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Nota di contenuto	Revievvs in Computational Chemistry 10; Contents; Genetic Algorithms and Their Use in Chemistry; Introduction; Natural Evolution as an Optimization Process; The Genetic Algorithm as a Metaphor; Overview; Genetic Algorithms Tutorial; The Simple Genetic Algorithm; Analysis of the Simple Genetic Algorithm; The Schema Theorem; Convergence; Known Problems; Estimating Parameter Values; Variations on the Simple Genetic Algorithm; Is It Real or Is It a Genetic Algorithm?; Examples of Chemical Applications (With Emphasis on the Genetic Algorithm Method); Conformational Searching: Molecular Clusters Conformational Searching: Small MoleculesConformational Searching: Proteins; Conformational Searching: Docking; Conformational Searching: DNA/RNA; Protein NMR Data Analysis; Protein X-ray Data Analysis; Molecular Similarity; QSAR; Design of Molecules; DNA and Protein Sequence Applications; Data Clustering; Spectral Curve Fitting; General Model Fitting; Potential Energy Functions; Summary and Comparison with Other Global Optimization Methods; Brief Overview of Other Global Search Methods; Summary of Comparison Between

Genetic Algorithm and Other Methods; Appendix 1. Literature Sources
Appendix 2. Public Domain Genetic Algorithm CodesAcknowledgments; References; Does Combinatorial Chemistry Obviate Computer- Aided Drug Design?; Introduction; Fragments vs. Whole Molecules; Similarity and "Property Space"; Properties; Experimental Design; Selecting Substituent Sets; Template Diversity; SecondGeneration Libraries; Structure-Based Library Design; Calibration of Diversity Score; Evaluating Efficiency of Experimental Design; Comparison to Clustering Corporate Archives; Diversity Space; Comparing Diversity Among Libraries; Synthesis and Testing of Mixtures; Conclusions; References
Visualizing Molecular Phase Space: Nonstatistical Effects in Reaction DynamicsMolecular Dynamics in Phase Space; Introduction; What We Hope to Gain: Semiclassical Insight; Reaction Rates from Dynamics Simulations; Initial Conditions; Rate Constants; Chemical Kinetics, Chaos, and Molecular Motions; A Brief Review of Absolute Rate Theory; Overview of Nonlinear Dynamics and Chaos Theory; Visualizing Uncoupled Isomerization Dynamics in Phase Space; Technical Overview of Nonlinear Dynamics; Some Essential Theorems; Visualizing Phase Space on PoincarC Maps: Practical Aspects
Interpreting Poincari MapsLinear Stability Analysis of Periodic Orbits; Numerical Reconstruction of the Separatrix; Visualizing Coupled lsomerization Dynamics in Phase Space; Isomerization in Two Coupled Degrees of Freedom; Reactive Islands Kinetic Theory; Isomerization in Many Coupled Degrees of Freedom; The Poincare Integral Invariants; A Note on Arnold Diffusion; Summary and Conclusions; Acknowledgments; References; Computational Studies in Nonlinear Dynamics; Introduction: Nonlinear Dynamics and Universal Behavior; Homogeneous Systems; Multiple Steady States
Autocatalysis as a Source of Bistability

Sommario/riassunto

Not only a major reference work for sale to the library market, Reviews in Computational Chemistry is now a purchase by individuals due to the explosive growth in the use of computational chemistry throughout many scientific disciplines. In an instructional and nonmathematical style, these books provide an access to computational methods often outside a researcher's area of expertise. Volumes 9 & 10 represent the next two volumes in the successful series designed to help the chemistry community keep current with the many new developments in computational techniques. Many chapters are written a