

Book Reviews

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BOOK REVIEWS

Topics in Stereochemistry, Volume 21. Ed. by ERNEST L. ELIEL and SAMUEL L. WILEN, John Wiley & Sons, Inc., 605 Third Avenue, New York, NY 10158-0012. 1994. xii + 533 pp. 16×23.5 cm. \$135.00. ISBN 0-471-521205.

In the first contribution by Vedejs and Peterson titled "Stereochemistry and Mechanism of the Wittig Reaction" (150 pages), a semblance of order is brought to the chaos surrounding the mechanism(s) of this classical reaction. Just how confusing the mechanistic picture is can be appreciated by reading the sections on allylic and benzylic ylides and carbonyl-stabilized ylides, respectively. The authors have done a commendable job of highlighting those trends in reactivity that are clear, and pointing out areas in which no generalizations are possible. The text is interspersed with a number of extensive tabulations of examples of the reaction, similar to what one finds in *Organic Reactions*. This is one of the most useful features of the chapter. The brief summaries on pp. 13, 31, and 44 make the reader's task much easier. This reviewer particularly enjoyed the lucid description of the effect of lithium ion on the selectivity of the reaction (p. 32), the clear discussion of the oxido ylide approach to *E*- and trisubstituted alkene synthesis (p. 38), and the very nice discussion (pp. 34–35) detailing the kinetically controlled decomposition of *cis*-disubstituted oxaphosphetanes. Less helpful were sections XIX–XXI in which an attempt is made to relate transition state geometry and characteristics to the stereochemical outcome of the reaction. The authors cannot be faulted for this, since the available information in the primary literature is fragmented and of uneven quality, obscuring any clear patterns.

There were a few typographical errors in the text (p. 34, line 7, and p. 107, paragraph 2, line 2). The references could have benefited from a more careful proofreading (errors in 29, 51, 137a, 141b). In summary, this chapter presents an illuminating discussion which will be of interest to a very broad audience.

The second chapter (190 pages), by Graczyk and Mikolajczyk, is titled "Anomeric Effect: Origin and Consequences." This is a thorough treatment from a physical organic chemist's point of view. Those looking to find a description of applications to synthetic planning will be disappointed. That having been said, the depth of detail, as well as the range of topics that are covered, is impressive. The organization of the material follows a logical sequence. After a discussion of the several meanings of the term "anomeric effect," interpretations of the origin of the effect according to the various levels of theory are discussed. The consequences of the anomeric effect on energy and structure are also mentioned. The discussion is not limited to the more familiar systems incorporating oxygen or nitrogen.

A minor criticism concerns the sequencing of numbered structures. For example, on p. 227, reference is made to structure **98** which appears on p. 297. Although the *section* in which the structure appears is referenced on p. 227, no *page* reference is given. Since the table of contents which appears immediately after the title in each of the chapters also does not list page numbers, one is required to leaf through the chapter in order to locate some of the structural drawings.

The third chapter (39 pages), by Dodziuk, is titled "Unusual Saturated Hydrocarbons: Interaction between Theoretical and Synthetic Chemistry." The title is somewhat misleading, since synthesis is not discussed. An attempt is made to interpret the influence of theory on the synthesis of strained organic molecules, as well as the impact of synthesis of these systems in shaping the theory. This chapter provides more of an overview than an analysis. A number of the structural formulas in this chapter could be improved. For example, the structure of tetrahedrane (**3**, p. 352) is shown without perspective with a crossed bond. On p. 362, structures **51–55** are hard to interpret because stereochemistry is not indicated by means of wedged and dashed bonds. The same is true of **58** and **64–70**. The structural drawings for **98** and **99** are reversed. On p. 357 *MM2* calculations of strained molecules are described, and it is stated that qualitative conclusions regarding energy and geometry could be drawn even though the parametrization which was used was developed for non-strained hydrocarbons. On p. 364 this statement is contradicted. There were a few typographical errors (references 121, 130, and p. 354, bottom).

The fourth chapter (85 pages) by Young is titled "Stereochemistry of Metabolic Reactions of Amino Acids." The chapter includes more than the title would suggest. The chemicoenzymatic syntheses of many of the materials which were used to probe the mechanisms are also shown, so that the reader will find a great deal of imaginative preparative chemistry. The major enzymic reactions of pyridoxal and pyridoxamine are discussed in a short introduction, following which the reactions of most of the common amino acids, starting with glycine, are covered. The structural drawings were rendered clearly. In Scheme 45 (p. 415) one of the enzymes has been mislabeled. The correct enzyme is *O*-acetylserine sulphydrase (not synthetase). There were a very few typographical errors (pp. 405, 418, 440).

