

## Approval: 8<sup>th</sup> Senate Meeting

**Course Name:** Mathematics for Chemist

**Course Number:** CY521

**Credits:** 3-0-0-3

**Prerequisites:** None

**Intended for:** UG/PG

**Distribution:** Elective

**Semester:** Odd/Even

**Course Preamble:** The course forms an elective course for the M. Sc. (Chemistry) degree program. The aim of the course is to give the techniques and skills of mathematics to students to be prepared for their advanced classes of quantum chemistry, molecular simulation, group theory etc. Especially for the students of Physical Chemistry and certain branch of inorganic chemistry, the knowledge of mathematics is essential to understand and interpret scientific data and mathematical expressions.

**Course Outline:** This course will cover the topics of Linear Algebra, Differential and Integral calculus, Analytical Geometry and data Analysis. This course is the pre-requisite course for quantum chemistry and group theory. The mathematical course content will be taught in conjunction with the advanced concept of physical chemistry outlined here as applications.

### **Modules:**

#### **Module 1: Linear Algebra [14 Lectures]**

Scalars and Vectors: vector, a summary of vectors and representation of 3-D co-ordinates, Vector Products, Vector Spaces, orthonormal basis set, vector functions, differentiation and integration of vector functions, gradient, divergence and Curl, line integral, Surface integral, volume integrals, Linear independence, basis, curvilinear coordinates, Laplacian, Greens theorem, Stokes theorem, Tensors

Matrix Algebra: Matrix and determinants, Rank, Matrix Algebra, diagonalization, Matrix property, Matrix functions, Eigen values, Eigen vectors,

Applications: Visualization in quantum chemistry, Symmetry and group theory, Spectroscopy

#### **Module 2: Calculus [14 Lectures]**

Functions, Variables, Bessel functions, basic rules of differentiation, maxima and minima, exact and inexact differential, partial differentiation (limits), rules of integration, definite and indefinite integrals, first and second order differential equations, linear homogeneous/inhomogeneous equations, general solution and particular solution, polynomials, Taylor and McLaurin series, Fourier series and Fourier transforms, power series method

Calculus of Several Variables: Functions of More Than One Variable, An Introduction to Partial Derivatives, Differentiability and the Gradient, The Chain Rule, Derivatives of Integrals, The Total Differential, the method of Lagrange Multipliers, multiple integrals

Applications: Kinetics, Quantum Chemistry, thermodynamics

Special Functions: integral functions, interpolation, delta function

### **Module 3: Analytical geometry and Data Analysis [14 Lectures]**

Analytical geometry: Properties of different graphs and plotting of them, understanding of any kind of scientific equation- plotting of them and interpreting the physical significance of the plot. Relevant especially for thermodynamic, kinetic and radioactive study, general application in all fields of chemistry

Data Analysis: Data Plotting, least square fitting, concept of floating points, interpolation, asymptotic analysis, error analysis, random numbers, correlations.

#### **Text books:**

1. Mathematics for Physical Chemists –R.G.Mortimer, Academic Press, 10<sup>th</sup> Jun2005, ISBN :9780080492889
2. Mathematics for Chemists, Charles L. Perrin, Wiley-Inter science, New York 1970.
3. Mathematical Methods for Scientists and Engineers Donald A. McQuarrie, University Science Books (May 2003)

#### **References Books:**

1. The Chemical Maths Book, E. Steiner, Oxford University Press, 2 edition (31 January 2008)
2. Maths for Chemists, Volumes 1 and 2, Martin C. R. Cockett and Graham Doggett, Royal Society of Chemistry , Cambridge Press (2003)