

## Symmetry and Spectroscopy (C003973)

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

**Credits** 5.0                      **Study time** 135 h

**Course offerings in academic year 2024-2025**

### Lecturers in academic year 2024-2025

Bultinck, Patrick	WE06	lecturer-in-charge
Acke, Guillaume	WE06	co-lecturer

### Offered in the following programmes in 2024-2025

	crdts	offering
<a href="#">Bachelor of Science in Chemistry</a>	5	A
<a href="#">Linking Course Master of Science in Chemistry (main subject Materials and Nano Chemistry)</a>	5	A
<a href="#">Preparatory Course Master of Science in Chemistry (main subject Materials and Nano Chemistry)</a>	5	A

### Teaching languages

Dutch

### Keywords

symmetry, group theory, chemical bonding, spectroscopy

### Position of the course

This course is part of the physical chemistry learning track and aims to familiarize the students with group theoretical methods and their applications for electronic states and spectroscopic properties of atoms and molecules.

### Contents

- Group theory and symmetry: Symmetry elements and operations, Group theoretical approach to symmetry, Representations and their reduction to irreducible representations, The great orthogonality theorem and projection operators, Symmetry adapted linear combinations.
- Symmetry and molecular orbital theory: Hückel theory, Ligand field theory, Jahn-Teller effect.
- Symmetry and vibrational spectroscopy: Spectroscopic transitions, Vibrational energy levels of diatomic molecules, Vibrational selection rules, Vibrations of polyatomic molecules.
- Symmetry and electronic transitions: Electronic selection rules, Frank-Condon principle, Vibronic transitions.

### Initial competences

This course builds further on certain final competences of the courses:

- General chemistry
- Chemical structures
- Mathematics: basic concepts
- Mathematics: advanced techniques
- Physics: mechanics
- Physics: waves, optics and thermodynamics

Students must have taken the course on Electronic Structure (C003972) in the same academic year or earlier prior to taking this course.

### Final competences

- 1 The student has knowledge of the fundamental aspects of group theory.
- 2 The student understands the power and limitations of these methods.

- 3 The student understands the importance of symmetry for the preparation of qualitatively correct MO diagrams.
- 4 The student understands the relationship between symmetry and spectroscopic selection rules.

#### **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

#### **Extra information on the teaching methods**

On campus lecture, online seminar: guided exercises with support via Ufora and MS Teams. Because of COVID19, changed working methods can be rolled out if this proves necessary.

#### **Learning materials and price**

An integrated course is available. Course notes and assignments from tutorials are supplemented with web lectures and knowledge clips. Each student is required to have their own computer with a webcam and microphone.

#### **References**

- "Group Theory Applied to Chemistry", A. J. Ceulemans (Springer), ISBN: 978-9402406139
- "Symmetry: An Introduction to Group Theory and Its Applications", R. McWeeny (Dover Publications), ISBN: 978-0486421827
- "Group Theory and Chemistry", D. M. Bishop (Dover Publications), ISBN: 978-0486673554

#### **Course content-related study coaching**

Interactive support through Ufora 'Discussions'. Individual guidance by teachers / assistants: by electronic appointment via MS Teams.

#### **Assessment moments**

end-of-term assessment

#### **Examination methods in case of periodic assessment during the first examination period**

Oral assessment, written assessment with open-ended questions

#### **Examination methods in case of periodic assessment during the second examination period**

Oral assessment, written assessment with open-ended questions

#### **Examination methods in case of permanent assessment**

#### **Possibilities of retake in case of permanent assessment**

not applicable

#### **Extra information on the examination methods**

The exam consists of the theory part, of which one part is oral with written preparation and one part purely written, and an exercise part, of which the only part is purely written.

#### **Calculation of the examination mark**

Both the theory part and the exercise part are each assessed for ten out of twenty points. Students who do not participate in the evaluation of one or more components or who achieve less than a four out of ten for one of the components, can no longer pass the whole of the course. If in that case the final score would still be ten or more, this will be reduced to a no-pass score.