# UAB Universitat Autônoma de Barcelona

## Crystallography

Code: 101059 ECTS Credits: 6

2024/2025

Degree	Туре	Year
2500254 Geology	ОВ	1

# Contact

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## Teachers

Lluis Casas Duocastella

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## **Teaching groups languages**

You can view this information at the <u>end</u> of this 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 and Contextualisation**

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.

#### Competences

- Learn and apply the knowledge acquired, and use it to solve problems.
- Relate the physical properties of matter to its structure.
- Work independently.

#### Learning Outcomes

- 1. Learn and apply the knowledge acquired, and use it to solve problems.
- 2. Relate the physical properties of matter to its structure.
- 3. Work independently.

### Content

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, in particular those requiring the use of a computer lab.)

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

## Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Practical sessions	25	1	1, 2, 3
Theory classes	26	1.04	1, 2
Type: Autonomous			
Autonomous work	88	3.52	1, 2, 3

The theory classes are developed as classic sessions with teacher explanations, questions and discussions with the students and solving exercises and problems.

Practical sessions are held in groups (in principle 3 or 4), in a classrooms with large tables where students can easily work in groups. Some of the practical sessions are carried out in the computer room using crystallographic software. The students have a script for the work they have to carry out. The teaching staff helps, solves doubts in groups or personally, and gives the correct result of the practice, either in the classroom itself, or on the subject's virtual campus.

The students' independent work consists of personal work on all the aspects raised in the classroom, both in the theory classes and in the practical sessions; that is why it has class notes, reference material, bibliography, exercises/practices and crystallographic software (the latter, either available in the classrooms of the computer service, either software free).

The Virtual Campus is used as a means of communication with students and is the place where practical scripts, specific reference material, theory class scripts, grades, etc. are stored. The scripts of the theory classes constitute a basis for the classes, but they do not replace the need for attendance in 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

## **Continous Assessment Activities**

Title	Weighting	Hours	ECTS	Learning Outcomes
Deliveries	20 - 30%	4	0.16	1, 2, 3
Mid-term exam 1	35 - 40%	2	0.08	1, 2, 3
Mid-term exam 2	35 - 40%	2	0.08	1, 2, 3
Second chance exam: repetition of one or both mid-term exams	35 - 40% for each mid-term exam	3	0.12	1, 2, 3

The avaluation includes two mid-term exams, one by the middle of the course and the other in the end. The avaluation will include also the delivery of several assignments. The evaluation of the subject includes the continuous evaluation and the final or recovery exam. Continuous assessment comprises two mid-term exams, the first of which is planned for early April and the second towards the end of May. Continuous assessment will also include the assessment of assignments, be it some practice, exercise, assignment or quiz set in class. These assignments will represent 25% of the overall grade. The subject can be approved by continuous assessment without the need to sit for the final exam if an overall grade of 5 is reached.

The second-chance exam is the opportunity of repeating one or two of the mid-term exams. In this case, the qualification obtained in the second-chance exam will replace the corresponding mid-term exam. The second-chance exam do not affect the qualifications of the assignments delivered.

In the event that the student requests a single assessment (in the form and date determined by the Faculty), an assessment will be carried out preferably coinciding with the date of the assessment of the second part of the subject by the rest of the students This assessment will consist of:

1-Passing an exam for the entire subject (70% of the overall grade).

2-The delivery of a work to be done with crystallographic software (10%  $\alpha$  3-An oral test where models of crystals will be presented and questions  $\nu$  In the event of not passign the single assessment, students will be entitle

## 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/web/la-divulgacio/grups-puntuals-de-simetria-1345664584325.html https://play.google.com/store/apps/details?id=aax.uab.guiztallography&hl=ca App Quiztallography http://www.iucr.org International Union of Crystallography http://www.iucr.org/education/pamphlets Teaching pamphlets http://reference.iucr.org/dictionary/Main\_Page http://it.iucr.org/ International Tables for Crystallography http://www.xtal.igfr.csic.es/Cristalografia/ Instituto de Química Física Rocasolano http://rruff.geo.arizona.edu/AMS/amcsd.php American Mineralogist Crystal Structure Database

Gender perspective:

https://riull.ull.es/xmlui/bitstream/handle/915/15048/CL\_05\_%282006%29\_08.pdf?s

### Software

interactive PDF files: https://www.uab.cat/web/la-divulgacio/grups-puntuals-de-simetria-1345664584325.html

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

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

# Language list

Name	Group	Language	Semester	Turn
(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
(TE) Theory	1	Catalan	second semester	morning-mixed