Universitat Autònoma de Barcelona

2023/2024

Crystallography

Code: 101059
ECTS Credits: 6

Degree	Type	Year	Semester
2500254 Geology	OB	1	2

Contact

Name: Ignacio Ramon Mata Martínez

Email: ignasi.mata@uab.cat

Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

Teachers

Lluis Casas Duocastella

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

Methodology

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), 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.

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.

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% o
3-An oral test where models of crystals will be presented and questions w
In the event of not passign the single assessment, students will be entitle

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

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

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

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