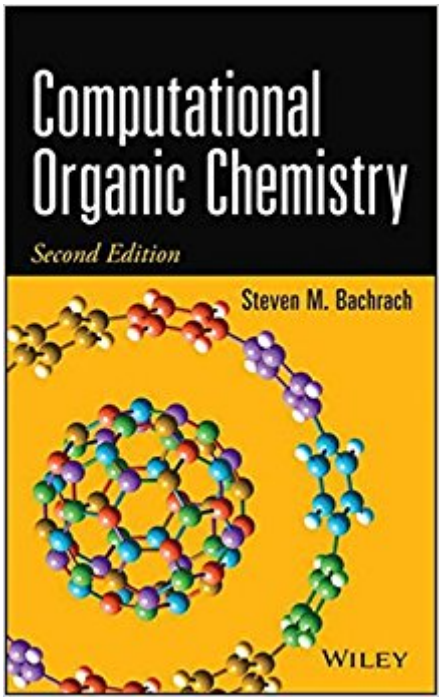
Ebook Directory
the best source of ebook

The book was found

Computational Organic Chemistry



PDF
Adobe
DOWNLOAD EBOOK

Synopsis

The Second Edition demonstrates how computational chemistry continues to shed new light on organic chemistry The Second Edition of author Steven Bachrachâ ™s highly acclaimed Computational Organic Chemistry reflects the tremendous advances in computational methods since the publication of the First Edition, explaining how these advances have shaped our current understanding of organic chemistry. Readers familiar with the First Edition will discover new and revised material in all chapters, including new case studies and examples. Thereâ ™s also a new chapter dedicated to computational enzymology that demonstrates how principles of quantum mechanics applied to organic reactions can be extended to biological systems. Computational Organic Chemistry covers a broad range of problems and challenges in organic chemistry where computational chemistry has played a significant role in developing new theories or where it has provided additional evidence to support experimentally derived insights. Readers do not have to be experts in quantum mechanics. The first chapter of the book introduces all of the major theoretical concepts and definitions of quantum mechanics followed by a chapter dedicated to computed spectral properties and structure identification. Next, the book covers: Fundamentals of organic chemistry Pericyclic reactions Diradicals and carbenes Organic reactions of anions Solution-phase organic chemistry Organic reaction dynamics The final chapter offers new computational approaches to understand enzymes. The book features interviews with preeminent computational chemists, underscoring the role of collaboration in developing new science. Three of these interviews are new to this edition. Readers interested in exploring individual topics in greater depth should turn to the bookâ ™s ancillary website www.comporgchem.com, which offers updates and supporting information. Plus, every cited article that is available in electronic form is listed with a link to the article.

Book Information

Hardcover: 632 pages
Publisher: Wiley; 2 edition (April 7, 2014)
Language: English
ISBN-10: 1118291921
ISBN-13: 978-1118291924
Product Dimensions: 6.4 x 1.6 x 9.3 inches
Shipping Weight: 2.1 pounds (View shipping rates and policies)
Average Customer Review: 5.0 out of 5 stars 3 customer reviews

Best Sellers Rank: #931,176 in Books (See Top 100 in Books) #85 inÂ Books > Science & Math > Chemistry > Molecular Chemistry #709 inÂ Books > Science & Math > Chemistry > Physical & Theoretical #868 inÂ Books > Science & Math > Chemistry > Organic

Customer Reviews

â œValuable forÂ anyone wishing to learn how to carry out quantum chemistry computations. . .Highly recommended. Upper-division undergraduates and above.â •Â (Choice, 1 June 2015) Â â œThe Second Edition of author Steven Bachrachâ ™s highly acclaimed Computational Organic Chemistry reflects the tremendous advances in computational methods since the publication of the First Edition, explaining how these advances have shaped our current understanding of organic chemistry.â •Â (Chemistry Views, 23 October 2014)

"[This book] collects together, largely for the first time, a series of chapters dedicated to all the ways in which molecular modeling/computational chemistry can impact organic chemistry."--Christopher J. Cramer, author of Essentials ofComputational Chemistry: Theories and ModelsComputational Organic Chemistry provides a practical overview of the ways in which computational modeling methods and applications can be used in organic chemistry to predict the structure and reactivity of organic molecules. After a concise survey of computational methods, the book presents in-depth case studies that show how various computational methods have provided critical insight into the nature of organic mechanisms. With a focus on methodologies, this unique resource: Discusses simple molecular properties, pericyclic reactions, carbenes and radicals, anion chemistry, solvent effects, and moreFeatures sidebars that offer a personal look at some of the leading practitioners in the fieldConveys the strengths and limitations of each method, so that readers develop a feel for the correct "tool" to use in the context of a specific problemFurther informs readers with a supporting Web site that provides links to materials cited and features a blog that discusses and provides links to new relevant articles at www.trinity.edu/sbachrac/coc/ This is a great reference for practicing physical organic and computational chemists, as well as a thought-provoking textbook for graduate-level courses in computational chemistry and organic chemistry.

