

3.0 credits	0 h + 45.0 h	1+2q
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Teacher(s) :	Hermans Sophie ; Filinchuk Yaroslav ; Elias Benjamin ;
Language :	Français
Place of the course	Louvain-la-Neuve
Inline resources:	CrysAlis and Shelx- single crystal diffraction Fit2D, ICDD database - powder diffraction Mercury- visualisation of crystal structures and simulation of powder diffraction patterns
Prerequisites :	- Basic chemistry and physics - Practical experience in chemistry laboratories.
Main themes :	The students in small groups will work on a project, which will lead them to state the problem, synthesize the necessary products to solve it, and to characterize them with the appropriate experimental method to solve the problem. This experimental method will be advanced in the sense that it requires technical means usually devoted to research, which are not available in the teaching laboratories. Nuclear Magnetic Resonance, Mass Spectrometry, gas or liquid phase chromatography, X-ray diffraction assisted by molecular modelling are the main methods envisaged in this course.
Aims :	- The use of modern methods of characterization in chemistry; - The identification of unknown substances by physico-chemical methods. The goal of this course is to teach the students how to analyze advanced problems in chemistry and to familiarize them with advanced instrumental techniques. The students will integrate and critically analyze the obtained experimental results to find a solution to the given chemistry problem. <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>
Evaluation methods :	The academic who is responsible for the manipulation will evaluate the students on written reports. The course coordinator will combine all marks in a unique final note for this course.
Teaching methods :	After expressing the problem, the synthesis of organic and/or inorganic products will be carried out. Then and in general, the students will familiarize themselves with the experimental techniques used by analyzing the synthesized samples. This familiarization comprises an introduction to the technique, measurements and an advanced interpretation of the results. These results are written up in a formal report. As an example, but not limited to this, mass spectrometry will allow to determine the structure and stability of coordination complexes; NMR will allow to determine the stability constants of several families of complexes; to compare them on the basis of specific factors and to compare with other experimental techniques; HPLC will allow to follow the kinetics and to determine the yield of reactions involving catalysts, irradiation, etc. In the crystallographic part of the course, we follow a chemical reaction induced by high energy ball milling. We study different mixtures and products after different milling times using X-ray powder diffraction. Databases and simulations are used for data interpretation. Moreover, in a separate experiment, a crystal structure is determined by single-crystal diffraction. The work is done in small groups of 2-3 people. The same exercise is repeated with two groups.
Content :	After expressing the problem, the synthesis of organic and/or inorganic products will be carried out. Then and in general, the students will familiarize themselves with the experimental techniques used by analyzing the synthesized samples. This familiarization comprises an introduction to the technique, measurements and an advanced interpretation of the results. These results are written up in a formal report. As an example, but not limited to this, mass spectrometry will allow to determine the structure and stability of coordination complexes; NMR will allow to determine the stability constants of several families of complexes; to compare them on the basis of specific factors and to compare with other experimental techniques; HPLC will allow to follow the kinetics and to determine the yield of reactions involving catalysts, irradiation, etc. Diffraction methods are presented in the context of the analysis of the reaction products, as well as aiming for a characterization of a completely unknown substance
Bibliography :	Scientific papers are recommended on the subject of the study and the literature search is encouraged. An updated syllabus is given to students, containing all the information.
Cycle and year of study :	<a href="#">&gt; Bachelor in Chemistry</a>

Faculty or entity in charge:	CHIM
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