UCLouvain

lchm1232

2025

Mathematics applied to chemistry

The version you're consulting is not final. This course description may change. The final version will be published on 1st June.

3.00 credits	30.0 h + 30.0 h	Q1

Teacher(s)	Bieliavsky Pierre ;Caprace Pierre-Emmanuel ;Vitale Enrico ;
Language :	French
Place of the course	Louvain-la-Neuve
Prerequisites	Mathematical concepts as covered in LMAT1101 and LMAT1102
Main themes	The Mathematics applied to chemistry course covers and develops the mathematical tools needed to understand physical chemistry, complementing and deepening those already covered in Block 1 courses. The course includes the linear algebra required for quantum chemistry, and the series development and function transforms needed for spectroscopy.
Learning outcomes	
Evaluation methods	Written exam including both closed MCQ-type questions and open questions that aim to test both the understanding of the subject (theoretical and reflection questions) and the mastery of calculation techniques (questions similar to the exercises seen in the practical work type). The written exam will be supplemented by an optional oral exam, open to any student who has obtained at least 8/20 in the written exam. In the event of participation in the oral exam, the result of the latter counts for 50% of the final grade.
Teaching methods	The lecture aims to introduce the theory from simple problems and to illustrate it by exercises solved in the audience. The lecture, the syllabus available online, the note-taking and their personal development should help you to strengthen your analysis and synthesis skills. The practical sessions should allow you to appropriate the tools introduced in the lecture through exercises of different levels (calculation, reflection, synthesis, contextualization, etc.). Both in the lecture and in the practical session, your questions are always welcome. After each supervised activity (lecture or practical session) independent revision work is necessary to be able to take full advantage of the following activity. An overview of the chemical applications (and especially in quantum chemistry and crystallography) of the mathematical concepts presented in the course will be presented.
Content	The following topics will be covered: - Complex numbers. - Linear algebra: vector spaces and subspaces, bases and dimension, matrix calculus, rank theorem and applications to systems of linear algebraic equations, determinant and invertible matrices, diagonalization of linear operators. - Spectral theorem - Linear differential equations - Group theory: group of isometries of a molecule, linear representation of a group, characters, irreducible representations, decomposition of a representation into a sum of irreducibles and application to molecular systems.
Faculty or entity in charge	CHIM

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Additionnal module in Chemistry	APPCHIM	3		🔍