The second edition of Bachrach’s book is even better, and more detailed, than the first. It is written for the organic experimentalist, not the mathematician or theorist. It is a superb introduction to the computational tools and techniques available to help plan experiments, and to interpret the results. It should be on the bookshelf of every student of organic chemistry, and every practicing organic

chemist.

(See also my review of the first edition.) This updated edition corrects the few errors that I noticed in the earlier one, and includes newer results that appeared in the literature after the publication of the first edition.Of the dozens of books on computational modeling that I have read, all of the rest seem to be aimed at an audience of mathematicians who develop computational methods. In contrast, this is the only book I have found aimed at an audience of chemists who are primarily interested in using extant computational tools to answer "chemistry" questions without necessarily worrying about what is "under the hood." At the same time, sufficient theoretical background is included to give users a firm grasp of the scope and limitations of any particular method.An exceptional work, a Magnum Opus, meticulously thorough and rigorously documented. I recommend it without hesitation or qualification.

The second edition of Bachrach's book (for comments about the 1-st edition see my older review) is a nice addition to the collection of computational quantum chemistry books which comes with extended and updated chapters along with two brand-new chapters.The new chapters are one about "Computed Spectral Properties and Structure Identification" and another about "Computational Approaches to Understanding Enzymes". The former is especially important for the identification of natural organic compounds which are extracted from plants or living organisms and do require an identification of their molecular structure using spectroscopic/crystallographic methods - computed spectroscopic properties represent a powerful tool for the identification process because upon comparing them against the experimental data it is possible to assign the correct 3D structure to the novel compound.The latter chapter is useful for those intending to study biological systems with the aid of QM/MM methods. With these methods one can treat the important residues in the active site and the substrate at the QM level while the remaining atoms of the enzyme can be treated at the MM level. On his website, the author maintains a blog with novel information and a lively discussion about the topics treated inside the book. Both students and professionals will benefit from reading this book.

Download to continue reading...

Study Guide: Ace Organic Chemistry I - The EASY Guide to Ace Organic Chemistry I: (Organic Chemistry Study Guide, Organic Chemistry Review, Concepts, Reaction Mechanisms and Summaries) Simulating Enzyme Reactivity: Computational Methods in Enzyme Catalysis (Theoretical and Computational Chemistry Series) Experimental Organic Chemistry: A Miniscale &

Microscale Approach (Cengage Learning Laboratory Series for Organic Chemistry) The Organic Chemistry of Drug Synthesis, Volume 3 (Organic Chemistry Series of Drug Synthesis) Computational Organic Chemistry Computational Fluid Mechanics and Heat Transfer, Third Edition (Series in Computational and Physical Processes in Mechanics and Thermal Sciences) Current Topics in Computational Molecular Biology (Computational Molecular Biology) Theoretical Neuroscience: Computational and Mathematical Modeling of Neural Systems (Computational Neuroscience Series) Computational Approaches to Protein Dynamics: From Quantum to Coarse-Grained Methods (Series in Computational Biophysics) The Power of Computational Thinking:Games, Magic and Puzzles to Help You Become a Computational Thinker What is Organic Chemistry? Chemistry Book 4th Grade | Children's Chemistry Books Ace General Chemistry I and II (The EASY Guide to Ace General Chemistry I and II): General Chemistry Study Guide, General Chemistry Review Organic Homemade Lotion Recipes - For All Skin Types (The Best Lotion DIY Recipes): Lotion Making For Beginners (organic lawn care manual, organic skin care, beauty and the beast) Molecular Visions (Organic, Inorganic, Organometallic) Molecular Model Kit #1 by Darling Models to accompany Organic Chemistry A Microscale Approach to Organic Laboratory Techniques (Brooks/Cole Laboratory Series for Organic Chemistry) Organic Chemistry (with Organic ChemistryNOW) (Available Titles OWL) Cycloaddition Reactions in Organic Synthesis, Volume 8 (Tetrahedron Organic Chemistry) Review of Organic Functional Groups: Introduction to Medicinal Organic Chemistry Organic Structure Analysis (Topics in Organic Chemistry) Examkrackers MCAT 101 Passages: Chemistry: General & Organic Chemistry

Contact Us

DMCA

Privacy

FAQ & Help