Syllabus of the Graduate Course CHEM 652 'Chemical Kinetics and Reaction Dynamics'

1. **Kinetics**

   1.1. Basic concepts: reaction order, molecularity, rate laws
   1.2. Reaction mechanisms: time dependence of reactance, intermediates, and products
   1.3. Rate constants: Arrhenius rate law and deviation; activation energy versus entrance barriers
   1.4. Experimental determination of rate constants

2. **Macroscopic and microscopic processes**

   2.1. Cross section and impact parameter
   2.2. Relationship between rate constants and cross sections
   2.3. Attractive interaction potentials in bimolecular reactions
   2.4. Experimental determination of cross sections

3. **Potential energy surfaces**

   3.1. Two dimensional representation
   3.2. Features on potential energy surfaces
   3.3. Experimental probing of potential energy surfaces and reaction mechanisms
   3.4. Molecular dynamics calculations

4. **Transition state theory**

   4.1. Partition functions and chemical equilibrium
   4.2. Transition state theory
   4.3. Application of transition state theory to unimolecular decomposition
   4.4. RRKM theory

5. **Classical versus quantum mechanical treatment of elastic and reactive scattering**

Required Textbooks

1. Molecular Reaction Dynamics and Chemical Reactivity, R.D. Levine, R.B. Bernstein (Oxford, New York).
2. Chemical Kinetics and Reaction Dynamics, Paul L. Houston (Mc Graw Hill, New York).

Optional Textbooks

1. Mathematical Methods for Physicists, G. Arfken, (Academic Press, New York).
2. Chemical Kinetics and Dynamics, J.I. Seinfeld, J.S. Francisco, W.L. Hase (Prentice Hall, New Jersey).