CH-310

Dynamics and kinetics

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Cursus	Sem.	Type
Chemical Engineering	BA5	Obl.
Chemistry	BA5	Obl.
HES - CGC	H	Obl.

Language of teaching	English
Credits	3
Session	Winter
Semester	Fall
Exam	Written
Workload	90h
Weeks	14
Hours	**3 weekly**
Courses	2 weekly
Exercises	1 weekly
Number of positions	

Summary

The course covers the principles of chemical kinetics, including differential rate laws, derivation of exact and approximate integral rate laws for common elementary and composite reactions, fundamentals of collision and transition state theories, and applications such as enzymatic catalysis.

Content

1. Definition

- Nomenclature.

2. Macroscopic aspects of chemical kinetics

- Variation of reaction rates with concentrations.
- Variation of reaction rates with temperature.
- Composite reactions.
- Introduction to enzyme catalysis.
- Kinetic aspects of polymerisation.

3. Kinetic theory of gases and molecular beams.

4. Collision theory

- Bimolecular reactions.
- Unimolecular reactions.

5. Statistical thermodynamics

- Distribution of molecular states.
- Thermodynamic properties.

6. Transition state theory

- Statistical approach.
- Thermodynamic formulation.
- Potential energy surfaces.
- Extention of transition state theory

7. Reactions rates in solutions

- Influence of the solvent on reaction rates.
- Reactions between ions.

- Diffusion controlled reactions.
- Influence of solvation on electron transfer reactions.

Learning Prerequisites

Required courses

Quantum Chemistry
Spectroscopy
Thermodynamics
Statistical Thermodynamics
Mathematical Methods in Chemistry

Learning Outcomes

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

- Express differential rate laws for elementary and composite chemical reactions.
- Derive and apply integral rate laws for the most common elementary and composite reactions.
- Apply correctly the steady-state approximation for the rate constant.
- Derive and apply the rate law for the Michaelis-Menten mechanism of enzymatic catalysis.
- Compute the thermodynamic properties of a gas from the kinetic theory.
- Compute the rate constants of unimolecular and bimolecular reactions from the collision theory.
- Apply the transition state theory to derive a general expression for the rate constant.
- Use the transition state theory to compute rate constants of elementary reactions.

Assessment methods

Written final exam (100 %)

Resources

Bibliography

Steinfeld, J. I., Francisco, J. S. & Hase, W. L. *Chemical Kinetics and Dynamics*. (Prentice Hall, 1989).
McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach*. (University Science Books, 1997).
Laidler, K. J. *Chemical Kinetics*. (Prentice Hall, 1987).

Ressources en bibliothèque

- Chemical kinetics and dynamics / Steinfeld
- Chemical kinetics / Laidler
- Physical chemistry / McQuarrie

Notes/Handbook

Lecture notes
H. Girault: Cinétique chimique