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The Generation of Conformations of a Simple Molecule Using Distance Geometry and Some Applications of the MethodEnergy Embedding; Related Approaches: Target Function Minimization, the Diffusion Equation Method, and the Ellipsoid Algorithm; Molecular Dynamics; The Molecular Dynamics Method; Using Molecular Dynamics to Search Conformational Space; Restrained Molecular Dynamics; Summary and Conclusions; References; Simplified Models for Understanding and Predicting Protein Structure; Introduction; Molecular Mechanics Modeling; Knowledge-Based Modeling; Semiempirical and Polymer Models
ConclusionReferences; Molecular Mechanics: The Art and Science of Parameterization; Introduction; Molecular Mechanics Theory; History of Molecular Mechanics; Formulation of Molecular Mechanics; Bond Stretching; Angle Bending; Torsional Angles; van der Waals; Electrostatics; Cross Terms; Heats of Formation; Parameterization; References; New Approaches to Empirical Force Fields; Force Fields and Their Physical Significance; Introduction; The Basic Paradigm; System of Coordinates, Spectroscopic versus Empirical Force Fields, and the Assumption of Transferability; The Energy Expression
Determining Force ConstantsDerivation of "Quantum Mechanical" Force Fields from Ab Initio Data: The Theory of Energy Derivatives; Specific Force Constant Analysis and Computational Observables; Applications of the Theory of Energy Second Derivatives; An lnitio Dihedral Potentials; Nonbonded Interactions; Conclusions; References; Calculating the Properties of Hydrogen Bonds by ab Initio Methods; Definition of a Hydrogen Bond; Geometry; Energetics; Electronic Rearrangement; Spectroscopic Criteria; Exceptions Make the Rules; Theoretical Framework; Perturbation Theory vs. Supermolecular Approach
Components of Interaction Energy

Sommario/riassunto

This second volume of the series 'Reviews in Computational Chemistry' explores new applications, new methodologies, and new perspectives. The topics covered include conformational analysis, protein folding, force field parameterizations, hydrogen bonding, charge distributions, electrostatic potentials, electronic spectroscopy, molecular property correlations, and the computational chemistry literature. Methodologies described include conformational search strategies, distance geometry, molecular mechanics, molecular dynamics, ab initio and semiempirical molecular orbital calculations, and quan