1. Record Nr. UNINA9910143987903321

Titolo	Reviews in computational chemistry . V / / edited by Kenny B. Lipkowitz and Donald B. Boyd
Pubbl/distr/stampa	New York, : Wiley-VCH, 1994
ISBN	1-282-30818-1 9786612308185 0-470-12582-9 0-470-12609-4
Descrizione fisica	1 online resource (482 p.)
Collana	Reviews in computational chemistry ; ; 5
Altri autori (Persone)	LipkowitzKenny B BoydDonald B
Disciplina	542.85 542/.8
Soggetti	Chemistry - Data processing Chemistry - Mathematics Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	Reviews in Computational Chemistry V; Contents; The Development of Computational Chemistry in the United States; Introduction; Beginnings; Stored Program Digital Computers; The Introduction of Computers to Chemistry; The Development of Model-Based Computationally Intensive Methods; Expansion and Extension; Number Crunching; Artificial Intelligence; Questions of Patronage; The Quantum Chemistry Program Exchange; Government Funding of Chemistry; The Westheimer Report; A Bid for Big Science; Computational Support for Theoretical Chemistry Efforts to Create a National Center for Computation in ChemistryThe National Resource for Computation in Chemistry; Epilogue; Acknowledgments; References; Applications of Post-Hartree-Fock Methods: A Tutorial; Introduction; Independent Particle Model; Correlation Problem; Methods for Electron Correlation; Methods; Numerical Results for Potential Energy Curves; Basis Sets; Molecular Geometries; Vibrational Spectra; Photoelectron Spectra; Ionization

Potentials; Electron Afinities; Electronic Spectra; Molecular Properties; First-Order Properties; Second-Order Properties
Nuclear Magnetic ResonanceAcknowlegments; Appendix on Quadratic Configuration Interaction (QCI); References; Population Analysis and Electron Densities from Quantum Mechanics; Introduction: Defining the Grail; Computational Approaches: Pathways to the Grail; Orbital-Based Methods; Spatially Based Methods; Alternative Methods; Examples, Comparisons, Benefits, and Faults: Where Is the Grail?; Basis Set Dependence; Effect of Electron Correlation on Populations; Comparisons of Population Analysis of Small Organic Compounds; Organolithium Compounds
Resonance in hides , Carboxylic Acids, and Related CompoundsSuggestions for the User: Avoiding Traps Along the Path; Conclusion: Is the Pursuit of the Grail Doomed?; References; Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations; Introduction; Electrostatics; Theory of Poisson-Boltzmann (PB) Methods; Short-Range Electrostatic Interactions; Brownian Dynamics Simulations; Theory; Examples; Conclusion; Acknowledgments; References; Computer Simulation of Lipid Systems; Introduction; Polymorphism in Lipid-Water Systems; Modeling Strategies
Monte Carlo Importance Sampling38Molecular Dynamics41; Brownian Dynamics and Stochastic Boundary Molecular Dynamics; Interaction Potentials; Parameterization; Modeling of Lipid-Water Systems; Lipid Aggregation Studies; Dynamic Simulations with Atom-Atom Potentials; Bilayer Simulations; Membrane Transport; Nonlamellar Phases; Long-Time Dynamics of Bilayers; Lipid-Cholesterol Interactions; Conclusions and Future Prospects; Acknowledgment; References; Distance Geometry in Molecular Modeling; Introduction; Overview of Distance Geometry as a General Model Builder
Where Do Distance Constraints Come from?

Sommario/riassunto

This series is reviewing advances in the rapidly growing and evolving field of computational chemistry. It was established to keep track of the many new developments and is therefore providing a valuable service to the scientific community.