

CH-250

Mathematical methods in chemistry

Lorenz Ulrich, Vanicek Jiri

| Cursus | Sem. | Type |
|------------------------------------|------|------|
| Chemistry and chemical engineering | BA4 | Obl. |
| HES - CGC | E | Obl. |

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|----------------------------|---------------------|
| Language of teaching | English |
| Credits | 4 |
| Session | Summer |
| Semester | Spring |
| Exam | During the semester |
| Workload | 120h |
| Weeks | 14 |
| Hours | 4 weekly |
| Lecture | 2 weekly |
| Exercises | 2 weekly |
| Number of positions | |

Summary

This course consists of two parts. The first part covers basic concepts of molecular symmetry and the application of group theory to describe it. The second part introduces Laplace transforms and Fourier series and their use for solving ordinary and partial differential equations in chemistry & c.e.

Content*Part I*

Molecular symmetry and point groups

Group theory

Representations of groups, the Great Orthogonality Theorem, character tables

Group theory and quantum mechanics, applications to molecular orbital theory and normal modes of vibration

Part II

Laplace transform, convolution, and solution of ordinary differential equations

Fourier series, separation of variables, and solution of partial differential equations

Applications of integral transforms in chemical kinetics, chemical engineering, and physical chemistry

Assessment methods

Part I (Lorenz): midterm exam 100%

Part II (Vanicek): homeworks 30% + midterm exam 70%

The points from the two parts are combined to form the final grade.

Resources**Bibliography**

1. Cotton, F. A. *Chemical Applications of Group Theory*. (John Wiley & Sons, 1990).
2. Walton, P. H. *Beginning Group Theory for Chemistry*. (Oxford University Press, 1998).
3. P. Dyke, *An introduction to Laplace transforms and Fourier series*, Springer, 2014.

Ressources en bibliothèque

- [An introduction to Laplace transforms and Fourier series / Dyke](#)
- [Chemical applications of group theory / Cotton](#)
- [Beginning group theory for chemistry / Walton](#)

Références suggérées par la bibliothèque

- [Chimie et théorie des groupes / Walton](#)

Moodle Link

- <https://go.epfl.ch/CH-250>