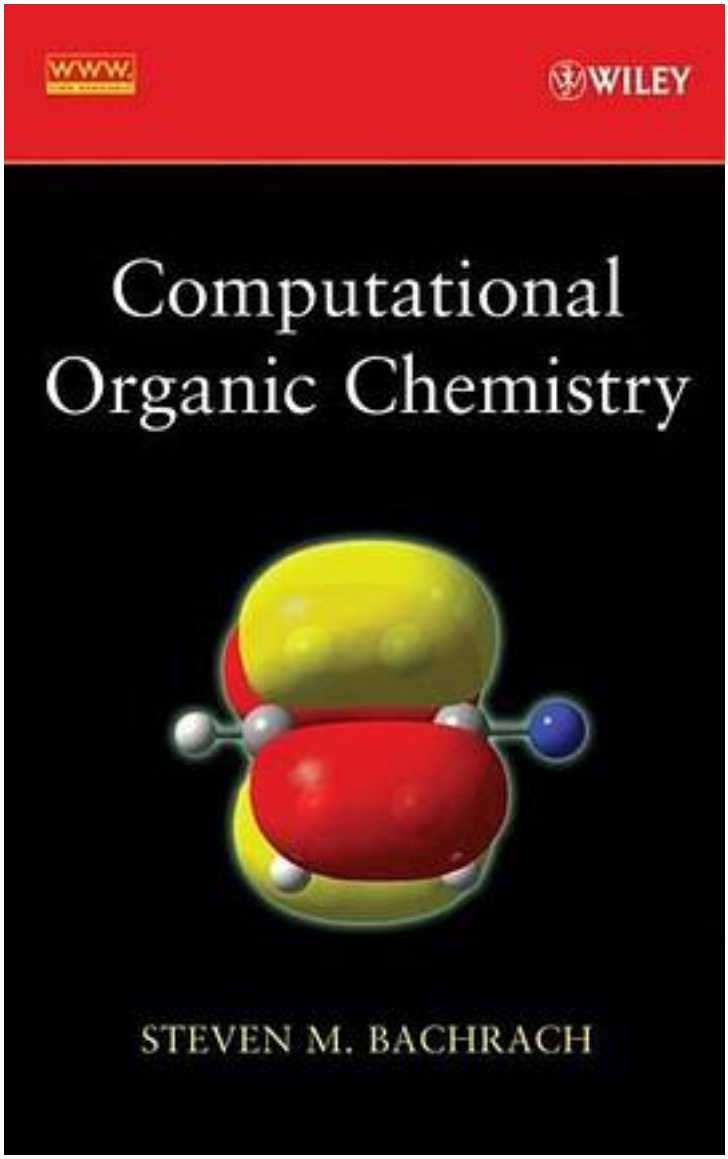
Computational Organic Chemistry



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著者:Bachrach, Steven M.

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"[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."

*Computational 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 more

*Features sidebars that offer a personal look at some of the leading practitioners in the field

*Conveys 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 problem

*Further 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.

作者介绍:

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