Book Reviews

The Alkaloids: Chemistry and Pharmacology, Vol. 48. Edited by G. A. Cordell (University of Illinois at Chicago). Academic Press, Inc., San Diego, CA. 1996. ix + 374 pp. 15 × 23 cm. $99.95. ISBN 0-12-469548-5.

This volume consists of four chapters, of which the first is a survey of the medicinal plants of New Caledonia, by Sévenet and Pusset. The presentation is arranged taxonomically, beginning with the Gymnosperms (Taxaceae) and proceeding to the Angiosperms (Magnoliidae, Dilleniidae, Rosiidae, and Asteridae), of which the last, containing the Apocynaceous family, is by far the most prolific in alkaloid content. There is a good deal of interesting information concerning the uses of many of these plants in traditional, ethnic medicine, which presumably prompted the examination of these plants in the first place. However, the survey is purely factual, and is presented from a botanist's point of view; there is, therefore, no reference to the chemistry and laboratory synthesis of the alkaloids. Although not all the alkaloids isolated are listed, over 450 are mentioned by name, and over 250 structures are illustrated.

The second chapter, by Bosch, Bonjoch, and Amat, is an invaluable review of the *Strychnos* alkaloids, which begins with a list of skeletal types followed by an alphabetical list of *all* known alkaloids, and a further list, which includes the structures and references to physical data and occurrences; some 224 alkaloids are listed. There follows an authoritative review of all the synthetic approaches to the *Strychnos* alkaloids published during the last 7 years. The discussion is arranged according to the ring that is formed last in the synthetic sequence; this has the advantage that, in general, it allows a unified presentation of the various strategies adopted by the major workers in this area.

The third chapter, by Borschberg, consists of an exhaustive account, covering the period 1983−1995, of the isolation, structure determination, and total synthesis of the *Aristotelia* alkaloids, in order of increasing complexity. Speculative proposals for the biogenesis of the alkaloids are presented in four schemes, which contain several interconversions that have already been mimicked *in vitro*, and the chapter concludes with what is known of the pharmacology of these alkaloids.

In the final chapter on *Erythrina* and related alkaloids, Tsuda and Sano present a brief summary of the occurrence of these alkaloids, with a tabular survey of the structures, names, and sources of all 94 erythrina and 67 homoerythrina alkaloids. The biosynthesis is also briefly discussed, followed by a relatively comprehensive section on structure determination. The construction of the erythrinan and homoerythrinan ring systems is then discussed in general terms, and the chapter ends with a survey of syntheses of the natural alkaloids. The period covered in this chapter is from 1979 to 1994.

This volume covers a vast amount of recent synthetic work, which is neatly summarized in over 120 reaction schemes, and in summary, it constitutes a notable addition to the Manske−Cordell series of monographs. Although none of the authors is a native English speaker, the standard of writing is impeccable throughout. This volume has a good subject index, but the practice of including an author index in this series appears regrettably to have been abandoned. Misprints are rare (I have only spotted five so far), and the presentation of the book is superb; it is a pleasure to handle.

This volume will be indispensable to anyone working in any of the areas covered, but in view of the wide-ranging and brilliant synthetic work discussed in three of the chapters, it will have a much wider appeal, since it illustrates in an impressive manner the state of the art of heterocyclic synthesis.

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Modeling Molecular Structures. Edited by Alan Hinchcliffe (University of Manchester Institute of Science and Technology). John Wiley & Sons, New York, NY. 1996. xv + 256 pp. 18.5 × 24 cm. $29.95. ISBN 0-471-95923-5.

This book, a part of the Wiley Tutorial Series in Theoretical Chemistry, gives a good survey of computational methods that have been utilized to describe molecular structure. The topics covered range from Molecular Mechanics through the Huckel Theory and Differential Overlap Models to the Ab-Initio package−Gaussian 92−and Electron Correlation. It also surveys a sampling of physical properties that have been calculated using the methods discussed.

The level of the book is for chemists who already have a grounding in computational methods and are interested in some of the computational details as well as how computational chemistry can be used to supplement experiments. There are a number of very good chapters. A chapter on Primary Properties that discusses Electric Multipole Moments and the Electric Potential is of interest as is the chapter on Induced Properties, which includes discussion of Induced Dipoles, Interaction Polarizabilities, and Magnetizabilities. Particularly noteworthy is the chapter on Potential Energy Surfaces. In this chapter the author uses simple examples to give an excellent feel for the methods currently used to find minima on potential energy surfaces. He also extends the methods to a discussion of using the Berny optimization technique to find minima on multidimensional surfaces and mentions, almost in passing, that this method can be extended to find transition states on multidimensional surface. The transition-state discussion is so brief, however, that it would leave the reader

wondering about details of the method. He also fails to give the reader an appreciation of the difficulty of applying the transition-state seeker to chemical mechanisms in general. The book ends with a discussion of half a dozen applications that will give the reader some flavor of recent applications of calculational methods to problems of chemical interest.

