



# Mathematical Methods for Physical and Analytical Chemistry

By David Z. Goodson

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*Mathematical Methods for Physical and Analytical Chemistry* presents mathematical and statistical methods to students of chemistry at the intermediate, post-calculus level. The content includes a review of general calculus; a review of numerical techniques often omitted from calculus courses, such as cubic splines and Newton's method; a detailed treatment of statistical methods for experimental data analysis; complex numbers; extrapolation; linear algebra; and differential equations. With numerous example problems and helpful anecdotes, this text gives chemistry students the mathematical knowledge they need to understand the analytical and physical chemistry professional literature.

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## **Editorial Review**

### Review

“Finally it can be said that this book helps to refresh and extend the knowledge about mathematical and statistical methods to be used for physico-chemical or analytical applications.” (*Materials and Corrosion*, 1 November 2012)

### From the Back Cover

#### **Bridging the gap between undergraduate calculus and the mathematics of chemistry**

A focused presentation of statistical and advanced mathematical methods likely to be encountered by chemists, *Mathematical Methods for Physical and Analytical Chemistry* can serve as a text for a one-semester course at the undergraduate or graduate level, or as a resource for independent study by students and professionals in all areas of chemistry and in related fields such as environmental science, geochemistry, and chemical engineering.

*Mathematical Methods for Physical and Analytical Chemistry* covers:

**CALCULUS**—review of the basics, coordinate systems, degrees of freedom, special functions, numerical methods, complex numbers, singular points, improper integrals, Taylor series

**STATISTICS**—probability theory, distribution functions, confidence intervals, propagation of error, significance of difference, ANOVA, method of least squares, calibration, model testing, fits with error in both variables, experiment design, randomization, optimization

**DIFFERENTIAL EQUATIONS**—chemical reaction rate equations, Lagrangian and Hamiltonian mechanics, transport equations, the superposition principle, separation of variables, methods for exact, approximate, and numerical solutions

**LINEAR ALGEBRA**—groups, Hilbert spaces, basis sets, matrices, determinants, orthogonal polynomials, spherical harmonics, Fourier series, eigenvalue equations, diagonalization, Fourier transform, spectral lineshapes, convolution, principles of quantum mechanics, Schrödinger's equation, hydrogen orbitals, hybrid orbitals, molecular orbitals

*Mathematical Methods for Physical and Analytical Chemistry* features:

- Modern topics such as Monte Carlo simulation, robust estimation, and discrete Fourier transform, which are otherwise available only in more specialized texts
- Numerous figures and worked out examples and more than 200 exercises, many of which take advantage of computer algebra

- An annotated bibliography of references for further study

#### About the Author

**David Z. Goodson**, Associate Professor of Chemistry at the University of Massachusetts Dartmouth, has a BA in chemistry from Pomona College and a PhD in chemical physics from Harvard University. An interdisciplinary scientist, he is author of numerous articles on a wide range of topics including quantum chemistry, molecular spectroscopy, reaction rate theory, atomic physics, and applied mathematics.

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