Paper-V CHN-404 B
Mathematics for Chemists

I Vectors and Matrix Algebra — 10 Hrs

A *Vectors*

Vectors, dot, cross and triple products etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem etc.

B. *Matrix Algebra*

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, skew-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence.

Introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants (examples from Hückel theory).

Introduction to tensors; polarizability and magnetic susceptibility as examples.

II Differential Calculus — 10 Hrs

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc), exact and inexact differentials with their applications to thermodynamic properties.

Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. Reduction formulae, applications of integral calculus.

Functions of several variables, partial differentiation, co-ordinate transformations (e.g. cartesian to spherical polar), curve sketching.

III Elementary Differential Equations — 7 Hrs

Variables-separable and exact first-order differential equations, homogeneous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. Solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and Legendre equation etc., spherical harmonics, second order differential equations and their solutions.

IV Permutation and Probability — 3 Hrs

Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples from the kinetic theory of gases etc., curve fitting (including least squares fit etc.) with a general polynomial fit.