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Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	Reviews in Computational Chemistry 111; Contents; Optimization Methods in Computational Chemistry; Introduction; Mathematical Preliminaries; Notation; Problem Statement; Matrix Characteristics; Conditions at Minima; Analysis of Functions; Basic Approaches to Large-Scale Optimization; Size and Space Limitations; Search Techniques; Local and Global Methods; Basic Descent Structure of Local Methods; Descent Directions; Line Search and Trust Region Steps; Convergence Criteria; Convergence Characterization; Nonderivative Methods; Gradient Methods; Steepest Descent; Conjugate Gradient PreconditioningNonlinear Conjugate Gradient; Newton Methods; Overview; Discrete Newton; Quasi-Newton; Truncated Newton; Perspective and Computational Examples; Comparisons; Numerical Example I: Rosenbrock Minimization; Numerical Example II: Deoxycytidine; Numerical Example III: Water Clusters; New Technologies; Acknowledgments; References; Predicting Three-Dimensional Structures of Oligopeptides; Introduction; Theoretical Foundations; Generation of Oligopeptide Chain; Residue Geometry;

End-Group Geometry; Constructing a Molecule; Ring Closure without Symmetry; Ring Closure with Symmetry
Early Use of Hard-Sphere PotentialMore Realistic Potentials; Potential Functions; Optimization Methods; Ancillary Techniques; Application to Simple Systems; Multiple-Minima Problem; Build-up Methods; Optimization of Electrostatics (Self-consistent Electric Field); Monte Carlo plus Minimization; Electrostatically Driven Monte Carlo; Adaptive Importance Sampling Monte Carlo; Increase in Dimensionality; Deformation of the Potential Energy Hypersurface; Mean-Field Theory; Simulated Annealing; Extension of Methodology to Large Polypeptides and Proteins; Build-up Method
Build-up with Limited ConstraintsCalculations with Constraints; Use of Homology; Pattern-Recognition Importance Sampling Minimization (PRISM); Outlook for the Future; Acknowledgments; References; Molecular Modeling Using Nuclear Magnetic Resonance Data; Introduction; Scope and Definitions; Historical Perspective; Molecular Representation; Generating Initial Structures; Metric Matrix Method; Variable Target Function Method; Other Methods for Generating Initial Structures; Modeling of Experimental Data; Distance Restraints; Averaging over Discrete Conformations
Time-Averaged Distance RestraintsDirect NOE Refinement; Dihedral Angle Restraints; Refinement, Minimization, and Dynamics; Molecular Dynamics; Other Derivative-Based Dynamics Schemes; Other Non-Derivative-Based Schemes; Force Field; Force Field Parameters and Accuracy; Force Field Modifications; Systematic Errors and Biases; Quality of Structures; Future Directions; Acknowledgment; References; Computer-Assisted Methods in the Evaluation of Chemical Toxicity; Introduction; Computer-Based Methods for Toxicity Evaluation; Quantitative Structure-Activity Relationship
Pattern Recognition Techniques

Sommario/riassunto

From reviews of the series:'Many of the articles are indeed accessible to any interested nonspecialist, even without theoretical background.'Journal of the American Chemical Society'...an invaluable resource for the serious molecular modeler.' Chemical Design Automation News