

## Molecular Reaction Dynamics

Professor Etienne Garand  
email: [egarand@chem.wisc.edu](mailto:egarand@chem.wisc.edu)  
office : 6365

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*

## Molecular Reaction Dynamics

Professor Etienne Garand  
email: [egarand@chem.wisc.edu](mailto:egarand@chem.wisc.edu)  
office : 6365

### 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.