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Altri autori (Persone)	LipkowitzKenny B BoydDonald B
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Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	Reviews in Computational Chemistry; Contents; Basis Sets for Ab Initio Molecular Orbital Calculations and Intermolecular Interactions; Introduction; Some Terminology; Gaussian Compared to Exponential Functions; Contracted Gaussians; Polarization Functions; Complete Sets; The Basis Set Superposition Error; Choosing a Basis Set; Molecular Geometries; Energy Differences; One-Electron Properties; In-Depth Discussion; Sources of Gaussian Primitives and Contraction Coefficients; Even-Tempered Gaussians; Well-Tempered Gaussians; MINI-i, MIDI-i and MAXI-i etc.; Still Others; Atomic Natural Orbitals Functions for Augmenting Basis Sets; Weak Interactions; Conclusion; References; Semiempirical Molecular Orbital Methods; Introduction; History of Semiempirical Methods; Complete Neglect of Differential Overlap; Complete Neglect of Differential Overlap Version 2; Intermediate Neglect of Differential Overlap; Neglect of Diatomic Differential Overlap (NDDO); Modified Neglect of Diatomic Overlap; Austin Model 1; Parametric Method Number 3; Self-consistent Field Convergors; Strong and Weak Points of NDDO Semiempirical Methods;

MIND0/3; MNDO, AM1, and PM3; Theoretical Experiments; Stationary Points

General Procedure for Characterizing a Reaction; Reaction Path; Time-Dependent Phenomena; Future of Semiempirical Methods; Summary; References; Properties of Molecules by Direct Calculation; Introduction; Overview of Quantum Mechanical Properties; Correspondence between Energy Derivatives and Properties; Differentiation of the Schrodinger Equation; The Development of Methods for Property Determinations; Semiempirical Approaches; Ab Initio Methods; Detailed View of Ab Initio Methods; Hamiltonians and Operators; Computational Organization of the Differentiation Process

Derivatives of Electronic Wavefunctions; Local Space Concepts for Extended Systems; Vibrations and Rotations; Direct Property Calculations; Electrical Properties; Magnetic Properties; Force Constants; Transition Probabilities and Optical Properties; Summary; References; The Application of Quantitative Design Strategies in Pesticide Discovery; Introduction; The Selection of a Strategy; The Well-Designed Substituent Set; The Ideal Substituent Set Should Cover All Factors That Control Activity; The Ideal Substituent Set Should Cover the Selected Factor Space as Completely as Possible

The Ideal Substituent Set Should Span Orthogonal Dimensions of Parameter Space; The Ideal Set Should Contain the Minimum Number of Substituents Necessary to Avoid Chance Correlations and Still Meet the Desired Goal; Target Compounds Should Be Chosen to Preserve Synthetic Resources But Should Not Be Chosen Just Because They Are Easy to Synthesize; The Derivatives Must Be Stable under the Conditions of Bioevaluation; Analysis Strategies; The Topliss Tree; Free-Wilson Analysis; A Strategy for Lead Optimization Using Multiple Linear Regression Analysis; Choose the Optimal Pattern for Substitution; Choose the Factors (Parameters) That Are Likely to Be Important

Sommario/riassunto

This book is an account of current developments in computational chemistry, a new multidisciplinary area of research. Experts in computational chemistry, the editors use and develop techniques for computer-assisted molecular design. The core of the text itself deals with techniques for computer-assisted molecular design. The book is suitable for both beginners and experts. In addition, protocols and software for molecular recognition and the relationship between structure and biological activity of drug molecules are discussed in detail.
