology and other courses in the following years.

As a consequence, the objectives are:

I. Acquisition of basic knowledge about:

1 - The crystal lattice and its mathematical description, as a basis for the description of the crystal structures of minerals.

2 - The crystal symmetry and its mathematical description, as a basis for the description of the crystal structures of minerals.

II. To know the basics of X-ray diffraction in crytals, for applying this knowledge in second year Mineralogy.

III. To visualize in 3D crystal structures in their symmetry.

IV. To perform simple tasks with crystallography software.

V. To have the basis for relating the physical properties of solids with their crystal structure.

Learning outcomes

- KM24 (Identify the physical and chemical principles that condition the crystal structure of minerals.) Identify the physical and chemical principles that condition the crystal structure of minerals.
- KM26 (Describe the main techniques and instruments used in the investigation of crystal structures.) Describe the main techniques and instruments used in the investigation of crystal structures.
- KM27 (Identify the main current challenges related to the potential application of different geological materials.) Identify the main current challenges related to the potential application of different geological materials.

Contents

Theory

(the order of the topics could change)

I. Crystal morphology

II. Point symmetry

III. Lattice theory

IV. Close packing types

V. Space symmetry

VI. X-ray diffraction in crystals

Practical sessions

(the order of the practical sessions could change)

Session 1: Crystal morphology

Session 2: Point symmetry I, Crystal models

Session 3: Point symmetry II, Crystal models

Session 4: Computer work. Point symmetry III, Interactive 3D Adobe files of point groups

Session 5: Projection of crystal structures

Session 6: Metric tensor and its applications

Session 7: Computer work. 3D representation of crystal structures with crystallographic software.

Session 8: Lattice planes and directions

Session 9: Space symmetry. Symmetry elements

Session 10: Space symmetry. Analysis of crystal structures

Session 11 - Computer work. Crystal structure databases

Session 12 - Computer work. X-ray diffraction, examples to illistrate different aspects of X-ray diffraction

Learning activities and methodology

Title	Hours	ECTS	Learning outcomes
Autonomous work	88	3.52	
Practical sessions	25	1	
Theory classes	26	1.04	

Theory classes are conducted as traditional classroom sessions, including lectures by the instructor, questions and discussions with students, and the solving of exercises and problems.

Practical sessions are carried out in groups (expected to be 3 or 4 students per group) in a classroom with large tables where students can easily work together. Some practical sessions require the use of computers (and will take place in computer-equipped classrooms), including the use of specific crystallographic software. Students are provided with a guide describing the work they must complete. The instructor assists students, answers questions either in groups or individually, and provides the correct solutions to the practical exercises, either during the session itself or through the course's virtual campus.

Independent student work consists of personally working on all the topics and activities covered in class, both in theory lectures and practical sessions. To support this work, students have access to lecture notes, reference materials, bibliographic resources, exercises/practical assignments, and crystallographic software (either available in the university's computer labs or as free software).

For this course, the use of Artificial Intelligence (AI) technologies is permitted exclusively for support tasks, such as literature searches, information gathering, proofreading, or translations. However, AI may not be used for the complete preparation of assignments or coursework submissions. If AI is used, the student must clearly identify which parts were generated with this technology and specify the tools used. A lack of transparency regarding the use of AI in assessed work will be considered a breach of academic integrity and may result in a partial or total penalty in the grade for the activity, or more severe sanctions in serious cases.

The Virtual Campus is used as the primary means of communication with students and is where practical guides, specific reference materials, theory lecture notes, grades, and other course materials are made available.

The theory lecture notes serve as a basis for the classes, but they do not, under any circumstances, replace attendance at class.

Annotation: within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continuous assessment activities

Title	Weight	Hours	ECTS	Learning outcomes
Mid-term exam 1	35 - 40%	2	0.08	KM24, KM27
Deliveries	15%	4	0.16	KM24, KM26
Second chance exam: repetition of one or both mid-term exams	35 - 40% for each mid-term exam	3	0.12	KM24, KM26, KM27
Mid-term exam 2	35 - 40%	2	0.08	KM24, KM26, KM27

The assessment for this course consists of continuous assessment and a final or resit examination.

