Semester	**1**
Programme	**CHEMISTRY**
Course	**MULTIDISCIPLINARY (ABC OF CRITICAL SCIENTIFIC THINKING)**
Paper Code	**M1CH230111T**
Credits	**3 (THEORY: 3)**
Hours/week	**3 (THEORY: 3)**
Category: Core/MDC/SEC/VEC	**MDC**
Theory/Practical/Composite	**THEORY**
Number of Modules	**3**
Syllabus	**Group A** **Module 1: Mathematics for Chemists 1 12 Lecture** 1. Equation of a straight line in different forms, slope and intercept. Graphical interpretation of the X and Y- intercepts. Effect of variation in slope: steepness of a straight line. Area under a straight line by geometric and integration methods. 2. A nonlinear plot. Representation by polynomial function. Curve fitting method. Slope and curvature of the function. Point-wise slope and curvature. Difference from a linear function. 3. Change in origin and how does it affect a function. 4. Exponential and Gaussian function. Discontinuity and continuity at x=0. Asymptote of a function. 5. Sigmoid function and the point of inflection. Generating first and second differential of a function. 6. Equation of circle, parabola, rectangular hyperbola. 7. Optimization of a function. Maximum and minimum condition: pictorial interpretation. 8. Predicting shape of a product function and its optimization. 9. State functions and path functions. Condition of a function to qualify as a state function. 10. Line integral and path integral 11. Total differential and Partial differential. Euler condition, inverse rule, cyclic rule. 12. Differentiation of a polynomial, trigonometric function, exponential function, logarithmic function and product function. 13. Displacement, velocity, acceleration and force in differentiation terms. 14. Newton’s second law as a second order differential equation.

	15. Solution of first and second order differential equation. Example of linear motion, simple harmonic motion. 16. Integration by parts. **Module 2: Mathematics for Chemists 2 12 Lecture** 1. Introduction to standalone graph plotting program like GNUPLOT/grace and wolfram alpha. 2. Introduction to probability: Permutation and Combination. 3. Mathematical modeling of pressure of an ideal gas. Ideal gas laws from the pressure expression. 4. Mathematical modeling of Bohr's atom. 5. Distribution function, their applicability and interpretation. 6. Calculation of average value and most probable value using distribution function: Beta and Gamma function 7. Taylor series expansion and it's interpretation. 8. Lagrange transformation and application. 9. Matrix representation of a vector. Representation matrix of simple (C_3, C_4 and i) symmetry operation. **Group B** **Module 3: Structural and behavioral aspects of molecules** **12 Lecture** ***Electronic effects*** and their influence on acidity-basicity: Inductive effect, field effect, resonance, resonance energy, hyperconjugation, bond polarization and bond polarizability; electromeric effect; steric effect, steric inhibition of resonance. Concept of hybridization, shapes of molecules; orbital pictures of bonding (sp^3, sp^2, sp: C-C, C-N and C-O systems and *s-cis* and *s-trans* geometry for suitable cases). Influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle. Polarity of molecules and dipole moments. ***MO theory:*** Qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about σ, σ^*, π, π^*, n – MOs; basic idea about Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; interpretation of chemical reactivity in terms of FMO interactions; sketch and energy levels of π MOs of (i) acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems) (ii) cyclic p orbital system (neutral systems: [4], [6]-annulenes; charged systems: 3-,4-,5-membered ring systems); Hückel's rules for aromaticity up to [10]-annulene

	(including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram.
Course Overview	**Theory:** 1. Students will be able to apply mathematical tools to tackle common problems in physical chemistry, including solving ordinary and partial differential equations, calculating differentials, solving multiple integrals, operating with vectors, matrices, determinants, and eigenvalue equations. Students will also be able to solve basic chemistry-related mathematical problems using the gnuplot and Wolfram Alpha 2. Student will learn about basic structural and fundamental aspects of molecules.
Course Outcomes	Upon successful completion of this multidisciplinary course, the student will be able to: **CO1 [Geometric & Linear Function Analysis]**: Interpret geometric features of linear, non-linear (polynomial), exponential, Gaussian, and sigmoidal functions; calculate slopes, intercepts, inflection points, asymptotes, and optimize functions using maxima/minima conditions. **CO2 [Conic Sections & Curve Fitting]**: Identify and analyze equations of circle, parabola, and rectangular hyperbola; represent nonlinear data using polynomial functions; apply curve fitting methods to interpret scientific data. **CO3 [Calculus & Differential Equations]**: Perform total and partial differentiation, evaluate Euler's condition, inverse rule, and cyclic rule; differentiate state functions from path functions; solve first and second-order differential equations (linear motion, SHM); evaluate line and path integrals; apply integration by parts. **CO4 [Mathematical Modeling in Physical Chemistry]**: Apply mathematical modeling to derive ideal gas laws from pressure expressions, model Bohr's atomic structure, and interpret displacement, velocity, acceleration, and force using differentiation; apply Newton's second law as differential equations. **CO5 [Probability, Distribution Functions & Series]**: Apply permutation and combination rules, interpret distribution functions (Maxwell-Boltzmann), calculate average and most probable values using Beta and Gamma functions; apply Taylor series expansion; understand Lagrange transformation and its applications. **CO6 [Digital Tools & Matrix Algebra]**: Utilize standalone graph plotting programs (GNUPLOT, Grace, Wolfram Alpha) for mathematical visualization; perform matrix representations of vectors and simple symmetry operations (C_3, C_4, inversion). **CO7 [Electronic Effects & Molecular Polarity]**: Explain fundamental electronic effects (inductive, resonance, field, electromeric, hyperconjugation, steric) and their influence on acidity-basicity, bond polarization, polarizability, and molecular dipole moments.

