

In view of the health context linked to the spread of the coronavirus, the methods of organisation and evaluation of the learning units could be adapted in different situations; these possible new methods have been - or will be - communicated by the teachers to the students.





4 credits

30.0 h + 10.0 h

Q1

Teacher(s)	Filinchuk Yaroslav ;
Language :	French
Place of the course	Louvain-la-Neuve
Prerequisites	knowledge of basic algebra <i>The prerequisite(s) for this Teaching Unit (Unité d'enseignement – UE) for the programmes/courses that offer this Teaching Unit are specified at the end of this sheet.</i>
Main themes	<ul style="list-style-type: none"> - 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	<p>1 - understanding the symmetry and in particular of the molecular symmetry</p> <p>- understanding the foundations of modern crystallographic analysis and results they deliver</p> <p>-----</p> <p><i>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".</i></p>
Evaluation methods	<p>Due to the COVID-19 crisis, the information in this section is particularly likely to change.</p> <p>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).</p>
Teaching methods	<p>Due to the COVID-19 crisis, the information in this section is particularly likely to change.</p> <p>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.</p>
Content	<p>Symmetry</p> <ol style="list-style-type: none"> 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 <p>Methods</p> <ol style="list-style-type: none"> 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) <p>Results</p> <ol style="list-style-type: none"> 11. Use and presentation of results, interpretation of literature data 12. Introduction to structural chemistry

	<p>13. In-situ studies: Chemistry by diffraction</p> <p>14. "large facilities instruments" - synchrotrons and neutron sources: the great opportunities</p> <p>Symmetry+</p> <p>15. Character tables, irreducible representations</p>
Inline resources	<p>http://symmetry.otterbein.edu/- interactive guide to molecular symmetry</p> <p>http://escher.epfl.ch/mobile/- crystallography on a mobile phone, 2D periodic groups</p> <p>http://nanocrystallography.research.pdx.edu/index.py/links- collection of useful links</p> <p>http://escher.epfl.ch/eCrystallography/- electronic crystallography course</p>
Bibliography	<p>1. J.-J. Rousseau, A. Gibaud, <i>Cristallographie géométrique et radiocristallographie</i> (Dunod, 3e édition, 2007).</p> <p>2. R. Tilley, <i>Crystals and crystal structures</i> (Wiley, 2006).</p>
Other infos	<p>Skills to be acquired:</p> <ul style="list-style-type: none"> - understanding the symmetry and in particular of the molecular symmetry - understanding the foundations of modern crystallographic analysis and results they deliver
Faculty or entity in charge	CHIM

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Aims
Master [120] in Chemistry	CHIM2M	4		
Master [120] in Biochemistry and Molecular and Cell Biology	BBMC2M	4		
Master [60] in Chemistry	CHIM2M1	4		
Bachelor in Chemistry	CHIM1BA	4	LMAT1101 AND LMAT1102	
Minor in Chemistry	LCHIM100I	4		