

Course Specifications

From the academic year 2017-2018 up to and including the

Structural Analysis (C003975)

Course size (nominal values; actual values may depend on programme)

Credits 5.0 Study time 140 h Contact hrs 50.0 h

Course offerings and teaching methods in academic year 2018-2019

A (semester 2)	Dutch	seminar: coached	25.0 h
		exercises	
		lecture	25.0 h

Lecturers in academic year 2018-2019

Geudens, Niels WE07 lecturer-in-charge

Offered in the following programmes in 2018-2019

Bachelor of Science in Chemistry	crdts	offering
	5	A

Teaching languages

Dutch

Keywords

Spectroscopy, Nuclear Magnetic Resonance, Infrared, Mass Spectrometry, Structure analysis, Conformation

Position of the course

To acquire knowledge en practical expertise in structural analysis of chemical substances, via analysis of experimental data obtained from, infrared (IR), Nuclear Magnetic Resonance spectroscopy and Mass spectrometry. The student realises that advance in chemical synthesis is intricately linked with spectroscopic and spectrometric structural analysis.

Contents

The following techniques are introduced:

- Infrared spectroscopy - relationships with characteristic functional groups
- Nuclear Magnetic Resonance Spectroscopy (NMR):
 - the nuclear spin as the basis for a spectroscopic technique, NMR active nuclei in the Periodic Table of the elements
 - Empirical correlations with chemical structure: chemical shift, scalar coupling.
- Mass spectrometry:
 - ionisation methods, low and high resolution
 - molecular formulas from mass spectra
 - fragmentation
 - interpretation

Particular attention is paid to the strong and weak points of each technique in structural analysis. Strategies for structural analysis using a combination of the above techniques are demonstrated via exercises. The emphasis lies on practical application rather than theory.

Initial competences

To have obtained a credit - or to have obtained the competences associated with these credits through equivalent courses - for the following :

Physics I: mechanics,

Introduction to Organic Structures

The following courses should already feature in the curriculum: Physics II: waves, optics and thermal physics;

Electromagnetism

Applied mathematics for chemists.

Final competences

- 1 The student can predict the most important spectral properties of chemical substances.
- 2 The correct or most probable structure can be derived from experimental data.
- 3 Strategies for the choice and application of spectroscopic and spectrometric techniques can be formulated and executed for the more complex problems.
- 4 Structure analysis can be integrated with synthesis during practical sessions.
- 5 Analytical reasoning and problem solving capabilities have been further developed.
- 6 Have an insight in the fundamental mechanisms that provide the foundations for the different spectroscopic techniques used for 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

Lecture, seminar: coached exercises

Learning materials and price

Dutch syllabus and exercise package
 On-line exercises via ELO (<http://minerva.UGent.be>)
 Each student disposes of their own computer

References

None of these are compulsory (55 €)
 Organic Spectroscopic Analysis, Anderson, Bendell and Groundwater, Royal Society of Chemistry, ISBN 0-85404-476-0
 Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 4th Edition, Pavia, Lampman, Kriz and Vyvyan, Harcourt Brace College Publishers, ISBN-10: 0495114782 ISBN-13: 9780495114789 [about ten copies are available during practicals and tutorials]
 Organic Structures from Spectra, 4th Edition, Field, Sternhall and Kalman, John Wiley and Sons, ISBN: 978-0-470-31927-7

Course content-related study coaching

Through tutored exercises: aims at developing the skills to solve structure analyses problems.
 Additional exercises for self-evaluation offered through the ELO
 Individual coaching and feedback by the lecturer.
 Interactive guidance via the Forum of the ELO

Evaluation methods

end-of-term evaluation

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

Written examination with open questions, oral examination

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

Written examination with open questions, oral examination

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation

not applicable

Extra information on the examination methods

Periodic: oral exam with written preparation for part of the exercises, written exam for the theory and the other part of the exercises.

Permanent: the correlation between structure and spectral parameters and vice versa are continuously evaluated through guided exercises and via additional exercises offered via the ELO.

Calculation of the examination mark

Exam questions cover the relation between structure and spectral parameters (8/20 points), as well as practical skills and problem solving capabilities through structure analysis exercises (12/20)