DESCRIPTION

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 quantitative structure-activity relationships (QSAR) using topological and electronic descriptors.

A compendium of molecular modeling software will help users select the computational tools they need. Each chapter in 'Reviews in Computational Chemistry' serves as a brief tutorial for organic, physical, pharmaceutical, and biological chemists new to the field. Practitioners will be interested in the recent advances.

ABOUT THE AUTHOR

Kenny B. Lipkowitz, PhD, is a retired Professor of Chemistry from North Dakota State University.
Donald B. Boyd was appointed Research Professor of Chemistry at Indiana University - Purdue University Indianapolis in 1994. He has published over 100 refereed journal papers and book chapters.

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