Course Type	Course Code	Name of Course	L	T	P	Credit
DE	NCYD533	Mathematics for Chemists	3	0	0	3

Course Objective
• Revision of the mathematical concepts of complex number, vectors and tensors to chemical systems by solving eigen value and eigenvector problems. Solving first and second order differential equations that are used for solving elementary model problems in physical chemistry; quantum mechanics (e.g., particle in a potential-free box, particle on a ring, harmonic oscillator, etc.) as well spectroscopy, thermodynamics, statistical thermodynamics, and kinetics. Developing advanced mathematical skills (series solutions, numerical analysis) which are used in computational chemistry and spectroscopy.
Learning Outcomes
• At the end of the course, the learners should be able to: • Use mathematical techniques in linear algebra for eigen values and eigenvectors and first and second order differential equations with series solutions not only in quantum chemistry and spectroscopy but in other areas of physical and theoretical chemistry that will be offered during the whole programme. • The students should be able to solve all the model problems in physical chemistry (quantum mechanics, statistical thermodynamics, kinetics, spectroscopy, etc.) for which exact analytical methods and solutions are available. Using the solutions to analyse the basis behind the philosophy of the method developments and also the limitation of each methods if any.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Error Analysis: Error, precision, accuracy, significant figures, mean, standard deviation, propagation of errors. Complex Number: Modulus and Conjugate, Argand Plane and Polar representation. Vectors: Dot product, cross product, gradient, divergence, continuity equation, curl. Vector integration: Stokes' and Gauss' theorems. Determinants and Matrices: coordinate transformation, Jacobian, system of linear equations, inverse of a matrix, Cramer's rule, Gaussian elimination and its variants, eigenvalues and eigenvectors.	13L	A brief discussion of solutions of quadratic equations and errors, followed by loss of determinism and its solutions. In-depth discussion of the complex number, vector, and matrices and how to use all of these to represent and solve quantum mechanics, statistical, and spectroscopic problems.
2	Differential Equations: General and particular solutions of a differential equation. Partial Differential equations.First order equations and their applications. Separation of variables, equations reducible to separable form. Exact differential equations, non-homogeneous differential equations,	15L	Comprehensive discussions on various methods to solve different types of differential equations that are commonly used in physical chemistry problems. Learn how to use special functions to solve quantum mechanics and spectroscopic problems.

	integrating factors. Second order linear differential equations: homogeneous with constant coefficients, characteristic equation, general solution, particular solution. Special functions such as Lagrange, Legendre and Hermite polynomials.		
3	Fourier series and transform, basic theorems, convolution. Laplace transform and its properties, Applications of Fourier and Laplace transforms. Introduction to Numerical Methods: Numerical differentiation and interpolation, Newton-Raphson method, Numerov Method, Numerical solution of differential equations.	14L	This module emphasizes the integral transform of various differential equations. Discussion on how to solve differential equations using numerical methods.
TOTAL		**42**	

Text Books:

1. Mathematical Methods for Physicists, G. B. Arfken and H.J. Weber, Academic Press (2001).
2. Mathematical Methods in the Physical Sciences, M. L. Boas, John Wiley, India (2007).

Reference Books:

1. Mathematics for Physical Chemistry, Robert G. Mortimer, 3rd Edition, Academic Press (2005).
2. Advanced Engineering Mathematics, E. Kreyszig, John Wiley, New York (1999).