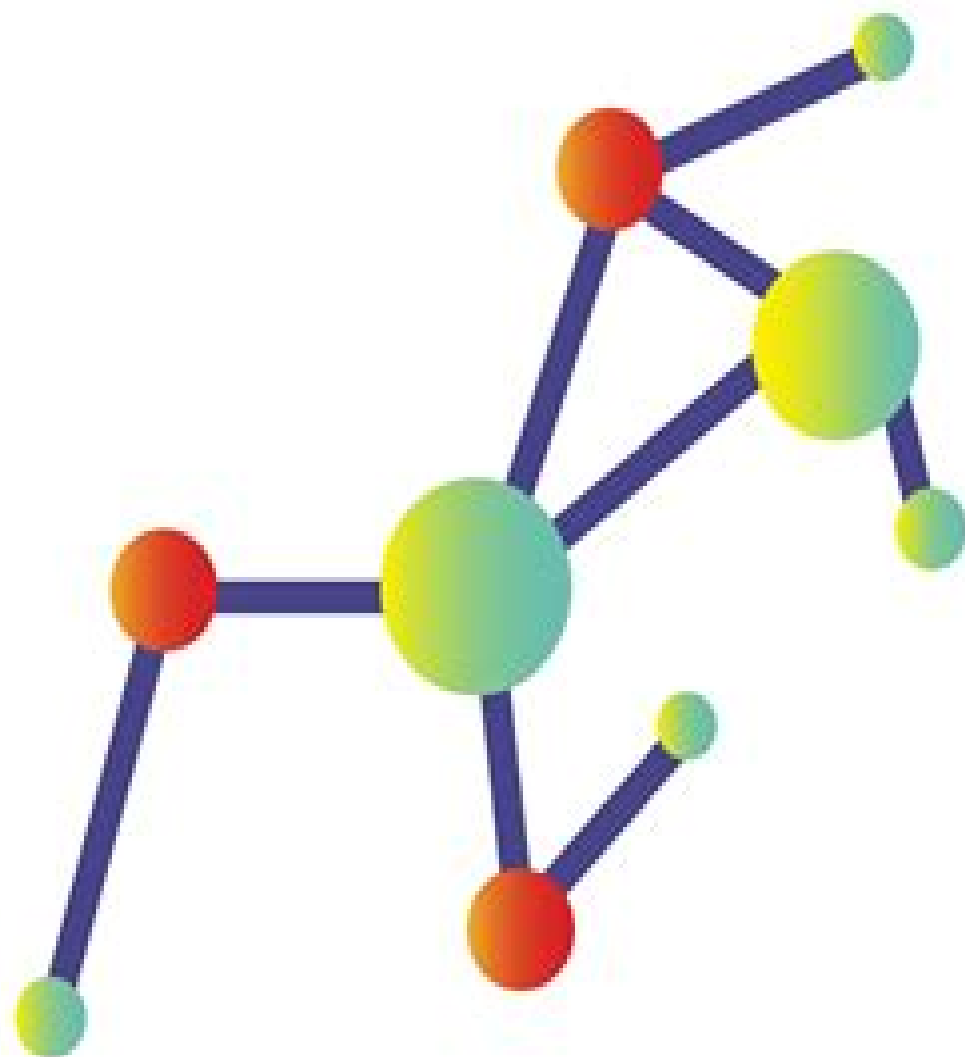




Construction And Use Of Atomic And Molecular Models

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Mislow, 2012-06-11 Molecular shape form and symmetry play a central role in organic chemistry and this text presents a brief introduction to the conceptual basis of stereochemistry. Its focus lies in the fundamentals of structural stereochemistry rather than the dynamic aspects that are more relevant to reaction mechanisms. The three part treatment deals with structure and symmetry, stereoisomerism and the separation and configuration of stereoisomers. The first section reviews molecular architecture relating empirical bonding geometries to the hybridization of the central carbon atom. Students receive a nonrigorous treatment of symmetry elements and point groups with particular focus on the presence or absence of reflection symmetry. The second section classifies stereoisomers according to symmetry properties and to the nature of their barriers; it also discusses the dependence of optical activity on structure and concludes with an examination of topological isomerism. The third and final section explores the conceptual basis of asymmetric syntheses and kinetic resolutions. Each of the major sections features a series of exercises that reinforce and extend the preceding material and answers are provided. Preface to the Dover edition. Answers to Exercises. Bibliography. Index. Genetic Algorithms in Molecular Modeling James

Devillers, 1996-06-07 Genetic Algorithms in Molecular Modeling is the first book available on the use of genetic algorithms in molecular design. This volume marks the beginning of a new series of books Principles in QSAR and Drug Design which will be an indispensable reference for students and professionals involved in medicinal chemistry, pharmacology, ecotoxicology and agrochemistry. Each comprehensive chapter is written by a distinguished researcher in the field. Through its up to the minute content, extensive bibliography and essential information on software availability, this book leads the reader from the theoretical aspects to the practical applications. It enables the uninitiated reader to apply genetic algorithms for modeling the biological activities and properties of chemicals and provides the trained scientist with the most up to date information on the topic. Extremely topical and timely. Sets the foundations for the development of computer aided tools for solving numerous problems in QSAR and drug design. Written to be accessible without prior direct experience in genetic algorithms.

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Barati, Mustafa M. Alhubail, 2020-12-03 A comprehensive textbook presenting techniques for the analysis and characterization of shale plays. Significant reserves of hydrocarbons cannot be extracted using conventional methods. Improvements in techniques such as horizontal drilling and hydraulic fracturing have increased access to unconventional hydrocarbon resources, ushering in the shale boom and disrupting the energy sector. Unconventional Hydrocarbon Resources: Techniques for Reservoir Engineering Analysis covers the geochemistry, petrophysics, geomechanics and economics of unconventional shale oil plays. The text uses a step by step approach to demonstrate industry standard workflows for calculating resource volume and optimizing the extraction process. Volume highlights include: Methods for rock and fluid

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Molecular Modeling Hans-Dieter Höltje, Gerd Folkers, 2008-07-11 Written by experienced experts in molecular modeling this book describes the basics to the extent that is necessary if one wants to be able to reliably judge the results from molecular modeling calculations Its main objective is the description of the various pitfalls to be avoided Without unnecessary overhead it leads the reader from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules A textbook for beginners as well as an invaluable reference for all those dealing with molecular modeling in their daily work

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