

1. Record Nr.	UNINA9911019825003321
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Titolo	Computational chemistry using the PC // Donald W. Rogers
Pubbl/distr/stampa	Hoboken, N.J., : Wiley-Interscience, c2003
ISBN	9786610344727 9781280344725 1280344725 9780470236642 0470236647 9780471474913 0471474916 9780471474906 0471474908
Edizione	[3rd ed.]
Descrizione fisica	1 online resource (371 p.)
Disciplina	541.2/2/02855365
Soggetti	Chemistry - Data processing Chemistry - Mathematics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes bibliographic references (p. 333-338) and index.
Nota di contenuto	Computational Chemistry Using the PC Third Edition; Contents; Preface to the Third Edition; Preface to the Second Edition; Preface to the First Edition; Chapter 1. Iterative Methods; Iterative Methods; An Iterative Algorithm; Blackbody Radiation; Radiation Density; Wien's Law; The Planck Radiation Law; COMPUTER PROJECT 1-1 Wien's Law; COMPUTER PROJECT 1-2 Roots of the Secular Determinant; The Newton-Raphson Method; Problems; Numerical Integration; Simpson's Rule; Efficiency and Machine Considerations; Elements of Single-Variable Statistics; The Gaussian Distribution COMPUTER PROJECT 1-3 Medical Statistics Molecular Speeds; COMPUTER PROJECT 1-4 Maxwell-Boltzmann Distribution Laws; COMPUTER PROJECT 1-5 Elementary Quantum Mechanics; COMPUTER PROJECT 1-6 Numerical Integration of Experimental Data Sets; Problems; Chapter 2. Applications of Matrix Algebra; Matrix Addition;

Matrix Multiplication; Division of Matrices; Powers and Roots of Matrices; Matrix Polynomials; The Least Equation; Importance of Rank; Importance of the Least Equation; Special Matrices; The Transformation Matrix; Complex Matrices; What's Going On Here?; Problems
Linear Nonhomogeneous Simultaneous Equations Algorithms; Matrix Inversion and Diagonalization; COMPUTER PROJECT 2-1 | Simultaneous Spectrophotometric Analysis; COMPUTER PROJECT 2-2 | Gauss-Seidel Iteration: Mass Spectroscopy; COMPUTER PROJECT 2-3 | Bond Enthalpies of Hydrocarbons; Problems; Chapter 3. Curve Fitting; Information Loss; The Method of Least Squares; Least Squares Minimization; Linear Functions Passing Through the Origin; Linear Functions Not Passing Through the Origin; Quadratic Functions; Polynomials of Higher Degree; Statistical Criteria for Curve Fitting Reliability of Fitted Parameters COMPUTER PROJECT 3-1 | Linear Curve Fitting: KF Solvation; COMPUTER PROJECT 3-2 | The Boltzmann Constant; COMPUTER PROJECT 3-3 | The Ionization Energy of Hydrogen; Reliability of Fitted Polynomial Parameters; COMPUTER PROJECT 3-4 | The Partial Molal Volume of ZnCl₂; Problems; Multivariate Least Squares Analysis; Error Analysis; COMPUTER PROJECT 3-5 | Calibration Surfaces Not Passing Through the Origin; COMPUTER PROJECT 3-6 | Bond Energies of Hydrocarbons; COMPUTER PROJECT 3-7 | Expanding the Basis Set; Problems; Chapter 4. Molecular Mechanics: Basic Theory
The Harmonic Oscillator The Two-Mass Problem; Polyatomic Molecules; Molecular Mechanics; Ethylene: A Trial Run; The Geo File; The Output File; TINKER; COMPUTER PROJECT 4-1 | The Geometry of Small Molecules; The GUI Interface; Parameterization; The Energy Equation; Sums in the Energy Equation: Modes of Motion; COMPUTER PROJECT 4-2 | The MM3 Parameter Set; COMPUTER PROJECT 4-3 | The Butane Conformational Mix; Cross Terms; Problems; Chapter 5. Molecular Mechanics II: Applications; Coupling; Normal Coordinates; Normal Modes of Motion; An Introduction to Matrix Formalism for Two Masses The Hessian Matrix

Sommario/riassunto

Computational Chemistry Using the PC, Third Edition takes the reader from a basic mathematical foundation to beginning research-level calculations, avoiding expensive or elaborate software in favor of PC applications. Geared towards an advanced undergraduate or introductory graduate course, this Third Edition has revised and expanded coverage of molecular mechanics, molecular orbital theory, molecular quantum chemistry, and semi-empirical and ab initio molecular orbital approaches. With significant changes made to adjust for improved technology and increased computer literacy, Computational
