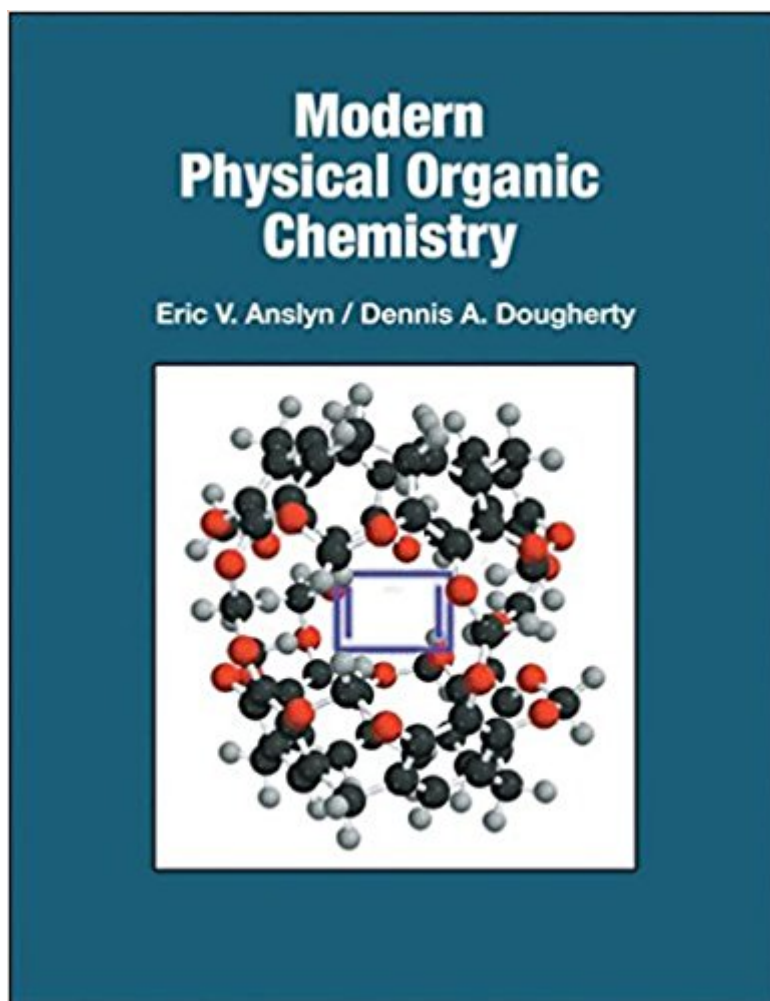


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# Modern Physical Organic Chemistry



## Synopsis

This is the first modern textbook, written in the 21st century, to make explicit the many connections between physical organic chemistry and critical fields such as organometallic chemistry, materials chemistry, bioorganic chemistry, and biochemistry. In the latter part of the 20th century, the field of physical organic chemistry went through dramatic changes, with an increased emphasis on noncovalent interactions and their roles in molecular recognition, supramolecular chemistry, and biology; the development of new materials with novel structural features; and the use of computational methods. Contemporary chemists must be just as familiar with these newer fields as with the more established classical topics. This completely new landmark text is intended to bridge that gap. In addition to covering thoroughly the core areas of physical organic chemistry &#x96; structure and mechanism &#x96; the book will escort the practitioner of organic chemistry into a field that has been thoroughly updated . The foundations and applicabilities of modern computational methods are also developed. Written by two distinguished researchers in this field, Modern Physical Organic Chemistry can serve as a text for a year-long course targeted to advanced undergraduates or first-year graduate students, as well as for a variety of shorter courses on selected aspects of the field. It will also serve as a landmark new reference text, and as an introduction to many of the more advanced topics of interest to modern researchers. An accompanying Student Solutions Manual will become available.

