DISCIPINE SPECIFIC ELECTIVES-IV (DSE-III)

Title: Mathematical Methods in Chemistry (DSE -III, Semester-VII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the Course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Mathematical Methods in Chemistry (DSE -III, Semester-VII, 30 Lectures)	04	02	---	02	Class 12th with Physics, Chemistry, Mathematics	---

Course Objectives:

- To build a working knowledge of essential mathematical tools used in physical chemistry.
- To develop confidence in applying calculus, algebra, and probability in thermodynamics, kinetics, and spectroscopy.
- To illustrate concepts with examples relevant to chemical phenomena.

Learning outcomes: After completing the course, the student will be able to:

- Use vector and matrix operations to solve chemical problems (e.g., molecular orbitals, symmetry).
- Understand and apply vector calculus to thermodynamic and electrostatic systems.
- Solve differential and integral problems relevant to kinetics and quantum chemistry.
- Apply probability and curve-fitting concepts to experimental data analysis.
- Understand the role of eigenvalues and coordinate transformations in physical chemistry models.

Course Contents (Theory): **Credit: 2 (30 Lectures)**

Unit I: Vectors and Matrix Algebra (10 lectures)

Vectors: Dot, cross, and triple products

Vector calculus: Gradient, divergence, and curl.

Integral theorems: Gauss' and Stokes' theorem (physical interpretation only).

Matrices: Types (square, diagonal, identity), operations (addition, multiplication, transpose), Inverse and adjoint.

Special matrices: Symmetric, skew–symmetric, Hermitian, skew- Hermitian, unitary-properties and physical relevance (e.g., Hermitian in quantum mechanics).

Determinants: Evaluation (2x2, 3x3 only), properties, Cramer's rule.

Eigenvalues and eigenvectors: Definition and physical meaning, Diagonalization with examples from Hückel theory and moment of inertia tensor.

Second-rank tensors (conceptual only): Brief mention of how second-rank tensors like polarizability and magnetic susceptibility help describe molecular properties.

Unit II: Differential and Integral Calculus (8 lectures)

Functions, continuity and differentiability, rules for differentiation. Exact and inexact differentials with their applications to thermodynamic properties.

Differentiation and chemical applications, including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution, etc).

Partial differentiation, coordinate transformations (for example, cartesian to spherical polar).

Basic rules for integration, integration by parts, substitution, partial fractions and substitution, reduction formulae. Applications of integral calculus.

Curve sketching and thermodynamic functions.

Unit III: Differential Equations (7 lectures)

First order differential equations: separable, linear, exact.

Applications to rate laws and chemical equilibrium.

Second-order differential equations: harmonic oscillator, Legendre equation (qualitative)

Introduction to Fourier series and boundary value problems (qualitative).

Examples from quantum chemistry (H-atom, angular momentum)

Unit IV: Probability, Statistics, and Curve Fitting (5 lectures)

Permutations and combinations

Probability distributions, RMS, mean, most probable values (Maxwell-Boltzmann distribution).

Error analysis in chemical experiments (standard deviation, RMS error)

Least squares fitting, polynomial trendlines (chemical data)

Recommended Texts/References:

1. Martin C. R. Cockett and Graham Doggett, Math for Chemist: Volume 1&2, Royal Society of Chemistry, Thomas Graham House, Cambridge, UK, 2003.
2. Robert G. Mortimer, Mathematics for Physical Chemistry, Elsevier

Supplementary Reading

1. McQuarrie, D. A., Mathematical methods for scientists and engineers, University Science Books, 2003.
2. Arfken, G., Weber, H., and Harris, F., Mathematical methods for physicists, Academic Press, 7th Ed., 2012.
3. Boas, M. L., Mathematical methods for the physical sciences, Kaye Pace, 3rd Ed., 2006.

Laboratory Exercises (Practical)/Tutorials: **Credit: 2**

1. Least-squares fit: Linear regression for absorbance vs. concentration data.
2. Matrix multiplication: Three-matrix multiplication, Group theory example.
3. Diagonalization: Secular determinant from Hückel Theory
4. Error analysis: Calculate SD, RMS error, correlation from experimental data.
5. Differential calculus: Maxima/minima problems (e.g., Boltzmann populations).
6. Integral calculus: Evaluation of thermodynamic integrals (e.g., partition functions).
7. Differential Solve and interpret rate equations, harmonic oscillator.
8. Curve fitting: Polynomial fit using spreadsheet or Python (optional).

Recommended Texts/References:

1. Cockett & Doggett, *Maths for Chemists*, Vols 1 & 2 (Royal Society of Chemistry)
2. Robert G. Mortimer, *Mathematics for Physical Chemistry*
3. McQuarrie & Simon, *Physical Chemistry: A Molecular Approach* (selected examples)
4. Excel or Google Sheets for plotting; Python (optional)

DISCIPLINE SPECIFIC ELECTIVE COURSE-IV (DSE-IV):

Title: Interfacial Electrochemistry (DSE-IV, Semester-VIII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Interfacial Electrochemistry (DSE-IV, Semester-VIII, 30 Lectures)	04	02	---	02	Class 12th with	---