UCL Université catholique de Louvain

LCHM1251B

2014-2015

Eléments de cristallographie et de spectroscopie moléculaire

4.0 credits	30.0 h + 10.0 h	1q

Teacher(s) :	Filinchuk Yaroslav ;
Language :	Français
Place of the course	Louvain-la-Neuve
Inline resources:	> http://symmetry.otterbein.edu/- interactive guide to molecular symmetry > http://escher.epfl.ch/mobile/- crystallography on a mobile phone, 2D periodic groups > http://nanocrystallography.research.pdx.edu/index.py/links- collection of useful links > http://escher.epfl.ch/eCrystallography/- electronic crystallography course
Prerequisites :	knowledge of basic algebra
Main themes :	- Symmetry Elements - Crystal lattice - Point Groups - Space groups - Use of the International Tables for Crystallography - Principles of diffraction, reciprocal space - Intensity diffracted by a crystal - Single-crystal diffraction, powder diffraction - Experimental methods and instruments - Information obtained from the diffraction - Introduction to structural chemistry, contribution of crystallography to chemistry knowledge
Aims :	- understanding the symmetry and in particular of the molecular symmetry - understanding the foundations of modern crystallographic analysis and results they deliver *The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".*
Evaluation methods :	oral exam with a written preparation. It includes two theoretical questions: one with and one without a written preparation (15 points). The practical part is examined by the engineer, Dr. Koen Robeyns, and is evaluated with a maximum of 5 points. One more point students can get for the creative home work (the task is given).
Teaching methods :	The course is taught with the use of PowerPoint slides, available at iCampus. The lecture course also includes demonstration software and the use of interactive material. Exercises are provided to facilitate the understanding.
Content :	Symmetry 1. Introduction, molecules and crystals, symmetry elements 2. Point groups, chirality 3. Translation, planar groups, lattice, elements of periodic symmetry 4. Space groups, International Tables for Crystallography Methods 5. X-rays, neutrons, principles of diffraction, reciprocal space 6. Structure factor, Fourier synthesis, phase problem 7. Diffraction methods: single crystal and powder diffraction 8. Information obtained by diffraction 9. Solution and refinement of crystal structures 10. Introduction to modern software (Crysalis, Fullprof, Shelx, Fox) Results 11. Use and presentation of results, interpretation of literature data 12. Introduction to structural chemistry 13. In-situ studies: Chemistry by diffraction 14. "large facilities instruments" - synchrotrons and neutron sources: the great opportunities Symmetry+ 15. Character tables, irreducible representations

Bibliography :	1. J.-J. Rousseau, A. Gibaud, Cristallographie géométrique et radiocristallographie (Dunod, 3e édition, 2007). 2. R. Tilley, Crystals and crystal structures (Wiley, 2006).
Cycle and year of study :	> Bachelor in Chemistry > Bachelor in Biology
Faculty or entity in charge:	CHIM