

MATHEMATICS AND NUMERICAL TECHNIQUES FOR CHEMISTS (CY515)

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✓ Contents

- ⊗ Ordinary and Partial Differential equations and Special functions
- ⊗ Fourier and Laplace transforms
- ⊗ Matrix Methods: Orthogonal and Unitary matrices, Diagonalization, Eigenvalues and Eigenvectors, Roots of equations, Algorithms for Matrix inversion and diagonalization
- ⊗ Group theory and representations of symmetry operations by Matrices, Character tables
- ⊗ Numerical methods: Errors in data, Distribution of errors, Central limit theorem
- ⊗ Power series and conversions, Interpolation and curve fitting
- ⊗ Use of computer software for Numerical Methods

✓ Grading

Midsem I	20 points
Midsem II	20 points
Endsem	50 points
Assignments	10 points
Total	100 points

- ⊗ Present your assignments clearly and they have to be detailed enough. Assignment submission dates are non-negotiable.
- ⊗ Assignment problems are NOT an exhaustive list of problems. One should be doing more problems in addition to the assignment problems. Refer standard books.

✓ Text Book

- ⊗ *Advanced Engineering Mathematics*, E. Kreyszig, Wiley, 9th Edition (2011).

✓ Reference Books

- ⊗ *Chemical Applications of Group Theory*, F. A. Cotton, Wiley India Private Limited, 3rd edition (2008).
- ⊗ *A Practical Guide to Data Analysis for Physical Science Students*, L. Lyons, Cambridge University Press (1991).
- ⊗ *Mathematics for Science Students*, L. Lyons, Cambridge University Press (2005).
- ⊗ *Mathematical Methods for Physicists*, G. B. Arfken, H. J. Weber, and F. E. Harris, Elsevier, 7th edition (2012).

□ *A Chemist who does not know mathematics is seriously handicapped*

— Irving Langmuir

□ *In so far as Quantum Mechanics is correct, chemical questions are problems in applied mathematics*

— Henry Eyring