CHEMICAL KINETICS AND TRANSITION STATE THEORY

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TYPE OF COURSE : New | Elective | UG/PG
COURSE DURATION : 8 Weeks (18 Jan' 21 - 12 Mar' 21)
EXAM DATE : 21 Mar 2021

PRE-REQUISITES : Introduction to chemical kinetics and dynamics

INTENDED AUDIENCE : Any Interested Learners

COURSE OUTLINE :
This course will cover calculating rate constants using two basic models: collision theory and transition state theory (TST). TST will particularly be discussed in detail with solving multiple examples and discussion of limitations and extensions. The course assumes knowledge of basic statistical mechanics, particularly Boltzmann distribution and partition functions. These concepts will be briefly revised, but not derived in detail. Knowledge of basic rate theory will be helpful, although will be covered in the course.

ABOUT INSTRUCTOR :
Dr. Amber Jain is an assistant professor at IIT Bombay since 2018. He did MSc (Integrated) from IIT Kanpur, PhD. from University of Wisconsin, Madison and postdoc from University of Pennsylvania. His main research interests are in chemical dynamics.

COURSE PLAN :

Week 1 : 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?

Week 2: 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

Week 3: 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?

Week 4: 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 H+HBr • Lecture 24: Collision theory as a special case of TST • Lecture 25: TST: an intuitive proof in one dimension

Week 5: 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 • Lecture 30: Problem solving session 3 • Lecture 31: Problem solving session 4

Week 6: 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 molecualr dynamics • Lecture 37: Problem solving session 5

Week 7: 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 micrononical RRKM model • Lecture 42: Sum and density of states

Week 8: 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