Book Reviews

Classics in Hydrocarbon Chemistry. Syntheses, Concepts, Perspectives. By Henning Hopf (Technische Universität Braunschweig, Germany). With a Foreword by W. von Eggers Doering. Wiley-VCH: Weinheim. 2000. xiii + 547 pp. Hardcover: $79.95. ISBN 3-527-30216-6. Paperback: $49.95. ISBN 3-527-29606-9.

This impressive monograph, "written primarily for readers who are not specialists in hydrocarbon chemistry", provides a fascinating and admirably accessible overview of what might be termed "nonstandard" hydrocarbons—a rich diversity of molecules and families of structures characterized by novel bonding characteristics, geometries, and topological signatures. Some of the hydrocarbons included are tetrahedranes and cubanes, prismanes and radialenes, adamantanes and propellanes, fenestranes, small-ring alkynes and cumulenes, rotanes, dendralenes and iptycenes, annulenes, geometrically distorted olefins and twisted polycyclic aromatic hydrocarbons, cyclophanes, phenacenes and rylenes, non-Kekulé hydrocarbons, staffanes and triangulanes, and many more.

Whether hydrocarbon chemistry should be considered a "separate field of chemistry" or simply one of many indispensable components within the canon of organic chemistry—one element in an alloy providing essential strength and character—depends on personal perspectives and value judgments. What is beyond question is that research on nonstandard hydrocarbons has been a significant component in the history of organic chemistry from the beginning and has led to spectacular achievements in organic synthesis and to valuable new synthetic methods, especially over the past 40 years. The nonstandard hydrocarbon structures secured through target-directed syntheses have, in turn, provided opportunities to illuminate and clarify fundamental concepts related to bonding, stereochemistry, electronic interactions, and reactivity—concepts appropriate to extreme structures as well as to standard molecules.

Hopf's judiciously selective and deeply informed exposition concentrates on synthetic chemistry, and it is supported with numerous, exceptionally clear flowcharts and outlines of synthetic routes. Details of the structural parameters, spectroscopic features, chemical propensities, mechanistic tendencies, and computationally derived insights for the hydrocarbons considered are less prominently included, but excellent leads to relevant articles and reviews are provided, often with useful notes and comments. The literature coverage is first-rate. Drawn from a wide range of sources, it includes the work of many chemists in many countries as well as historically significant papers and the latest journal articles.

Any chemist reading this book and working through the schemes will be rewarded with fresh insights, introductions to or reminders of powerful but uncommon synthetic transformations, and renewed appreciation for the innovative chemists whose great imagination, curiosity, bravery, and diligence created this body of work based on novel transformations and nonstandard hydrocarbon structures. This universe of chemical compounds provided by creative intelligence, deliberately selected synthetic targets, and successful synthetic endeavors has allowed organic and physical chemists to test theories and refine concepts in ways not accessible through syntheses and studies of standard structures alone.

New synthetic challenges, hypothetical structures yet to be envisaged and synthesized, mechanistic issues still unaddressed, and new ambitions toward projected applications and desired material properties will stimulate and drive further work in hydrocarbon chemistry. This monograph will serve for some time as an indispensable guide and inspiration toward that future.

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Protein Structure Prediction: Methods and Protocols. Edited by David M. Webster (Southern Cross Molecular, Bath, UK). Methods in Molecular Biology 143. Humana Press: Totowa, NJ. 2000. x + 422 pp. $89.50. ISBN 0-89603-637-5.

Protein structure prediction is a daunting place to start for someone who is new to the field of computer modeling. Unlike, say, electronic structure or molecular dynamics, which offer large commercial software packages and textbook-level introductions, predicting protein structure is an area that is currently undergoing an explosion of new methodology. This has led to a dizzying array of specialized programs by various research groups. Many of these programs are readily available via public web servers or as downloads, making much of the prediction process easily accessible to the nonspecialist. Thus, a comprehensive guide to the available tools is indeed a very timely offering.

The organization of this book is excellent. Eighteen chapters lead the reader through the entire process, beginning with initial sequence comparisons through different stages of model-building and culminating with protein−ligand docking. The range of topics covered also includes secondary-structure prediction, homology modeling, threading, scoring functions, loop modeling, side-chain placement, and fold classification, among others. Many of the authors are, in fact, the developers of some commonly used methods and offer a first-hand introduction to their software.

Most of the contributed chapters follow a common format. The emphasis is on providing a practical handbook, and with that goal in mind most chapters contain detailed tutorials and worked-through examples that give a real-life flavor to the explanations. Many sections will undoubtedly be read propped up next to a terminal with a target sequence in hand. A particularly nice feature is a final "Notes" section in many chapters, listing problems to look out for or providing helpful tips.

Naturally, this approach also has certain drawbacks. Much of the introductory material is rather cursory, so this is not a good place for a beginner to pick up much theoretical background. The focus of some sections is very narrow, reading much like a software user's guide; there are also a lot of raw input and output files and even several pages of C source code—plenty of detail for hands-on experimentation but unlikely to make much sense to a casual reader.

Placing a heavy emphasis on real-life detail carries with it the risk of becoming rapidly dated, and that can already be seen to some extent. There are very few references from 1998 or later, and some newer methods are overlooked. The many references to Web-based resources, while extremely useful for hands-on work, are also vulnerable to this trap and some of the URLs are already incorrect.

Overall, though, the quality of the book is high. There is a good index and relatively few typos; nearly half were concentrated in only two chapters. The book will certainly appeal to active practitioners, and I would recommend it to anyone who is interested in structure prediction and anxious to try out some of the latest methods. This insider's handbook will allow them to hit the ground running.

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