UCLouvain

lchm1253

2024

Elements of crystallography

4.00 credits	30.0 h + 10.0 h	Q1

Teacher(s)	Filinchuk Yaroslav ;
Language :	French
Place of the course	Louvain-la-Neuve
Prerequisites	algebraic knowledge base
Main themes	• Elements of symmetry • Crystal lattice • One-time groups • Space groups • Use of International Tables of Crystallography • Principles of diffraction, reciprocal space • Intensity diffracted by a crystal • Single crystal diffraction, powder diffraction Experimental methods and instruments • Information obtained by diffraction Introduction to structural chemistry, contribution of crystallography in the knowledge of chemistry
Learning outcomes	**At the end of this learning unit, the student is able to :** 1 • reasoned understanding (knowing how to explain) of symmetry and in particular of molecular symmetry • understanding the fundamentals of modern methods of crystallographic analysis and the results they provide
Evaluation methods	An oral exam with written preparation. It includes two theoretical questions with written preparation and the others without preparation (total of 15 points). The practical part is examined by the engineer, Dr. Koen Robeyns, and is evaluated with a maximum of 5 points. Students can earn one more point for creative homework.
Teaching methods	The course is given with the use of PowerPoint presentations, available on moodle. The court also includes software demonstration and the use of interactive material. Exercises are planned to facilitate understanding. **Exercises :** 1. One-off groups 2. Networks. Groups of the plan. Slip plane 3. Space Groups 4. Practical exercises in the laboratory : - Diffraction on single crystals, powder - Description and comparison of crystalline structures. - Types of structure
Content	Symmetry 1. Introduction, molecules and crystals, elements of symmetry 2. Point groups, chirality 3. Translation, plan groups, crystal lattice, elements of periodic symmetry 4. Space Groups, International Tables of Crystallography Methods 1. X-rays, neutrons, diffraction principles, reciprocal space 2. Structure factor, Fourier synthesis, phase problem 3. Information obtained by diffraction 4. Diffraction methods: single crystals and polycrystals (powders) 5. Resolution of structures, identification of known and unknown compounds 6. Refinement of crystalline structures 7. Presentation of modern software (CrysAlis, Fullprof, Shelx, Fox) Results 1. Use and presentation of results, interpretation of literature data 2. Introduction to structural chemistry 3. Diffraction chemistry: in situ studies

	4. The big "instruments" - synchrotrons and neutron sources: the great possibilities
Inline resources	> https://symmetry.otterbein.edu/ - interactive guide to molecular symmetry > https://escher.epfl.ch/mobile/ - crystallography on a mobile phone, 2D periodic groups > https://nanocrystallography.research.pdx.edu/index.py/links - collection of useful links > https://escher.epfl.ch/eCrystallography/ - electronic crystallography course
Bibliography	1. J.-J. Rousseau, A. Gibaud, *Cristallographie géométrique et radiocristallographie* (Dunod, 3e édition, 2007). 2. R. Tilley, *Crystals and crystal structures* (Wiley, 2006).
Faculty or entity in charge	CHIM

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Bachelor in Chemistry	CHIM1BA	4		🔍
Minor in Chemistry	MINCHIM	4		🔍
Master [120] in Biochemistry and Molecular and Cell Biology	BBMC2M	4		🔍