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Theory and Modelling in Chemistry

Chemical physics and its interface with biology, physics

Theochem Impact Factor

KJ Lindholm-Leary



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Reviews in Computational Chemistry, Volume 9 Kenny B. Lipkowitz, Donald B. Boyd, 2009-09-22 An Computational Chemistry f hrt heute in den meisten Disziplinen chemischer Forschung kaum noch ein Weg vorbei Die B nde 8 und 9 der erfolgreichen Reihe Reviews in Computational Chemistry helfen Ihnen durch ihr gewohnt verst ndliches mathematisch nicht beladenes Konzept den berblick ber Methoden und Programmen zu behalten gerade dann wenn Sie sich nicht t glich mit Quantenchemie und Gro rechnern besch ftigen Schritt f r Schritt werden Hintergr nde und Theorie von Molecular Modeling CAMD Quantenchemie Molek lmechanik und dynamik sowie Struktur Aktivit ts Beziehungen QSAR erkl rt Anwendungsgebiete Vor und Nachteile diskutiert Der Interessent findet aktuellste Literaturangaben Nicht nur f r Bibliotheken geeignet Issues in Chemistry and General Chemical Research: 2011 Edition, 2012-01-09 Issues in Chemistry and General Chemical Research 2011 Edition is a ScholarlyEditions eBook that delivers timely authoritative and comprehensive information about Chemistry and General Chemical Research The editors have built Issues in Chemistry and General Chemical Research 2011 Edition on the vast information databases of ScholarlyNews You can expect the information about Chemistry and General Chemical Research in this eBook to be deeper than what you can access anywhere else as well as consistently reliable authoritative informed and relevant The content of Issues in Chemistry and General Chemical Research 2011 Edition has been produced by the world s leading scientists engineers analysts research institutions and companies All of the content is from peer reviewed sources and all of it is written assembled and edited by the editors at ScholarlyEditions and available exclusively from us You now have a source you can cite with authority confidence and credibility More information is available at <http://www.ScholarlyEditions.com> **Reviews in Computational Chemistry, Volume 2** Kenny B. Lipkowitz, Donald B. Boyd, 2009-09-22 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 **Chemical Modelling** Alan Hinchliffe, 2007-10-31 Chemical Modelling Applications and Theory comprises critical literature reviews of molecular modelling both theoretical and applied Molecular modelling in this context refers to modelling the structure properties and reactions of atoms molecules materials Each chapter is compiled by experts in their fields and provides a selective review of

recent literature With chemical modelling covering such a wide range of subjects this Specialist Periodical Report serves as the first port of call to any chemist biochemist materials scientist or molecular physicist needing to acquaint themselves of major developments in the area Specialist Periodical Reports provide systematic and detailed review coverage in major areas of chemical research Compiled by teams of leading authorities in the relevant subject areas the series creates a unique service for the active research chemist with regular in depth accounts of progress in particular fields of chemistry Subject coverage within different volumes of a given title is similar and publication is on an annual or biennial basis Current subject areas covered are Amino Acids Peptides and Proteins Carbohydrate Chemistry Catalysis Chemical Modelling Applications and Theory Electron Paramagnetic Resonance Nuclear Magnetic Resonance Organometallic Chemistry Organophosphorus Chemistry Photochemistry and Spectroscopic Properties of Inorganic and Organometallic Compounds From time to time the series has altered according to the fluctuating degrees of activity in the various fields but these volumes remain a superb reference point for researchers

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