

CHEM 224

Math for Chemists

Introduction:

Description – This course introduces and reinforces mathematical methods needed to understand quantum chemistry, spectroscopy, thermodynamics, kinetics, etc. Subjects covered include: introduction to complex numbers; calculus; differential equations; vector spaces and vector algebra; matrices and determinants. Throughout the course an effort is made to illustrate mathematical concepts with chemical problems.

Course learning objectives – You will learn to work with the mathematical tools necessary to manipulate a thermodynamic equation of state, understand the vibration of a diatomic molecule, apply Hückel molecular orbital theory to small molecules, for example.

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Office hours: TBD and by appointment.

Teaching Assistant: Jikai Zhu will be leading tutorials and marking assignments.

Course material:

Required Text: Mathematical Methods for Molecular Science: Theory and Applications, Visualizations and Narrative. John Straub

Outline

Complex Numbers and Functions

- complex numbers and arithmetic, functions of complex variables

Topics from Calculus

- derivatives, chain rule, implicit functions, Leibnitz rule
- partial differentiation, total differentials, exact and inexact differentials
- integrals and integration

Differential Equations

- definitions, simple solution methods
- boundary conditions and eigenvalues
- solution by series
- partial differential equations and separation of variables

Vectors, Vector Spaces and Vector Algebra

- geometric vectors
- vector spaces, inner products
- functions as vectors and orthogonality
- Fourier series

Operators and Matrices

- matrix algebra
- determinants
- linear equations
- matrix eigenvalue problems

Numerical Methods (if there is time)

Assessment: Final Exam (50%), a Midterm test (30%), two quizzes (10%) and two homework assignments (10%).

