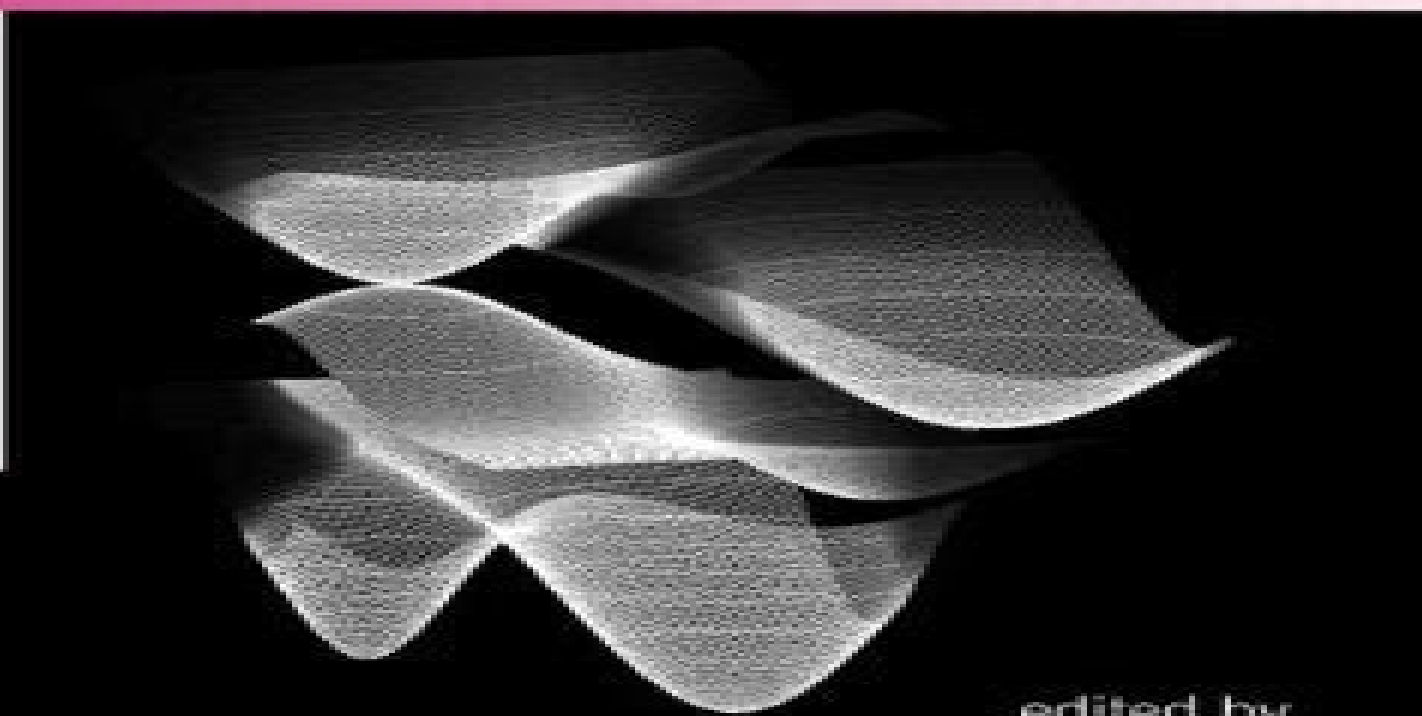


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VOLUME 13

Computational Methods in Photochemistry



edited by
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Computational Methods In Photochemistry Molecular And Supramolecular Photochemistry 2005 05 05

G. Wipff



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Computational Methods in Photochemistry Andrei G. Kutateladze, 2005-05-05 Addressing critical aspects of computational modeling in photochemistry Molecular Methods in Photochemistry is designed to familiarize researchers and practitioners with state of the art computational methods to predict the reactivity of excited molecules It provides practical guidelines and examples for the modeling of excited states and describes some of the latest approaches in the computational modeling of photochemistry in solutions and constrained media Presents research from experts in the top tiers of computational chemistry and photochemistry including chapters by recognized specialists such as Howard Zimmerman Josef Michl Matthew Platz Nina Gritsan Weston Borden Mike Robb Michael Bearpark Maccimo Olivucci Martin Klessinger Frank Weinhold Todd Martinez and others While the issue of excited states is discussed in specialized computational series these books address issues of organic photochemistry sparsely There has been until now no volume specifically devoted to the computational methods in photochemistry with an emphasis on organic photochemistry

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Computational Photochemistry Massimo Olivucci, 2005-10-20 Computational Photochemistry Volume 16 provides an overview of general strategies currently used to investigate photochemical processes Whilst contributing to establishing a branch of computational chemistry that deals with the properties and reactivity of photoexcited molecules the book also provides insight into the conceptual and methodological research lines in computational photochemistry Packed with examples of applications of modelling of basic photochemical reactions and the computer aided development of novel materials in the field of photodegradation paints photoprotection sunscreens color regulation photochromic devices and fluorescent probes this book is particularly useful to anyone interested in the effect of light on molecules and materials Provides an overview of computational photochemistry dealing with principles and applications Demonstrates techniques that can be used in the computer aided design of novel photo responsive materials Written by experts in computational photochemistry

Theoretical and Computational Photochemistry García Iriepa Cristina, Marco Marazzi, 2023-04-21 Theoretical and Computational Photochemistry Fundamentals Methods Applications and Synergy with Experimental Approaches provides a comprehensive overview of photoactive systems and photochemical processes After an introduction to photochemistry the book discusses the key computational chemistry methods applied to the study of light induced processes over the past decade and further outlines recent research topics to which these methods have been applied By discussing the synergy between experimental and computational data the book highlights how theoretical studies could facilitate

understanding experimental findings This helpful guide is for both theoretical chemists and experimental photochemistry researchers interested in utilizing computational photochemistry methods for their own work Reviews the fundamentals of photochemistry helping those new to the field in understanding key concepts Provides detailed guidance and comparison of computational and theoretical methods highlighting the suitability of each method for different case studies Outlines current applications to encourage discussion of the synergy between experimental and computational data and inspiring further application of these methods to other photochemical processes *Supramolecular photochemistry* Vincenzo Balzani,1996

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Computational Approaches in Supramolecular Chemistry G. Wipff,1994-03-31 Supramolecular chemistry has been defined by J M Lehn as a highly interdisciplinary field of science covering the chemical physical and biological features of chemical species of higher complexity that are held together and organized by means of intermolecular noncovalent binding interactions Science 1993 Recognition reactivity and transport represent three basic functional features in essence dynamics which may be translated into structural features The purpose of the NATO workshop which took place september 1 5 1993 at the Bischofsberg near Strasbourg was to present computations which may contribute to the atomic level understanding of the structural and thermodynamical features involved in the processes of molecular recognition and supramolecular organization of supramolecular modeling Other The main focus was therefore on the many facets applications of computers in chemistry such as automation simulation of processes procedures for fitting kinetic or thermodynamic data computer assisted synthetic strategies use of data bases for structure elucidation or for bibliographic searches have an obvious impact in supramolecular chemistry as well but were not presented at the workshop

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