The continuous assessment includes two midterm exams. The first is scheduled for early April and the second for late May. Continuous assessment will also include the evaluation of submitted work, such as practical assignments, exercises, projects, or quizzes assigned in class. These submissions will account for 15% of the final grade.

It is possible to pass the course through continuous assessment without taking the final exam if an overall grade of 5.0 or higher is achieved.

The June resit exam provides an opportunity to retake one or both midterm exams. In this case, the grade obtained in the resit exam will replace the grade from the corresponding midterm exam. Submitted and graded coursework cannot be retaken or recovered.

Attendance at practical sessions is mandatory. Missing 3 practical sessions without justification will result in a grade of "Not Assessed" (No Avaluable).

Failure to attend one of the two midterm exams and its corresponding resit exam will also result in a grade of "Not Assessed."

Attendance at theory lectures is highly recommended. The instructor may take note of particularly valuable class participation, which may positively influence the final grade of students whose marks fall on the boundary between two grade categories (for example, between "Good" and "Excellent"). However, such positive adjustments will never be applied if there is evidence of repeated absences from class.

If a student requests single assessment (following the procedure and deadlines established by the Faculty), an evaluation will be held, preferably on the same date as the assessment of the second part of the course for the rest of the students. This assessment will consist of:

1. Passing a comprehensive exam covering the entire course (70% of the final grade).
2. Submission of a project completed using crystallographic software (10% of the final grade).
3. An oral examination in which crystal models will be presented and questions will be asked about their symmetry (20% of the final grade).

If the student does not pass the single assessment, they will be entitled to a second exam, and the grade from this exam will replace the grade from the first exam. This second exam will preferably be held on the same day as the resit exam.

Neither the project nor the oral examination can be retaken or recovered.

Bibliography

• Cristal·lografia. Teoria Reticular, Grups Puntuals i Grups Espacials

SALVADOR GALÍ MEDINA, Edicions de la Universitat de Barcelona

Biblioteca Facultat de Ciències i ETSE

• International Tables for Crystallography. Volume A: Space-Group Symmetry (teaching edition)

T. HAHN, editor, The International Union of Crystallography, D. Reidel Publishing Company

Biblioteca Facultat de Ciències i ETSE

• Introduction à la Cristallographie et à la Chimie Structurale

M. VAN MEERSSCHE et J. FENEAU-DUPONT, Oyez

Biblioteca Facultat de Ciències i ETSE

• An Introduction to Crystal Chemistry

R.C. EVANS, Cambridge University Press

Biblioteca Facultat de Ciències i ETSE

· Estructura atómica y enlace químico

JAUME CASABÓ I GISPERT, Editorial Reverté

Biblioteca Facultat de Ciències i ETSE

· Introduction to Mineral Science

A. PUTNIS, Cambridge University Press

Biblioteca Facultat de Ciències i ETSE

· Crystallography

WALTER BORCHARDT-OTT, Springer Verlag

Biblioteca Facultat de Ciències i ETSE

Webpages

https://www.uab.cat/ca/geologia/grups-simetria

https://github.com/LluisCasas/GSP

http://www.iucr.org International Union of Crystallography

http://www.iucr.org/education/pamphlets Teaching pamphlets

http://reference.iucr.org/dictionary/Main_Page Diccionari de cristal·lografia

http://it.iucr.org/ International Tables for Crystallography, accés només al campus

http://www.xtal.iqfr.csic.es/Cristalografia/ Instituto de Química Física Rocasolano

http://www.crystallography.net/cod/ Crystallography Open Database

https://www.rruff.net/amcsd/ American Mineralogist Crystal Structure Database

Perspectiva de gènere

https://riull.ull.es/xmlui/bitstream/handle/915/15048/CL_05_%282006%29_08.pdf?s

Software

interactive PDF files: https://github.com/LluisCasas/GSP

VESTA: https://jp-minerals.org/vesta/en/

Quiztallography (Android) https://play.google.com/store/apps/details?id=aax.uab.quiztallography&pli=1

Course groups and languages

The information provided is provisional until November 30. After this date, you will be able to consult the language of each group through this link. To access the information, you will need to enter the course CODE

Type of teaching	Group	Language	Semester	Shift
(TE) Theory	1	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	1	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	2	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	3	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	4	Catalan	second semester	morning-mixed