

Mathematics for Chemistry - Video course

COURSE OUTLINE

This course will cover the standard mathematical techniques that are typically used by Chemists. In addition to illustration of the basic mathematical techniques, this course will showcase a large number of applications, typically used by Chemists.

The topics covered will include Linear Algebra, Ordinary Differential Equations, Partial Differential Equations, Integral Transforms, Group Theory, Data Analysis and Numerical Methods.

COURSE DETAIL

Module No.	Topic/s	Lectures
1	Scalars and Vectors: Scalars, Vectors, Vector Products, Vector Spaces, linear independence, basis, curvilinear coordinates, Tensors. Applications: Two body problem, Center of Mass and Relative coordinates.	4
2	Vector Integration and Differentiation: Gradient, Divergence and Curl, Line Integrals, Surface integrals, volume integrals, Greens theorem, Stokes Theorem. Applications: Force, Work and Potentials. Path integrals.	4
3	Matrix Algebra: Matrices, Rank, Determinants, Eigenvalues, Eigenvectors, System of Equations. Applications: Slater Determinants, Huckel MO theory.	4
4	1st order ODEs: Differential Equations of 1st order. Separation of variables, integrating factor, exact differentials, system of ODEs. Applications: Reaction rates.	4
5	2nd order differential equations: 2nd order differential equations with constant coefficients, general solution, particular solution, power series method. Applications: Angular Momentum Eigenfunctions for a single particle.	4
6	Integral Transforms: Sturm-Liouville problem, basis functions, Fourier and Laplace transforms, dirac-delta functions. Applications: Power spectrum, momentum and position basis.	4
7	Group Theory Basics: Group, subgroup, group	4



NP-TEL

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<http://nptel.iitm.ac.in>

Chemistry and Biochemistry

Pre-requisites:

- Basic linear algebra- scalars, vectors, matrices.
- Integration, Differentiation, BSc level Chemistry
- Complex variables

Additional Reading:

Mathematical Methods in Physical Sciences: Mary L. Boas

Hyperlinks:

- <http://www.mathworks.com/matlab>
- <http://mathworld.wolfram.com/>

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	multiplication table, symmetry operations, Great Orthogonality Theorem, Character Tables. Applications: This section is done with illustration of actual calculations.	
8	Symmetry adapted linear combinations, molecular motions, selection rules. Applications: This section is done with illustration of actual calculations.	4
9	Data Analysis, Interpolation, least square fitting, asymptotic analysis, error estimates, random numbers, correlations. Applications: Fluctuations, noise, signal processing, scattering experiments.	4
10	Numerical Methods: Taylor series, numerical differentiation and integration, matrix diagonalization methods. Applications: Perturbation method for radiation-matter interaction	4

References:

1. Mathematical Methods for Physicists: Arfken and Weber
2. Engineering Mathematics: EL Kreyszig
3. Chemical Applications of Group Theory: FA Cotton