

Symmetry and Spectroscopy (C003973)

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

Credits 5.0 **Study time 135 h**

Course offerings and teaching methods in academic year 2024-2025

A (semester 2)	Dutch	Gent	seminar lecture
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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
Bachelor of Science in Chemistry	5	A
Linking Course Master of Science in Chemistry(main subject Materials and Nano Chemistry)	5	A
Preparatory Course Master of Science in Chemistry(main subject Materials and Nano Chemistry)	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

Seminar, Lecture

Extra information on the teaching methods

On campus lecture, online seminar: guided exercises with support via Ufora and MS Teams.

Study material

Type: Syllabus

Name: Bachelor's Quantum Theory

Indicative price: € 20

Optional: no

Language : English

Number of Pages : 200

Available on Ufora : Yes

Online Available : Yes

Available in the Library : No

Available through Student Association : No

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.