1. Record Nr. UNINA9910830176203321

Autore	Young David C. <1964->
Titolo	Computational chemistry [[electronic resource]] : a practical guide for applying techniques to real-world problems / / David C. Young
Pubbl/distr/stampa	New York, : Wiley, c2001
ISBN	1-280-54168-7 9786610541683 0-470-88008-2 0-471-45843-0 0-471-22065-5
Descrizione fisica	1 online resource (408 p.)
Disciplina	542.85 542/.85
Soggetti	Chemistry - Computer simulation Chemistry - Data processing Chemistry - Mathematics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes glossary.
Nota di bibliografia	Includes bibliographical references and index.
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
12.5 Electrostatic Charges12.6 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

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

2.

Record Nr.	UNISANNIORAV0181788
Autore	Butler, Barry Conrad Milne
Titolo	Lettura e interpretazione delle carte geologiche / B.C.M. Butler, J.D. Bell ; edizione italiana a cura di Elvidio Lupia Palmieri e Maurizio Parotto
Pubbl/distr/stampa	Bologna, : Zanichelli, 1991
Titolo uniforme	Interpretation of geological maps.
ISBN	8808120341
Descrizione fisica	XIII, 307 p., \6! c. di tav. : ill. ; 25 cm
Altri autori (Persone)	Bell, John David
Disciplina	526 550 550.223 551.8
Soggetti	Carte geologiche
Collocazione	04-LT 526 BUT le0104-LT 526 BUT le
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Trad. di Paola Fredi Seguono appendici.

3. Record Nr. UNINA9910134010303321

Autore	Baldi Bernardino <1553-1617, >
Titolo	In mechanica Aristotelis problemata exercitationes
Pubbl/distr/stampa	Edition Open Access, 2011 [Place of publication not identified], : epubli GmbH, 2011
Descrizione fisica	1 online resource (273 p.)
Collana	Sources 4 (Italian version of Sources 3): Max Planck Research Library for the History and Development of Knowledge
Soggetti	Engineering & Applied Sciences Applied Mathematics
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Sommario/riassunto	_In mechanica Aristotelis problemata exercitationes_, scritte da Bernardino Baldi, vengono ristampate – provviste d'introduzione e commento – come quarto volume della collana _Sources_ della _Max Planck Research Library for the History and Development of Knowledge_, la versione Italiana di _Sources 3_. Il volume è disponibile in internet senza limitazioni d'accesso anche come pubblicazione elettronica _open-access_ all'indirizzo www.edition-open-access.de. Il testo venne pubblicato nel 1621, quattro anni dopo la morte dell' autore. Questo libro appartiene alla lunga tradizione rinascimentale concernente lo studio dei _Problemi Meccanici_ pseudo-aristotelici. A differenza della maggior parte delle altre opere scritte durante il XVI secolo, tuttavia, il testo di Baldi esprime una posizione critica nei confronti dell'approccio teorico presente nelle meccaniche pseudo-aristoteliche. Il testo delle _Exercitationes_ mostra una sistematica applicazione dei principi archimedei alla spiegazione delle questioni discusse nei _Problemi Meccanici_ e, dunque, illustra chiaramente la struttura a forma di patchwork della meccanica preclassica. Il testo, inoltre, presenta lunghe digressioni che ampliano considerevolmente i confini della meccanica. The _Exercitationes_ were first published in 1621, four years after the death of the author. The work belongs to the

long tradition of studies on the pseudo-Aristotelian _Mechanical Problems_ developed during the Renaissance but, unlike most other works written during the sixteenth century, it takes a critical position against the theoretical approach of the pseudo-Aristotelian text. The _Exercitationes_ display a systematic application of Archimedean principles to the explanation of the questions discussed in _Mechanical Problems_ illustrating the patchwork character of preclassical mechanics. Moreover, Baldi's work presents lengthy digressions that considerably widen the boundaries of mechanics.