

Molecular Reaction Dynamics

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This course covers the microscopic description and experimental investigation of chemical reactions in gases and liquids. The topics covered are:

1. Kinetics and rate laws

Differential and integrated rate laws, reaction mechanism, temperature dependence

2. Collision and encounters

Collision theory and cross-section, thermal averages, threshold and activation energy, transition-state theory

3. Interaction potentials

Intermolecular forces, potential energy surfaces, centrifugal barrier, molecular trajectories, Polanyi rules, scattering, transition-state spectroscopy

4. Energy transfer

Internal vibrational redistribution, intermolecular energy transfer, Landau-Teller model, Landau-Zener curve crossing

5. Reactions in solutions

Cage effect, diffusion control, solvation energy, Marcus theory of electron transfer, Kramer's theory

6. Photochemistry

Light absorption and emission, photodissociation dynamics, RRKM theory

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Meeting time:

Room 8335 Chemistry
8:50-9:40AM **Wednesday and Friday**

Except:

No class on Nov 4 and Nov 25

Required Assignments

- 1) Problems sets (4) 60%
- 2) In-class final exam 40%

Textbooks:

The recommended (but not required) textbooks for the course are *Chemical Kinetics and reaction dynamics* by Paul L. Houston.