	CO8 [Hybridization & Bond Properties]: Apply concepts of hybridization (sp^3, sp^2, sp) to predict molecular shapes, orbital pictures of bonding (C-C, C-N, C-O systems), s-cis and s-trans geometry; analyze the influence of hybridization on bond dissociation energy, bond distances, and bond angles. **CO9 [Molecular Orbital Theory]**: Apply qualitative MO theory to construct σ, σ, *π, π*, and n MOs; identify Frontier MOs (HOMO, LUMO, SOMO); sketch and analyze π MO energy levels of acyclic systems (C=C, conjugated diene, triene, allyl, pentadienyl) and cyclic systems ([4], [6]-annulenes, charged 3-, 4-, 5-membered ring systems). **CO10 [Aromaticity & Frost Diagrams]**: Classify organic and heterocyclic molecules as aromatic, anti-aromatic, homoaromatic, or non-aromatic using Hückel's rules (up to [10]-annulene including mononuclear heterocyclic up to 6-membered ring); construct Frost diagrams to rationalize molecular stability.
Program Outcomes	**PO1: Fundamental Knowledge:** Demonstrate a comprehensive understanding of core concepts in chemistry, including organic, inorganic, physical, analytical, and biochemistry. **PO2: Laboratory Skills:** Acquire hands-on experience in laboratory techniques and instrumentation, applying safety protocols and proper methodologies to conduct experiments and analyse results. **PO3: Problem Solving:** Develop critical thinking and problem-solving skills by applying chemical principles to real-world scenarios, including the ability to design experiments and interpret data. **PO4: Research Competency:** Engage in independent and collaborative research projects, employing scientific methods to formulate hypotheses, conduct experiments, and communicate findings effectively. **PO5: Interdisciplinary Applications:** Understand the interdisciplinary nature of chemistry, exploring its applications in fields such as medicine, environmental science, materials science, and nanotechnology. **PO6: Communication Skills:** Effectively communicate scientific information, both verbally and in written form, to diverse audiences, demonstrating the ability to present complex ideas clearly and concisely. **PO7: Ethics and Sustainability:** Recognize the ethical implications and responsibilities of scientific research and practice in chemistry, emphasizing the importance of sustainability and environmental stewardship in chemical practices.

CO #	Core Curriculum Domain	Bloom's Taxonomy (K-Level)	Mapped POs
CO1	Geometric & Linear Function Analysis	**K2 (Understand) K3 (Apply) K4 (Analyze)**	PO3, PO4, PO7
CO2	Conic Sections & Curve Fitting	**K3 (Apply) K4 (Analyze)**	PO3, PO4, PO7
CO3	Calculus & Differential Equations	**K3 (Apply) K4 (Analyze)**	PO3, PO4, PO7
CO4	Mathematical Modeling in	**K3 (Apply) K4 (Analyze)**	PO1, PO3,

	Physical Chemistry		PO4, PO5, PO7
CO5	Probability, Distribution Functions & Series	**K3 (Apply) K4 (Analyze)**	PO3, PO4, PO7
CO6	Digital Tools & Matrix Algebra	**K3 (Apply)**	PO2, PO3, PO4, PO5, PO6, PO7
CO7	Electronic Effects & Molecular Polarity	**K2 (Understand) K4 (Analyze)**	PO1, PO3, PO5
CO8	Hybridization & Bond Properties	**K3 (Apply) K4 (Analyze)**	PO1, PO3, PO5
CO9	Molecular Orbital Theory	**K3 (Apply) K4 (Analyze)**	PO1, PO3, PO5
C10	Aromaticity & Frost Diagrams	**K4 (Analyze) K5 (Evaluate)**	PO1, PO3, PO5

Reading/Reference Lists	1. Calculus made easy by Silvanus P. Thompson 2. Mathematics for Physical Chemistry by Robert G. Mortimer 3. Mathematical Methods for Scientists and Engineers by D. A. McQuarrie 4. Mathematics for Chemists by C. L. Perrin 5. Mathematics for Chemistry Dr. Madhav Ranganathan & Dr. P. P. Thankachan, NPTEL 6. http://mathworld.wolfram.com 7. A Guidebook to Mechanism in Organic Chemistry, P. Sykes, Pearson. 8. Advanced Organic Chemistry, J March, Wiley.
Evaluation	Theory: 50 Internal: 15 (Assessment: 10; Other form of Assessment: 3; Attendance: 2) Semester Exam: 35 (Group A: 20; Group B: 15)
Paper Structure for Theory Semester Exam	Group A: Answer FOUR out of FIVE questions of 5 marks each Group B: Answer THREE out of FOUR questions of 5 marks each