Although the book is well written, it is not clear what its primary intended audience would be. Unfortunately, the level of treatment is such that there is considerably more mathematical detail than the experimentalist interested in using the book as a compilation of what can be gained from using calculations would likely be interested in, but it is not sufficiently detailed to meet the needs of the person interested in mathematical aspects of the computations. It is probably best suited for use in an advanced undergraduate or beginning graduate course designed to introduce students to molecular modeling.

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Computer-Aided Molecular Design: Applications in Agrochemicals, Materials and Pharmaceuticals. Edited by C. H. Reynolds (Rohm and Haas Company), M. K. Holloway (Merck Research Laboratories), H. K. Cox (Zeneca Ag Products). American Chemical Society, Washington, DC. 1995. x + 428 pp. 15 × 22.5 cm. $109.95. ISBN 0-8412-3160-5.

Computer-Aided Molecular Design (CAMD) consists of many different methods aimed at solving a variety of chemical problems. As a collection, these methods form a set of powerful tools that are being used in a number of industrial and academic laboratories to design and develop new chemical products. This book brings together a number of examples in which CAMD has increasd the mechanistic understanding and/or provided energetic and structural information that has assisted in the design of new drugs, agrochemicals, and materials. The book is well organized and referenced (ca. 850), and each chapter is lucid. The balance between the theoretical bases behind the methods, the application of the methods, and results is well maintained.

Chapter one provides a short historic overview of computational chemistry and provides the reader with a brief description of the various CAMD techniques. The description covers the scientific underpinning of each method, what type of information can be obtained, and computational cost relative to other methods. In addition, modeling paradigms that have been found to be of general use such as structure-based design, novel lead generation, protein homology modeling, and catalysis simulation are discussed. The remainder of the book is divided into three sections. The sections contain case studies aimed at the understanding of the underlying mechanisms and/or design of new products in pharmaceutical, agrochemical, and material sciences. Molecular dynamics studies are presented on backbone-modified antisense oligodeoxynucleotides, drug diffusion in biomembranes, polyelectrolyte adsorption on mineral surfaces, and the behavior of organic molecules in zeolites. Studies using Genetic Algorithms (GA) to design a screen for antihinovirus agents and new materials are reported. In addition, case studies using Quantitative Structure Activity Relationships (QSAR), structure-based design, de novo design, and quantum mechanics are reported.

Overall, this book will be most useful to chemists who wish to apply CAMD to their own research. It provides a collection of examples that clearly demonstrate how CAMD can be used to assist in moving a project forward without setting up unrealistic expectations.

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Chemistry and Toxicology of Diverse Classes of Alkaloids. Edited by Murray S. Blum (University of Georgia). Alaken Incorporated, Fort Collins, CO. 1996. v + 386 pp. 15 × 22.5 cm. $99.50. ISBN 1-880293-06-4.

Five chapters on the chemical and toxicological properties of alkaloids from terrestrial and marine sources and one chapter describing alkaloids as anticancer agents comprise this book edited by M. S. Blum. *Chemistry and Toxicology of Diverse Classes of Alkaloids* is a companion volume to *The Toxic Action of Marine and Terrestrial Alkaloids* published recently by Alaken, Inc., which was reviewed in this journal (*J. Nat. Prod.* **1996**, *59*, 1218−1219).

In this book, G. T. Tan and J. M. Pezzuto describe *Toxic Alkaloids Pertinent to Cancer Chemotherapy* (711 references); Atta-ur-Rahman and M. I. Choudhary discuss *Toxic Alkaloids and Other Nitrogenous Compounds from Marine Plants* (87 references); M. S. Blum elaborates the *Chemistry and Toxicology of Arthropod Alkaloids* (112 references); W. Z. Antkowiak details *The Chemistry and Toxicology of Mushroom Alkaloids* (387 references); J. M. Jacyno delineates *The Chemistry and Toxicology of the Diterpene Alkaloids* (100 references); and T. Higa and J.-I. Tanaka survey *Bioactive Marine Alkaloids from Okinawan Waters* (125 references).

The chapter by Tan and Pezzuto focuses on specific alkaloids from the 15 families of antitumor alkaloids that have demonstrated clinical antitumor activity. Their survey provides insight into botanical source and occurrence, chemistry and structure−activity relationships, proposed biochemical mechanisms of cytotoxic/antitumor activity, clinical pharmacology and pharmacokinetics, clinical applications and toxicology, and mechanism of resistance to antitumor alkaloids. Pertinent alkaloids discussed include *Vinca* alkaloids, acronycine, camptothecin, *Cephalotaxus* alkaloids, ellipticine, indicine *N*-oxide, and swainsonine. This richly detailed presentation is accompanied by over 700 citations.