

Chemical Structures (C003964)

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 9.0 Study time 260 h Contact hrs 87.5 h

Course offerings and teaching methods in academic year 2020-2021

A (year)	Dutch	Gent	lecture	45.0 h
			seminar: coached	37.5 h
			exercises	
			guided self-study	5.0 h
			online seminar:	0.0 h
			coached exercises	
			online lecture	0.0 h

Lecturers in academic year 2020-2021

Martins, José	WE07	lecturer-in-charge
Bultinck, Patrick	WE06	co-lecturer
Hens, Zeger	WE06	co-lecturer

Offered in the following programmes in 2020-2021

	crdts	offering
Bachelor of Science in Chemistry	9	A

Teaching languages

Dutch

Keywords

atoms and molecules, spatial structure, electronic structure, chemical bond, quantum mechanics, stereochemistry, conformation

Position of the course

This is an annual course within the 'general chemistry' learning track.

It provides a thorough knowledge of the spatial structure and electronic structure of molecules, and the relationship between the two. This includes:

(1) a broad and detailed descriptive introduction to the concepts and ideas which form the basis of today's description of atoms, molecules and the chemical bond, followed by,

(2) an extensive overview of spatial and dynamic aspects of molecules, whereupon

(3) follows a thorough introduction to the basic principles of quantum mechanics, and its use in describing and understanding of electronic structure and the chemical bonding.

The emphasis is on teaching general knowledge with more specialized learning can build on. The course makes use of skills in modeling and simulation.

Contents

- Part 1 - Introduction to chemical structures
- Chemical structures - an introduction
- Electron in atoms: introduction and the hydrogen atom
- Electron in atoms: atoms of more than one electron
- From atom to molecule: molecules of elements of the 1st period
- Electrons in diatomic molecules, compounds of the 2nd period
- Electrons in the molecules: polyatomic compounds
- The chemical bond in the Periodic Table
- Isomerism, representation of chemical structures and naming
- Resonance
- Stereochemistry
- Conformational Analysis

- Symmetry and Chemical Structures

Part 2 - Quantum check chemical structures

- Functions and vectors; operators and matrices
- The Schrödinger equation - Chemical two-state systems
- Time-dependent systems
- More electrical systems
- Wave mechanics - exactly solvable problems
- Wave mechanics - spherical potentials
- Quantum mechanical description of atomic systems
- Quantum mechanical description of molecules

Initial competences

No specific requirements

Final competences

- 1 The student understands the description of atoms, molecules and chemical bonding and is familiar with the language and the related interpretations of the concepts at its base.
- 2 The student has insight into the way in which the above leads to the composition and structure of the Periodic Table.
- 3 The student has gained insight into the different types of chemical bonds and can recognize and describe them correctly.
- 4 The student is familiar with the concept of resonance and the precise meaning and application; he / she can derive the relevant resonance structures
- 5 The student can recognize, describe and name the different types of isomerism
- 6 The student is able to recognize and name the major functional groups of organic molecules and name
- 7 Derive the IUPAC name of simple inorganic and organic compounds and from the IUPAC name derive the associate structure formula.
- 8 Analyze the symmetry of a molecule and apply the insight in predicting physical properties, crystal forms and orbitals
- 9 The student is familiar with the concept of conformation and can perform simple conformational analysis and explain from this the dynamic behavior of molecules.
- 10 The student understands the basic principles of quantum mechanics and to apply them within the context of two-level systems.
- 11 The student has insight into the electronic structure of atoms and the quantum mechanical description thereof.
- 12 The student understands the chemical bond and the quantum mechanical description thereof.
- 13 The student is able to solve problems of chemical structure by reasoning from a quantum mechanical context.

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

Guided self-study, lecture, seminar: coached exercises, online lecture, online seminar: coached exercises

Extra information on the teaching methods

Due to the COVID19 pandemic changes may be required in didactic methods. Information on this is spread via Ufora.

Learning materials and price

Part 1: English textbook Chemical Structure and Reactivity (50€) is accompanied by dutch course notes (40 €) and PowerPoint material.

Part 2: English course notes and English reference material.

Background texts and links on Ufora.

Each student disposes of their own computer.

References

Part 1: Chemical Structure and Reactivity - an integrated approach, James Keeler and Peter Wothers, Oxford University Press, 2nd Edition ISBN 978-0-19-960413-5 (about 50 EUR) - mandatory.

Part 2: Leonard Susskind and Art Friedman, Quantum Mechanics, the theoretical minimum. Penguin Books, UK, 2015. ISBN 9780141977812 (about 15 EUR) - optional. Colleges (video) from this book, iTunes or YouTube (free) - required viewing.

Course content-related study coaching

Evaluation methods

end-of-term evaluation

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

Written examination with open questions

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

Written examination with open questions

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation

not applicable

Extra information on the examination methods

The partial exam concerns part 1 "introduction to chemical structures " during the first semester exam period.

A short question in connection with each of the above-mentioned final competences 1-9; two to three content questions concerning final objective 1 and 4.

Students who have passed the partial examination are exempted from part 1 during the second semester exam period.

The exam during the second semester exam period includes, subject to exemption, the entire lesson content.

The evaluation of part 2 includes both theory and exercises.

Calculation of the examination mark

For part 2, the theory accounts for 40%, while exercises account for 60%. The individual total scores for part 1 respectively part 2 are equally weighted in the final score.