UCL Université catholique de Louvain

LCHM2251

2010-2011

Structural chemistry by diffraction methods

3.0 credits	22.5 h + 7.5 h

Teacher(s) :	SOMEBODY ;
Language :	Anglais
Place of the course	Louvain-la-Neuve
Main themes :	1. Crystallisation. 2. X-ray diffraction, theory and experimental methods. 3. Crystalline and molecular structures determination methods. 4. Interpretation of results.
Aims :	1. Determination of molecular structures by X-ray diffraction. 2. Application to small molecules and biological macromolecules. *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".*
Content :	1. Crystallisation of small molecules and biological macromolecules. 2. Manipulation of crystals, cryogenic set-ups, preparation of heavy atom derivatives. 3. Reminder of basic relations of X-ray crystallography. 4. Experimental methods applicable to monocrystals. 5. Determination of direct and reciprocal reticular parameters 6. Determination of space groups. 7. Measure of crystal diffracted intensities. 8. Lorentz, polarisation, absorption corrections 9. How to go from diffraction data to the structure: structural factors and electronic density, Fourier transform, phase problems. Wilson statistic. 10. Patterson function, direct methods, isomorphous replacement, anomalous scattering, MAD (multiwavelength anomalous dispersion) and SAD methods (single wavelength anomalous dispersion). 11. Determination and use of non crystallographic symmetry. 12. Refinement and phase extensions by modifying electronic density. 13. Molecular replacement, classic methods and methods based on the "likelihood maximum". 14. Refining of molecular structures. 15. Quality, analysis and interpretation of results.
Other infos :	Background: Molecular symmetry and crystal structures (CHM 1251A) Evaluation mode: Oral exam with a written preparation The course could be partly or totally delivered by an invited lecturer.
Cycle and year of study :	> Master [120] in Chemistry
Faculty or entity in charge:	CHIM