Program: Chemistry (15025012071P6)

Course: CHEMICAL KINECTS

Code: PPGQU0057

Workload: 60 hours

Credits: 04

Syllabus:

Kinetics definitions, reaction rate, reaction order, and molecularity; Relationship with thermodynamics; Degree of advancement; rate equation and specific rate constant; Empirical laws: Determination of the rate equation; Experimental methods and data treatment; Complex reactions; Temperature dependence of reaction rate; Empirical equations; Arhenius equation and activation energy; Theories in Chemical Kinects; Biomolecular gas-phase reactions; Transition-state theory and activated complex; Potential energy surfaces; Energy versus reaction coordinate diagrams; Thermodynamic formulation; Unimolecular an bimolecular reactions; Termolecular reactions; Lindemann, Hinshelwood, Rice-Ramsperger-Kassel (RRK), and Marcu (RRKM) theories; Applications.

Bibliography:

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ATKINS, P. W. Physical Chemistry, 5th edition, Oxford University Press, 1994.

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STEINFIELD, J. I.; FRANCISCO, J. S.; HASE, W. L. Chemical Kinetics and Dynamics, Prentice Hall, New Jersey, USA, 1999.

LEVINE, R. D. Molecular Reaction Dynamics, Cambridge University Press, 2005.

BENSON, S. W. The Foundations of Chemical Kinetics, New York: McGraw-Hill, 1960.