CH-310

Dynamics and kinetics

Feldmann Sascha

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**
Lecture	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. Basic Concepts of Kinetics

- Order and molecularity of reactions
- Integrated reaction rate laws
- Arrhenius Equation

2. Complex reactions

- Composite reactions
- Exact analytical and approximate solution methods
- Enzymatic catalysis
- Polymerization reactions

3. Kinetic theory of gases

- Ideal gases
- Maxwell-Boltzmann distribution

4. Collisions

- Collision theory
- Bimolecular collisions
- Two-body scattering

5. Unimolecular reaction dynamics

- Lindemann-Hinshelwood theory of thermal unimolecular reactions
- RRK theory

6. Transition state theory

- Potential energy surfaces
- Postulates and derivation

- Thermodynamic formulation

Learning Prerequisites

Required courses

Quantum Chemistry
Spectroscopy
Thermodynamics
Statistical Thermodynamics

Recommended courses

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

Atkins, P., de Paula, J., and Keeler. J. *Atkins' Physical Chemistry* (Oxford University Press, any edition, e.g. 8th edition, 2006).
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
- Atkins' Physical Chemistry / Atkins, P. (2023)
- Chemical kinetics / Laidler
- Physical chemistry / McQuarrie

Notes/Handbook

Lecture notes
H. Girault: Cinétique chimique

Moodle Link

- https://go.epfl.ch/CH-310