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Nota di contenuto	CONTENTS; PREFACE; ACKNOWLEDGMENTS; SYMBOLS USED IN THIS BOOK; 1. Introduction; 1.1 Models, Approximations, and Reality; 1.2 How Computational Chemistry Is Used; Bibliography; Part I. BASIC TOPICS; 2. Fundamental Principles; 2.1 Energy; 2.2 Electrostatics; 2.3 Atomic Units; 2.4 Thermodynamics; 2.5 Quantum Mechanics; 2.6 Statistical Mechanics; Bibliography; 3. Ab initio Methods; 3.1 Hartree-Fock Approximation; 3.2 Correlation; 3.3 Moller-Plesset Perturbation Theory; 3.4 Configuration Interaction; 3.5 Multi-configurational Self-consistent Field; 3.6 Multi-reference Configuration Interaction 3.7 Coupled Cluster3.8 Quantum Monte Carlo Methods; 3.9 Natural Orbitals; 3.10 Conclusions; Bibliography; 4. Semiempirical Methods; 4.1 Huckel; 4.2 Extended Huckel; 4.3 PPP; 4.4 CNDO; 4.5 MINDO; 4.6 MNDO; 4.7 INDO; 4.8 ZINDO; 4.9 SINDO1; 4.10 PRDDO; 4.11 AMI; 4.12 PM3; 4.13 PM3/TM; 4.14 Fenske-Hall Method; 4.15 TNDO; 4.16 SAM1; 4.17 Gaussian Theory; 4.18 Recommendations; Bibliography; 5. Density Functional Theory; 5.1 Basic Theory; 5.2 Linear Scaling Techniques; 5.3

Practical Considerations; 5.4 Recommendations; Bibliography; 6. Molecular Mechanics; 6.1 Basic Theory; 6.2 Existing Force Fields
6.3 Practical Considerations6.4 Recommendations; Bibliography; 7. Molecular Dynamics and Monte Carlo Simulations; 7.1 Molecular Dynamics; 7.2 Monte Carlo Simulations; 7.3 Simulation of Molecules; 7.4 Simulation of Liquids; 7.5 Practical Considerations; Bibliography; 8. Predicting Molecular Geometry; 8.1 Specifying Molecular Geometry; 8.2 Building the Geometry; 8.3 Coordinate Space for Optimization; 8.4 Optimization Algorithm; 8.5 Level of Theory; 8.6 Recommendations; Bibliography; 9. Constructing a Z-Matrix; 9.1 Z-Matrix for a Diatomic Molecule; 9.2 Z-Matrix for a Polyatomic Molecule
9.3 Linear Molecules9.4 Ring Systems; Bibliography; 10. Using Existing Basis Sets; 10.1 Contraction Schemes; 10.2 Notation; 10.3 Treating Core Electrons; 10.4 Common Basis Sets; 10.5 Studies Comparing Results; Bibliography; 11. Molecular Vibrations; 11.1 Harmonic Oscillator Approximation; 11.2 Anharmonic Frequencies; 11.3 Peak Intensities; 11.4 Zero-point Energies and Thermodynamic Corrections; 11.5 Recommendations; Bibliography; 12. Population Analysis; 12.1 Mulliken Population Analysis; 12.2 Lowdin Population Analysis; 12.3 Natural Bond-Order Analysis; 12.4 Atoms in Molecules
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14. The Importance of Symmetry

Sommario/riassunto

A practical, easily accessible guide for bench-top chemists, this book focuses on accurately applying computational chemistry techniques to everyday chemistry problems.Provides nonmathematical explanations of advanced topics in computational chemistry.Focuses on when and how to apply different computational techniques.Addresses computational chemistry connections to biochemical systems and polymers.Provides a prioritized list of methods for attacking difficult computational chemistry problems, and compares advantages and disadvantages of various approximation techniques.<li