

NPTEL Video Lecture Topic List - Created by LinuXpert Systems, Chennai

NPTEL Video Course - Chemistry and Biochemistry - NOC:Chemical Kinetics and Transition State Theory

Subject Co-ordinator - Prof. Amber Jain

Co-ordinating Institute - IIT - Bombay

Sub-Titles - Available / Unavailable | MP3 Audio Lectures - Available / Unavailable

- Lecture 1 - Rate: the reaction velocity
- Lecture 2 - Its elementary - rate law equations
- Lecture 3 - Arrhenius equation: what's the fuss about?
- Lecture 4 - Dance of atoms: from Newton to Hamilton
- Lecture 5 - Boltzmann distribution: a story of Hamilton, Liouville and Boltzmann
- Lecture 6 - Maxwell Boltzmann distribution: how fast are molecules moving?
- Lecture 7 - Kinetic theory of collisions: initial estimate
- Lecture 8 - Boltzmann distribution and kinetic theory of collisions
- Lecture 9 - Kinetic theory of collisions: a discussion
- Lecture 10 - Kinetic theory of collisions: reactive cross section
- Lecture 11 - Problem solving session - 1
- Lecture 12 - Problem solving session - 2
- Lecture 13 - Kinetic theory of collision and equilibrium constant
- Lecture 14 - Critique of kinetic theory of collisions
- Lecture 15 - Transition state theory and partition functions
- Lecture 16 - Partitioning the partition function
- Lecture 17 - Translating, rotating and vibrating quantum mechanically
- Lecture 18 - Partition function and equilibrium constant
- Lecture 19 - What is a transition state?
- Lecture 20 - A puzzle: cars on highway
- Lecture 21 - Transition state theory: derivation 1
- Lecture 22 - Practical calculation of TST rate
- Lecture 23 - Calculating TST rate for the reaction $\text{H} + \text{HBr}$
- Lecture 24 - Collision theory as a special case of TST
- Lecture 25 - TST: an intuitive proof in one dimension
- Lecture 26 - Rate as a flux across a dividing surface
- Lecture 27 - Transition state theory: derivation 2 from dynamical perspective
- Lecture 28 - Discussion of the assumptions of TST
- Lecture 29 - Thermodynamic formulation of TST

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- Lecture 30 - Problem solving session - 3
- Lecture 31 - Problem solving session - 4
- Lecture 32 - Hills and valleys of potential energy surfaces
- Lecture 33 - Molecular dynamics: rolling spheres on potential energy surfaces
- Lecture 34 - Predictions from potential energy surfaces - rotational vs vibrational energies
- Lecture 35 - Free energy and potential of mean force
- Lecture 36 - Transmission coefficient and molecular dynamics
- Lecture 37 - Problem solving session - 5
- Lecture 38 - Microcanonical rate constant: putting balls in jars
- Lecture 39 - Microcanonical rate constant: RRK model
- Lecture 40 - Microcanonical rate constant: magic of Marcus - RRKM model
- Lecture 41 - Canonical TST from microcanonical RRKM model
- Lecture 42 - Sum and density of states
- Lecture 43 - Unimolecular decay - revisited
- Lecture 44 - Unimolecular decay: RRK's approach
- Lecture 45 - Unimolecular decay: RRKM's approach
- Lecture 46 - Problem solving session - 6