

Foundations of NMR and XRD for Structure Analysis (C004130)

Due to Covid 19, the education and evaluation methods may vary from the information displayed in the schedules and course details. Any changes will be communicated on Ufora.

Course size (nominal values; actual values may depend on programme)
Credits 4.0 Study time 120 h Contact hrs 37.5 h

Course offerings and teaching methods in academic year 2020-2021

A (semester 2)	English	Gent	seminar: coached exercises	15.0 h
			lecture	22.5 h

Lecturers in academic year 2020-2021

Martins, José	WE07	lecturer-in-charge
Van Hecke, Kristof	WE06	co-lecturer

Offered in the following programmes in 2020-2021

	crdts	offering
Master of Science in Teaching in Science and Technology (main subject Chemistry)	4	A
Master of Science in Chemistry (main subject (Bio)Organic and Polymer Chemistry)	4	A
Master of Science in Chemistry (main subject Analytical and Environmental Chemistry)	4	A
Exchange Programme in Chemistry (master's level)	4	A

Teaching languages

English

Keywords

Nuclear magnetic resonance spectroscopy, X-ray diffraction, Organic Structure analysis.

Position of the course

The course is aimed at master's students who pursue a deeper understanding of the foundations of NMR spectroscopy and XRD techniques with the prospect of 1) applying them to advanced structural analysis problems in the context of scientific research in organic chemistry or 2) designing new ones or further development of existing NMR and/or XRD methods in organic structure analysis. Attention is paid to both the theoretical background and the practical aspects that are associated with the implementation and execution of experiments on the respective equipment.

Contents

NMR

- Manipulating nuclear spins
- Nuclear spin relaxation
- Manipulation of two-core spin systems
- Introduce multiple dimensions
- In the wake of a measurement: NMR in practical terms
- Principle and use of pulsed magnetic field gradients for modern NMR spectroscopy
- Solvent suppression: work in the presence of an intense signal
- Dynamic effects and the NMR time scales
- Resolution without extra costs? "Pure shift" methods
- Translate conformation-sensitive parameters into a spatial structure
- New trends

XRD

- Crystallization procedures for organic molecules and (bio) macromolecules
- Data collection and processing
- Crystallography of small (organic) molecules
 - Direct methods

- Patterson
- Absolute configuration
- Crystallography of (bio) macromolecules
 - Molecular replacement
 - Anomalous scattering
 - Structure refinement
- Databases and structure validation

Initial competences

Fundamental and advanced aspects of structural analysis, spectroscopy, nuclear resonance and X-ray diffraction in agreement with the bachelor program Chemistry and the course Molecular Structure Analysis of the Master of Science in Chemistry.

Final competences

- 1 • Being able to read NMR pulse sequences and predict the spectrum.
- 2 To be able to read the scientific literature on NMR spectroscopy and X-ray diffraction and to understand the most important results.
- 3 To have insight into the different parameters that are required to correctly collect X-ray data and how these influence structural models (accuracy, validity,...).
- 4 To have insight into the NMR parameters that have an impact on a practical measurement and on signal processing.
- 5 To be able to use and apply different crystallization and solution methods in theory and practice to solve crystallographic problems.
- 6 Being able to draw up simple NMR pulse sequences and simulate their results.
- 7 To have insight into the way in which conformation-sensitive parameters obtained with NMR techniques can be converted into a spatial structure.
- 8 To have knowledge of recent trends in NMR spectroscopy for organic structure analysis.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Demonstration, lecture, seminar: coached exercises

Learning materials and price

- PowerPoint presentations (Ufora)
- Artikels and book chapters from recent literature

References

The following handbooks are relevant with regard to the NMR spectroscopy section but are not mandatory purchases:

High-Resolution NMR techniques in Organic Chemistry 2nd Edition. Timothy DW Claridge

Elsevier, ISBN-13: 978-0-08-054628-5.

This book is available electronically via Ufora.

Understanding NMR spectroscopy, J. Keeler, 2nd Edition, Wiley, ISBN: 1119964938.

This book is available electronically via Ufora.

Crystallography made Crystal Clear (Gale Rhodes)

Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology (Bernhard Rupp)

Crystal structure determination (William Clegg)

Course content-related study coaching

Interactive support via Ufora, or through interaction with the docent(s) or assistants during coached excercises or demonstrations.

Individual support after evaluation of the request by the docent(s) or assistants, on appointment.

Evaluation methods

end-of-term evaluation

Examination methods in case of periodic evaluation during the first examination period

Written examination, open book examination, oral examination

Examination methods in case of periodic evaluation during the second examination period

Written examination, open book examination, oral examination

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation
not applicable

Calculation of the examination mark

100% end-of-term evaluation:

- 65% NMR
- 35% XRD