CH-250

Mathematical methods in chemistry

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

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