## Book Information

Hardcover: 1104 pages

Publisher: University Science; illustrated edition edition (July 15, 2005)

Language: English

ISBN-10: 1891389319

ISBN-13: 978-1891389313

Product Dimensions: 8.9 x 2.2 x 11.1 inches

Shipping Weight: 6 pounds (View shipping rates and policies)

Average Customer Review: 4.8 out of 5 stars 51 customer reviews

Best Sellers Rank: #28,826 in Books (See Top 100 in Books) #9 in Ã Â Books > Science & Math > Chemistry > Physical & Theoretical > Physical Chemistry #77 in Ã Â Books > Science & Math > Chemistry > Organic #178 in Ã Â Books > Science & Math > Chemistry > General & Reference

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"It will certainly inspire." -- Barry Carpenter, Cornell University" This book is the new authoritative

physical organic resource that will benefit researchers, students, and teachers alike." -- Timothy Swager, Massachusetts Institute of Technology "This book is the new authoritative physical organic resource that will benefit researchers, students, and teachers alike." -- Timothy Swager, Massachusetts Institute of Technology "This much needed text places physical organic chemistry in its most modern context." -- Timothy M. Swager, MITI can enthusiastically recommend the text." -- Nicholas J. Turro, Columbia University

Eric V. Anslyn received his PhD in Chemistry from the California Institute of Technology under the direction of Robert Grubbs. After completing post-doctoral work with Ronald Breslow at Columbia University, he joined the faculty at the University of Texas at Austin, where he became a Full Professor in 1999. He currently holds four patents and is the recipient of numerous awards and honors, including the Presidential Young Investigator, the Alfred P. Sloan Research Fellow, the Searle Scholar, the Dreyfus Teacher-Scholar Award, and the Jean Holloway Award for Excellence in Teaching. He is also the Associate Editor for the Journal of the American Chemical Society and serves on the editorial boards of Supramolecular Chemistry and the Journal of Supramolecular Chemistry. His primary research is in physical organic chemistry and bioorganic chemistry, with specific interests in catalysts for phosphoryl and glycosyl transfers, receptors for carbohydrates and enolates, single and multi-analyte sensors; the development of an electronic tongue, and synthesis of polymeric molecules that exhibit unique abiotic secondary structure. Dennis A. Dougherty received a PhD from Princeton with Kurt Mislow, followed by a year of postdoctoral study with Jerome Berson at Yale. In 1979 he joined the faculty at the California Institute of Technology, where he is now George Grant Hoag Professor of Chemistry. Dougherty's extensive research interests have taken him to many fronts, but he is perhaps best known for development of the cation- interaction, a novel but potent noncovalent binding interaction. More recently, he has addressed molecular neurobiology, developing the in vivo nonsense suppression method for unnatural amino acid incorporation into proteins expressed in living cells. This powerful new tool enables physical organic chemistry on the brain; - chemical-scale studies of the molecules of memory, thought, and sensory perception and the targets of treatments for Alzheimer's disease, Parkinson's disease, schizophrenia, learning and attention deficits, and drug addiction. His group is now working on extensive experimental and computational studies of the bacterial mechanosensitive channels MscL and MscS, building off the crystal structures of these channels recently reported by the Rees group at Caltech.

I bought this for a graduate level physical organic chemistry course, but most of the material will be accessible to a Junior/Senior undergrad majoring in a relevant subject. The book begins with molecular orbital theory. It gives you a foundation for how to build simple molecular orbitals, and then how to mix simple molecular orbitals to generate the orbitals for more complex molecules. This is explained using intuition and visualizations rather than math. In fact, the book is surprising non-mathematical for a physical chemistry book. Acid-Base chemistry, stereochemistry, and stability are studying through the molecular orbital picture. The middle chapters are about reactivity, kinetics, and mechanisms. The reactivity and mechanisms emphasize frontier orbital interactions, while the kinetics sections allow you to develop an intuitive understanding of potential landscapes under different scenarios. The final chapters are in electronic structure. Computational methods are introduced for how to perform QM calculations, there is some photochemistry and electronic materials. While great introductions, if you are more interested in the computational aspects or mathematical derivations you will need to look somewhere else. I recommend this to anyone who wants to achieve an intuitive understanding of why molecules behave as they do, rather than just accepting dogmas from sophomore organic chemistry. If you have taken sophomore organic chemistry you will be able to understand most of this, and with physical chemistry you should have no trouble understanding the material.

