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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
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 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