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2. Record Nr.	UNINA9911019196703321
Autore	Young David C. <1964->
Titolo	Computational chemistry : a practical guide for applying techniques to real-world problems // David C. Young
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Descrizione fisica	1 online resource (408 p.)
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Soggetti	Chemistry - Computer simulation Chemistry - Data processing Chemistry - Mathematics

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Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes glossary.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	<p>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 Cluster 3.8 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 Considerations 6.4 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 Molecules 9.4 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 12.5 Electrostatic Charges 12.6 Charges from Structure Only; 12.7 Recommendations; Bibliography; 13. Other Chemical Properties; 13.1 Methods for Computing Properties; 13.2 Multipole Moments; 13.3 Fermi Contact Density; 13.4 Electronic Spatial Extent and Molecular Volume; 13.5 Electron Affinity and Ionization Potential; 13.6 Hyperfine Coupling; 13.7 Dielectric Constant; 13.8 Optical Activity; 13.9 Biological Activity; 13.10 Boiling Point and Melting Point; 13.11 Surface Tension; 13.12 Vapor Pressure; 13.13 Solubility; 13.14 Diffusivity; 13.15 Visualization; 13.16 Conclusions; Bibliography 14. The Importance of Symmetry</p>
Sommario/riassunto	<p>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</p>

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.
