CH-250

# Numerical methods in chemistry

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| 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** |
| Courses | 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

## Learning Outcomes

By the end of the course, the student must be able to:

- Work out / Determine the point group of molecules
- Understand basic concepts of group theory, representations of groups, and character tables
- Apply group theory to predict properties of symmetric molecules
- Work out / Determine analytically Laplace transforms, Fourier series, and convolutions of functions
- Solve linear ordinary and partial differential equations with Laplace transforms and Fourier series
- Apply Laplace transforms and Fourier series to solve the rate, heat-transport, and Schrödinger equations

## 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
- MATLAB : a practical introduction to programming and problem solving / Attaway