This textbook is great if you want to learn the principles behind the principles in organic chemistry. It really is a must have because a lot of colleges don't explain in detail why these concepts are relevant in today's understanding of chemistry. Also, this textbook goes in depth about the language of chemistry which sometimes other textbooks assume you might already know. It's extremely thorough. You must read the chapters in order though. If you skip a few chapters, it can get confusing in the long run. Read the stuff you already know because it will shed new light to the subject.

I have been a professional chemist for more than 30 years. This book is probably the best on physical organic chemistry that I have ever come across. The book is over 1000 pages in length. I read the book from cover to cover. There is not a single chapter that is boring. The book covers a wide range of topics in physical organic chemistry. These topics include molecular structures, stereochemistry, conformational analysis, molecular recognition and supramolecular chemistry, acid and base chemistry, thermodynamics, kinetics and mechanism, organometallic chemistry, polymers, organic electronic theory, pericyclic reactions, photochemistry and organic materials. The

treatment of each topics is well beyond elementary level. It is the intent of the authors that the book will be able to provide the necessary background for reading current research literature. Excercises are provided at the end of each chapter. The problems in the Excercises Section are interesting and challenging. I strongly encourage any graduate student to attempt these problems. Many interesting examples are given throughout each chapter. To illustrate, here is an interesting example given in the chapter of "Advanced Concepts in Electronic Structural Theory". Using the simple Huckel molecular orbital analysis, the two molecules cyclobutadiene (CBD) and trimethylenemethane (TMM) are known to have the same molecular orbital pattern for their pi electrons. In other words, these two molecules have one bonding orbital, two degenerate non-bonding orbitals and one anti-bonding orbital. Both are 4-electron systems. We therefore expect that there will be two unpaired parallel spin electrons in the degenerate non-bonding orbitals. Both molecules would have a triplet ground state. However, more advanced analysis shows that the spin preferences of the two systems are different. CBD is expected to exist as a singlet ground state while TMM is expected to exist as a triplet state. The authors provide an extremely clear explanation for such an analysis. In the case of CBD, the two non-bonding orbitals are disjoint. Two molecular orbitals are said to be disjoint when there are no atoms in common in their LCAO's. Consequently, the exchange integral of the two electrons in the two non-bonding orbitals are zero. When electron correlation is incorporated into the analysis, CBD is found have a singlet ground state with a rectangular structure, instead of a perfect square, of alternate double and single bond. This is sometimes known as pseudo Jahn-Teller distortion. In the case of TMM, the non-bonding orbitals are non-disjoint. The exchange integral consequently is non-zero and a triplet ground state is preferred. This concept of spin preference is used to explain one of the strategies used in the synthesis of magnetic organic material. Examples of applications of physical organic chemistry principles to biological systems and technologies (such as liquid crystal) are also found throughout the book. Beyond any doubts, this book is going to be the standard text for graduate students in organic chemistry for many years to come. If after reading this book and your interest in physical organic chemistry is not aroused, I do not believe that I will be able to find you a more interesting book on physical organic chemistry. The only criticism that I want to make is that I wish the authors would cover more on density functional theory. This part of theoretical chemistry is fast becoming more and more popular in current research. I also hope that the authors will update the book frequently.

I first heard of this book from an interview with one of my organic chemistry Professors, who chose this book when asked what one book he would take to a deserted island. I personally love this book

because I loved learning about how the introductory mechanisms learned in organic chemistry are vastly oversimplified, and there is really much more to the picture. Comes with a great appendix in the back with a great explanation of introductory quantum mechanics, with a focus on ab initio methods. ABSOLUTELY MY FAVORITE TEXTBOOK - Enthusiastic Chemistry Student.

Modern Physical Organic Chemistry is a must have book for anyone who studies Organic Chemistry at the graduate level and has a desire for better (and complete) understanding of the foundations for every underlying concept in the field. Without being heavily centered on the Maths and calculations behind every concept, the authors still manage to go excessively deep into each of the topic covered to give you a fantastic understanding of them. I couldn't imagine getting through a Advanced Physical Organic Chemistry class without this book as a resource, and I would recommend over any other of its kind.

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