20CY109 MATHEMATICS AND SYMMETRY FOR CHEMISTRY

Hours Per Week :

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2	1	-	3

Course Description and Objectives:

This course introduces the basic concept Symmetry elements and operations. Also explain the group theory and its applications for various molecules. Moreover, the students able to gain the knowledge on Numbers, Functions, Variables, Integral Calculus and Differential Equations, Special Functions, Matrices and Determinants. Also, able to analyse the mathematical model of Linear systems, Non-linear systems and Curve fittings

Course Outcomes:

The goal of this course is to provide an overview of the concept of mathematics. Upon completion of the course the student will gain the knowledge and able to:

COs	Course Outcomes
1.	Understand the concept of symmetry element, symmetry operation and point groups.
2.	Apply Numbers, Functions and Variables for various applications.
3.	Acquire the basic knowledge of Integral Calculus and Differential Equations.
4.	Apply characteristic equation, eigenvalues and corresponding eigenvectors of a given matrix.
5.	Analyze mathematical models of linear and nonlinear systems.

UNIT - I :

Symmetry of molecules: Symmetry elements and operations, point groups. Matrix representation of symmetry operations-Great Orthogonality Theorem-Character tables. Direct product representations. Projection operators and symmetry adapted linear combinations. Applications.

Unit - II :

Numbers, Functions and Variables :

Real and complex number systems and their properties, Vector Algebra – addition, scalar multiplication, vector products, Limits, Continuity, Differentiation – First and higher order derivatives, Application : Evaluation of Maxima and Minima (of functions of one variable)

Unit - III:

Integral Calculus and Differential Equations:

Integral Calculus: Indefinite and Definite integrals, improper integrals, Methods of integration, Numerical Integration: Trapezoidal Rule, Simpson's Rules

Differential Equations: Ordinary Differential Equations – order, degree, formation, First order equations: Variable Separable, Homogeneous, Non-homogeneous, Exact, Non-exact, Linear, Non-linear equations, Numerical Methods – Runge-Kutta method, Predictor and Corrector methods.

Unit - IV :

Matrices and Determinants :

Matrices, Determinants, Rank, Inverse, Eigen Values and Eigen Vectors, Orthogonal transformations

Unit - V :

Linear Systems and Curve fitting :

Solutions of Linear Systems – Cramer's rule, Gaussian elimination, Gauss-Jordan elimination, Gauss-Siedel method, Jacobi method, Relaxation method. Curve fitting – Least Squares method, Straight line fitting, Parabola fitting

Text Books:

1. Molecular Symmetry and Group Theory. Allan Vincent, John Wiley & Sons, LTD.
2. Symmetry: An introduction to group theory and its applications. R. McWeeny, Dover Publications, Inc.
3. Chemical Applications of Group Theory. F. A. Cotton, John Wiley & Sons, Inc.
4. Mathematics for Physical Chemistry. R. G. Mortimer, Academic Press.
5. Mathematics for Chemistry and Physics. G. Turrell, Academic Press.
6. Advanced Engineering Mathematics. E. Kreyszig, Wiley.

Reference Books

1. Symmetry and Structure. S. F. A. Kettle, Wiley.
2. Numerical Analysis: A Practical Approach. Melvin J. Maron, Macmillan Publishinh Co., Inc. NY & Collier Macmillan Publishers, London.