| Course Code | Course Name | Credits |
|---|---|---|
| 26CH503 | THERMODYNAMICS AND CHEMICAL KINETICS | 04 |

**Course Objectives**

- To understand the fundamental principles of thermodynamics, including energy changes, laws, and equilibrium concepts.
- To develop knowledge of thermochemical processes and calculation of heat changes in chemical reactions.
- To analyze reaction rates and mechanisms using chemical kinetics theories and experimental methods.

**Learning Outcomes**

Upon successful completion of this course, it is intended that a student will be able to:

- Understand basic thermodynamic laws, functions, and their applications.
- Apply entropy, free energy, and equations of state to assess spontaneity and equilibrium.
- Analyze thermochemical processes and heat changes using Hess's law.
- Evaluate reaction kinetics, rate laws, and reaction mechanisms.

**Unit 1 - Thermodynamics-I (12 Hrs.)**

Definitions; Different types of systems; Thermodynamic processes: reversible and irreversible, isothermal and adiabatic processes; Work of expansion at constant pressure and at constant volume; First law of thermodynamics: statement and limitations; Definition of internal energy (E), enthalpy (H), and heat capacity; Relationship between $C_p$ and $C_v$; Ideal and real gases under isothermal conditions of reversible and irreversible processes; Joule–Thomson effect; Adiabatic expansion of an ideal gas; Work done in adiabatic reversible expansion.

**Unit 2 – Thermodynamics-II (12 Hrs.)**

Second law of thermodynamics; Need for the second law; Different statements of the second law; Carnot cycle and efficiency of heat engine; Concept of entropy; Definition and physical significance of entropy; Entropy as a function of P, V, and T; Entropy changes during phase changes; Entropy of mixing; Entropy criterion for spontaneous and equilibrium processes in isolated systems; Gibbs free energy (G) and Helmholtz free energy (A); Variation of A and G with P, V, and T; Gibbs–Helmholtz equation and its applications; Thermodynamic equations of state; Maxwell's relations; $\Delta A$ and $\Delta G$ as criteria for spontaneity and equilibrium; Clapeyron equation; Clausius–Clapeyron equation and its applications.

**Unit 3 - Thermochemistry (12 Hrs.)**

Enthalpy of a Reaction; Heat of Reaction (Enthalpy of Reaction); Exothermic and Endothermic Reactions; Thermochemical Equations; Heat of Combustion; Heat of Solution; Heat of Neutralization; Energy Changes During Transitions or Phase Changes; Heat of Fusion; Heat of Vaporization; Heat of Sublimation; Heat of Transition; Hess's Law of Constant Heat Summation; Applications of Hess's Law; Measurement of the Heat of Reaction.

**Unit 4 – Chemical kinetics-I (12 Hrs.)**

Reaction Rate; Rate Equation; Order of Reaction; Molecularity of a Reaction; Rate Laws; Rate Constants; Derivation of First Order Rate Constant; Properties of Zero-Order, First-Order and Second-Order Reactions; Half-Life of Reactions (Derivation of Time for Half Change) with Examples; Methods for Determining the Order of Reactions (Experimental Methods); Determination of Rate Constant by Volumetry, Colorimetry and Polarimetry.

**Unit 5 - Chemical Kinetics-II (12 Hrs.)**

Simple Collision Theory and its Limitations; Absolute Reaction Rate Theory (ARRT); Thermodynamic Treatment of Reaction Rates; Potential Energy Surfaces; Application of ARRT to Simple Bimolecular Processes; Chain Reactions – General Characteristics; Kinetics of Chain Reactions ($H_2$–$Br_2$ Reaction, Decomposition of Acetaldehyde, Decomposition of $N_2O_5$); $H_2$–$O_2$ Explosive Reactions; Theory of Unimolecular Reactions (Lindemann, Hinshelwood, RRKM and Slater Treatments); Steady State Approximation; Kinetic Isotope Effect.

**Reference Books:**


1. Samuel Glasstone, Thermodynamics for Chemists 3rd Edn., 1974, East-West Edn.
2. J.Rajaram and JC Kuriacose, Thermodynamics for students of Chemistry, 1986, Lal Nagin Chand, New Delhi.
3. B.R. Puri, L.R. Sharma and M.S. Pathania, Principles of Physical Chemistry, 35th Edn., 2013, Shoban Lal Nagin Chand and Co, New Delhi.
4. S. Glasstone and D. Lewis, Elements of Physical Chemistry, Mac Millan & Co Ltd. London.
5. P.W. Atkins, Physical Chemistry, 5th Edn., 1994, Oxford University press.
6. M.V. Sangaranarayanan, V. Mahadevan, Text Book of Physical Chemistry, 2nd Edn., Hyderabad, Universities Press, India.


**Websites and eLearning Sources:**

1. https://nptel.ac.in/courses/104106094
2. https://www.youtube.com/watch?v=Ce9X4A7b94Q&list=PLII3zV64b7xRSd_iewlSMruH0PcwkXUjQ

| COs and Bloom's Taxonomy Mapping – 26CH503 | | |
|---|---|---|
| **Course Outcomes** | **On completing P.G. program the students will be able to** | **BTL** |
| **CO1** | Recall and explain fundamental concepts of thermodynamics, thermochemistry, and chemical kinetics. | K1, K2 |
| **CO2** | Apply thermodynamic principles and equations to determine energy changes, spontaneity, and equilibrium. | K3 |
| **CO3** | Analyze thermochemical data and reaction kinetics, including rate laws and mechanisms. | K4 |
| **CO4** | Evaluate reaction processes using kinetic theories and thermodynamic criteria. | K5 |
| **CO5** | Design and interpret experiments related to heat changes and reaction rates. | K6 |

**BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6- Create**

| Relationship Matrix – 26CH503 | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Course Outcomes** | **Programme Outcomes (POs)** | | | | | | **Programme Specific Outcomes (PSOs)** | | | | | **Mean Score of Cos** |
| | **PO1** | **PO2** | **PO3** | **PO4** | **PO5** | **PO6** | **PSO1** | **PSO2** | **PSO3** | **PSO4** | **PSO5** | |
| **CO1** | 1 | 3 | 2 | 1 | 2 | 1 | 2 | 3 | 1 | 2 | 1 | 1.72 |
| **CO2** | 2 | 3 | 2 | 3 | 2 | 1 | 2 | 3 | 1 | 3 | 1 | 2.09 |
| **CO3** | 3 | 2 | 2 | 2 | 1 | 2 | 3 | 1 | 2 | 3 | 1 | 2 |
| **CO4** | 3 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 2 | 2 | 2 | 1.81 |
| **CO5** | 1 | 2 | 3 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1.63 |
| | | | | | | | | | | | **Total** | 1.85 |

Mean Score: 3- High, 2- Medium/Moderate, 1-Low