

Molecular Reaction Dynamics

Professor Etienne Garand
8:50-9:40AM MWF
Room 8335 Chemistry
2 credits

This course covers the microscopic description and experimental investigation of elementary 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, ionic strength, Marcus theory of electron transfer

6. Photochemistry

Light absorption and emission, photodissociation dynamics, RRKM theory

7. Experimental techniques in reaction dynamics

Reactive scattering, velocity-map imaging, pump-probe spectroscopy, single-molecule fluorescence

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