Course Code	Course Title	C	H	I	E	T
17P2CMC6	PHYSICAL CHEMISTRY-II	4	4	25	75	100

UNIT I GROUP THEORY 12 Hrs

Rules of group -symmetry elements and symmetry operations – various operations with illustrations - matrix representation of symmetry operations - classification of groups - symmetry point groups - Groups and their basic properties — rotational (C), dihedral (D), tetrahedral (Td) and octahedral (Oh) point groups. Order of a group. Classes and similarity transformation - Group multiplication table(C_{2v}, C_{3v} and C_2h) –. Reducible and irreducible representations - decomposition procedure of reducible representation - Great orthogonality theorem - construction of character tables – C_2v, C_3v and C_2h point groups.

UNIT II APPLICATIONS OF GROUP THEORY 12 Hrs

Direct products- definition –types- triple product principle – Reduction formula- group theoretical analysis of IR and Raman active vibrations of H_2O and NH_3 Mutual exclusion principle – N_2F_2-selection rules for IR, Raman- symmetries of Molecular Orbitals -Application of group theory to electronic transitions to formaldehyde and ethylene - -selection rules – Formation of hybrid orbitals in molecules like BF_3, $[PtCl_4]^{2-}$ and CH_4.

UNIT III CHEMICAL KINETICS I 12 Hrs

Simple collision theory – modification-Absolute reaction rate theory (ARRT)-Statistical and thermodynamics formulation- Comparison of ARRT with collision theory-Significance of entropy of activation-Relation between ΔH and Ea-Transmission co-efficient-ARRT of termolecular reactions- Unimolecular reactions- Lindemann, Hinshelwood, RRKM and Slater treatments. Solution kinetics- ARRT of reaction in solution- primary and secondary - Salt effects.

UNIT IV CHEMICAL KINETICS II 12 Hrs

(a) *Chain reactions* - general characteristics, kinetics of chain reactions - steady state approximation - H_2 - Br_2 – reaction, Rice - Herzfeld mechanisms for the decomposition of ethane and acetaldehyde General characteristics of branched chain reactions explosion limits - H_2-O_2-reaction.

(b) *Fast reactions* - flow techinque - continuous and stopped flow methods - relaxation methods - pressure - jump and temperature - jump methods.Complex reactions – opposing, consecutive and parallel reactions.

UNIT V STATISTICAL THERMODYNAMICS 12 Hrs

Need for statistical thermodynamics – Definition of state of a system – assembly – ensemble-canonical and micro canonical ensembles – phase space – microstate – probability and distribution. Boltzman distribution law- Bose - Einstein and Fermi-Dirac distribution laws - derivation-partition function- Translational, rotational, vibrational and electronic partition funtions. Thermodynamic properties from partition functions for energy, heat capacity and entropy, Helmholtz free energy, pressure and chemical potential. Sackur-Tetrode equation-Thermodynamic properties of monoatomic gases.

Text Book(s):

1. Cotton, F.A., "Chemical Applications of Group Theory", Third Edition, Wiley Eastern Ltd., New Delhi, 2011.
2. Ramakrishnan, V. and Gopinathan, M.S., "Group Theory in Chemistry", Third Edition, Vishal Publication, New Delhi, 2011.
3. Atkins, P. and de Paula, J., "Physical Chemistry", Ninth Edition, Oxford University Press, New Delhi, 2011.
4. Berry, R.S., Rice, S.A and Ross. J, "Physical Chemistry", Second Edition, Oxford University Press, New York, 2007.
5. Laidler, K.J. "Chemical Kinetics" Sixth Edition, Pearson Education, New Delhi, 2011.
6. Rajaram, R. and Kuriacose, J.C., "Kinetics and Mechanism of Chemical Transformation", First Edition, Macmillan India Ltd., New Delhi, 2006.

Reference Books:

1. Ball, D. W., "Physical Chemistry", First Indian Edition, Cengage Rearing India Pvt., Ltd., New Delhi, 2009.
2. Mortimer, R.G. "Physical Chemistry", Third Edition, Academic Press – An imprint of Elsevier, London, 2009.
3. Puri, B.R., Sharma, L.R. and Pathania, M.S., "Principles of Physical Chemistry", Forty sixth Edition, Vishal Publishing Co., Jalandhar, 2013.
4. Bhal, A., Bhal, B.S. and Tuli, G.D., "Essentials of Physical Chemistry", First Edition, S.Chand & Company Ltd., New Delhi, 2012.