The last chapter, by Bures, Martin, and Willett, is titled "Searching Techniques for Databases of Three-Dimensional Chemical Structures" (44 pages). Screen set construction, similarity searching and substructure

ture searches are discussed, along with the dynamic relationship between molecular modeling and three-dimensional structure searching. The challenges of searching for a set of properties (i.e., interactions with a receptor), for a flexible molecule, are mentioned. As more nonspecialists use these tools, an appreciation of their limitations will be useful: failure to identify a hit within one's library of compounds is likely to be expensive. In section VII, the limitations of the computational methods and hardware, and some of the areas which will be important in the future are mentioned. The discussion of de novo structure design, in which molecular fragments are assembled into a three-dimensional molecule to fit a receptor, was particularly interesting.

Some familiarity with the common searching algorithms and software tools is assumed. Of necessity, this chapter makes mention of specific software packages, and is therefore likely to become outdated rather quickly. No matter; the chapter was thought-provoking and is likely to appeal to the dilettante within every chemist.

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Handbook of Natural Products Data. Volume 2. Pentacyclic Triterpenoids. VIQUAR U. AHMAD and ATTA-UR-RAHMAN. Elsevier Science BV, Sara Burgerhartstrasse 25, P.O. Box 211, 1000 AE Amsterdam, The Netherlands. 1994. vii+1556 pp. 16.5×24 cm. \$685.75. ISBN 0-444-88200-6.

This is a hefty (over 6 kg!) compendium of data on pentacyclic triterpenoids. The coverage includes ¹H- and ¹³C-nmr data (complete with assignments, if made), mass spectral data, infrared and ultraviolet spectra, melting points, and optical rotations. Source organisms are listed, although if the compound is very common the listing is not exhaustive. The data are keyed by footnotes to the abundant references to the primary data sources. This makes the pursuit of the original paper(s) quite rapid and convenient. If, for example, one wishes to examine the data supporting the ¹³C-nmr assignments, it is a simple matter to pick the relevant reference out of the list. Citations to X-ray crystallographic structure are also given where appropriate.

Each compound is listed in a separate monograph, with derivatives such as methyl esters listed under the parent compound. Entries are arranged by carbon skeleton; the most abundant class, the oleananes, occupy almost a third of the book. Within carbon skeletal types the compounds are ordered by increasing molecular weight. A complete set of indices makes access to known or unknown compounds relatively straightforward. Indices are provided to 1) compound name, 2) molecular formula, 3) molecular weight, 4) compound type, and 5) plant source. An Appendix gives the numbering systems for each of the 23 structural types and this numbering system is used consistently throughout the book. A few seco-triterpenes which are clearly derived from pentacyclic triterpenes are included, but otherwise the boundaries of the scope are clearly drawn. Sapogenins which fall into the category are given entries, with a notation that they occur in nature as the saponin.

While it has been my opinion for a long time that this sort of data is most useful when incorporated into a computerized database, this volume provides the maximum of utility and flexibility which can conceivably be attained in a book format. A comparison of several entries with the corresponding entries in the Chapman and Hall CD-ROM *Database of Natural Products* showed that the present book made a clearer distinction between epimers; e.g., Chapman and Hall indexes 3 α - and 3 β -substituted triterpenes under the same entry, while the present volume has separate entries for epimers. In addition, nmr and mass spectral data are simply not (yet) covered in the above-mentioned CD-ROM database.

The utility of the book in a practical situation can be illustrated by a recent application. I wished to locate ¹³C-nmr assignments for 3 α - versus 3 β -OH triterpenes. It was a matter of less than an hour to page through and locate compounds which had the respective substitutions and for which there were published ¹³C-nmr assignments. The original articles were rapidly assembled and the desired information was readily obtained.

As with any work of this magnitude, there are typographical errors and misspellings; however, none of any major consequence were detected. A few Latin names were misspelled (*ExCoecaria agallocha*, *Homonoia riparia*). Several graphics were cut off at the margins, but the quality of structure figures is otherwise excellent. The coverage extends into the literature of the early 1990s.

Any laboratory which must deal with triterpenes would be well advised to obtain this book. The rather large expense will be rapidly repaid by the time saved.

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