Semester	**1**
Course	**MULTIDISCIPLINARY**
Paper Code	**M1CH230111T**
Paper Title	ABC OF CRITICAL SCIENTIFIC THINKING
No. of Credits	**3**
Theory / Practical / Composite	**Theory**
Minimum No. of preparatory hours per week a student has to devote	3
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.
Learning Outcomes	**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.
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