

'Reaction Dynamics - Advanced Statistical Theory of Chemical Reactions' - 2004

1. Introduction

- 1.1 Statistical theory of canonical ensemble - review
 - Boltzmann statistics, Partition function, Chemical equilibrium, Transition-state theory
- 1.2 Statistical theory of microcanonical ensemble
 - Multiplicity, Density of states (Problem-1)

2. Density of states for molecular motions

- 2.1 Translational density of states
 - 1-Dimensional (1-D) translation, 3-D translation, 3-D relative translation (Problem-2.1)
- 2.2 Rotational density of states
 - Rotational motion, 1-D Rotator, 2-D Rotator, 3-D Rotator, Summary
- 2.3 Vibrational density of states
 - Vibrational motion, One vibrator, n_v Vibrators (Problem-2.2)

3. Prior distribution

- 3.1 Rotational distribution and rotational sum
 - (Problem-3.1)
 - Rotational sum (Problem-3.2)
- 3.2 Vibrational sum
 - Vibrational sum (Problem-3.3)
- 3.3 Degeneracy of the electronic states
 - Atoms, Linear molecules, Non-linear molecules
- 3.4 Number of optical isomers and rotational symmetry number
 - Number of optical isomers, Rotational distribution and nuclear spin statistics (Problem-3.4)

4. Microscopic rate coefficients and unimolecular reactions

- 4.1 Microscopic rate coefficients
 - $k(E)$ (Problem-4.1)
 - $k(E, J)$, sum of states, Whitten-Rabinovich approximation, Direct count (Problem-4.2)
- 4.2 Unimolecular reactions
 - Lindemann mechanism, Troe's formula
- 4.3 RRKM Theory
 - 'Lindemann' to RRKM, High-pressure limit (Problem-4.3)
 - Low-pressure limit, strong-collision RRKM, Weak collision correction (Problem-4.4)

[scheduling]

- (1) Dec. 8
- (2) Dec. 15
- (3) Dec. 22
- (4) Jan. 12
- (5) Jan 19
- (6) Jan 26

Deadline for the submission of reports: Wed., Feb. 9