Universitat Autònoma de Barcelona

2021/2022

Crystallography

Code: 101059
ECTS Credits: 6

Degree	Type	Year	Semester
2500254 Geology	OB	1	2

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

Contact

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Use of Languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: Yes
Some groups entirely in Spanish: No

Teachers

Juan Francisco Piniella Febrer
Lluís Casas Duocastella

Prerequisites

There are no formal prerequisites. However, a previous knowledge of the following topics is convenient:

1.- Chemical formulation

2.- Chemical valence and bonding types

3.- Matrix calculus

4.- Vector calculus

Objectives and Contextualisation

This is a basic course in first year, with direct application in second year Mineralogy 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 can be modified)

I. Introduction

II. Lattice theory

III. Crystal morphology

IV. Point symmetry

V. Space symmetry

VI. X-ray diffraction in crystals

Practical sessions

(the order of the practical sessions can change)

I: Projection of crystal structures

II: Lattice planes

III: Close packings

IV: Metric tensor and its applications

V: 3D representation of crystal structures with crystallographic software.

VI: Point symmetry. Crystal models I

VII: Point symmetry: 3D interactive PDF files

VIII: Point symmetry. Crystal models II

IX: Space symmetry. Symmetry elements

X: Space symmetry. Analysis of crystal structures

XI: X-ray diffraction

Methodology

Practical sessions will take place in in a space with large tables where the students can work in group. Some of the sessions will take place in computing classrooms using crystallographic software. The students will have a guide with the work to make. The teacher will provide assistance and will deliver the correct results, either during the session or in the virtual campus.

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.

Activities

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

Assessment

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 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.

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

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

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· Estructura atómica y enlace químico

JAUME CASABÓ I GISPERT, Editorial Reverté

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· Introduction to Mineral Science

A. PUTNIS, Cambridge University Press

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· Crystallography

WALTER BORCHARDT-OTT, Springer Verlag

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Webpages

http://departaments.uab.cat/geologia/PSG

https://play.google.com/store/apps/details?id=aax.uab.quiztallography&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.iqfr.csic.es/Cristalografia/ Instituto de Química Física Rocasolano

http://rruff.geo.arizona.edu/AMS/amcsd.php American Mineralogist Crystal Structure Database

Software

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