Master of Science, Chemistry
M. Sc. Chemistry, Semester – II

Course Code	PS02CCHE53	**Title of the Course**	Topics in Physical Chemistry-II
Total Credits of the Course	04	**Hours per Week**	04

Course Objectives:	The concepts developed are: 1. Chemical Kinetics and Group theory and chemical applications. 2. The course content and delivery takes the concepts further to study and understand the mechanistic aspects of complex reactions. The basis of reaction mechanism is dealt theoretically. 3. The fundamentals and concept based aspects of group theory and symmetry of molecules are taught to apply them to predict the spectroscopic and hybridization of some classical examples.

Course Content

Unit	Description	Weightage* (%)
1.	**Chemical Kinetics – II :** Complex reactions :- Opposing reactions, Consecutive reactions, Parallel reactions, Reactions in flow systems, Chain reactions, Ionic reactions and salt effect, enzyme catalyzed reactions, kinetics of fast reactions.	25
2.	**Chemical Dynamics :** Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory ; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of uni-molecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogenbromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction).	25
3.	**Group theory in Chemistry :** Concepts of symmetry in molecule:- Symmetry elements, symmetry operations, definitions and theorems in group theory, examples of groups, subgroups and classes, Molecular Point groups :- Identification and classification, notation of point groups, Matrix representation of symmetry operations, Types of matrices, matrix notations for symmetry elements : E, C_n, i, σ, S_n. Matrix representation of point groups : product and square rule, inverse rule, matrices for C_{3v}, C_{4v} etc., Construction of character tables :-rules, reducible and irreducible representations, character of a representation, properties of a irreducible representations, orthogonality theorem, character tables for C_{2v}, C_{3v}, C_{4v}, D_{nh}, uses of character tables.	25

4.	**Chemical Applications of Group Theory :** Molecular vibrations, molecular vibration of symmetrical AB_2 (bent) molecule, symmetry of normal modes of ethylene, tetrahedral hybridization, Hybridization in Boron Trifluoride (trigonal planar geometry), Bonding in water molecule, calculations on naphthalene and cyclic conjugated polyenes. Group theoretical selection rules for electronic transitions, infrared spectra and Raman spectra, Electronic spectra of carbonyl chromophore.	25

Teaching-Learning Methodology	We have forged over the last few years traditional and some of the innovative approaches as teaching learning methodologies such as: Direct Instruction; flipped classrooms; classroom discussion; unit based quizzes and assignments; problem solving activities; student presentations; project-based learning; problem-based learning; providing a repository of quality questions on a subject; reevaluation of - quizzes, scripts, assignments, online platforms etc. Self Study: The course coordinator may allot a segment of the syllabus (max-10% of the syllabus or equivalent to maximum 4 lecture hours) as self study by the students.

Evaluation Pattern:

Sr. No.	Details of the Evaluation	Weightage
1.	Internal Written / Practical Examination (As per CBCS R.6.8.3)	15%
2.	Internal Continuous Assessment in the form of Practical, Viva-voce, Quizzes, Seminars, Assignments, Attendance (As per CBCS R.6.8.3)	15%
3.	University Examination	70%

Course Outcomes: Having completed this course, the learner will be able to:

1.	Learn kinetic and mechanistic aspects of complex reactions, opposing reactions, consecutive reactions, parallel reactions, chain reactions, ionic reactions and salt effect, enzyme catalyzed reactions, fast reactions.
2.	Explain the theories for energy transfer among the molecules as they undergo collisions in gas-phase or condensed-phase environments.
3.	Discover group theory based mathematical methods by which aspects of a molecules symmetry can be determined and understood.

4.	Apply group theory and symmetry for predicting the molecular vibrations of Symmetrical molecules, selection rules for electronic transitions, infrared spectra and Raman spectra.

Suggested References:

Sr. No.	References
1.	Elements of Physical Chemistry, Peter Atkins, Julio De Paula, David Smith,(Oxford University Press, 6th Edition)
2.	Chemical Kinetics, K. J. Laidler, (McGrraw Hill Publication)
3.	Chemical Applications of Group Theory, F. A. Cotton, (Wiley Eastern Ltd., Third Edition)
4.	Group Theory and Its Chemical Applications, P. K. Bhattacharya (Himalya Publishing House, Mumbai, Second Revised Edition).
5.	Group theory in Chemistry, M. S. Gopinathan, V. Ramakrishnan (Vishal Publishing Co. Second Edition)
6.	Symmetry and Spectroscopy of Molecules, K. Veera Reddy (New Age International Publishers, Second revised Edition)
7.	Symmetry and Group Theory For Chemists, N. N. Das, (Asian Books Private Limited, New Delhi, First Edition)
8.	Physical Chemistry, Ira N Levine (Tata McGraw-Hill Publishing Company, New Delhi, Fifth Edition).
9.	Physical Chemistry, Alberty and Stilby, (John Wiley & Sons, New York)

On-line resources to be used if available as reference material:

On-line Resources: From time to time there are many Online resources, including web sites, databases, e-books, bibliographies and platforms that offer educational videos, lectures on a range of topics can be suggested or displayed to the students.
Major Web Sites used for chemical education such as: Education, American Chemical Society (ACS);ChemCollective; LearnChemistry; Chemical Education Digital Library (ChemEd DL); The Green Chemistry Education Network (GCEdNet); ACS Examinations Institute; Process Oriented Guided Inquiry Learning (POGIL) Curriculum Materials; Resources for Chemistry Education; NPTEL online resources etc.