Additions and Corrections

A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules [*J. Am. Chem. Soc.* **1995**, *117*, 5179−5197]. WENDY D. CORNELL, PIOTR CIEPLAK, CHRISTOPHER I. BAYLY, IAN R. GOULD, KENNETH M. MERZ, JR., DAVID M. FERGUSON, DAVID C. SPELLMEYER, THOMAS FOX, JAMES W. CALDWELL, AND PETER A. KOLLMAN*

Some of the reported results in Tables 3−6 were carried out with "semifinal" force field parameters. Thus, there are some small changes in these tables when the calculations are run with the parameters reported in the paper. The modified tables are available in the supporting information for this issue of the Journal. We thank Lisa Yan of Biosym Corp. for pointing this out. We reemphasize that there are no changes in the force field parameters reported in the paper.

Supporting Information Available: Tables 3−6 from the published paper modified with results obtained when the final force field parameters are used (8 pages). This material is contained in many libraries on microfiche, immediately follows this article in the microfilm version of the journal, can be ordered from the ACS, and can be downloaded from the Internet; see any current masthead page for ordering information and Internet access instructions.

JA955032E

Total Synthesis of the Unusual Marine Alkaloid (−)-Papuamine Utilizing a Novel Imino Ene Reaction [*J. Am. Chem. Soc.* **1995**, *117*, 10905−10913]. ROBERT M. BORZILLERI, STEVEN M. WEINREB,* AND MASOOD PARVEZ

The compounds labeled **15** and **16** are, in fact, identical and are not enantiomers. The rotation reported for lactone **15** in the Experimental Section should be positive.

JA965400U

Book Reviews

Introduction to Molecular Electronics. Edited by M. C. Petty, M. R. Bryce, and D. Bloor (University of Durham, U.K.). Oxford University Press: New York. 1995. xiv + 387 pp. $42.50. ISBN 0-19-521156-1.

The mission of this book is to provide a solid overview of molecular electronics, a rapidly growing field of cross-disciplinary interest. The book is arranged as follows: (1) Molecular Electronics Overview, (2) Theory, (3) Piezo- and Pyroelectrics, (4) Molecular Magnets, (5) Organics for Nonlinear Optics, (6) Photochromism, (7) Physics of Conductive Polymers, (8) Conductive Charge-Transfer Complexes, (9) Liquid Crystals and Devices, (10) Langmuir-Blodgett (LB) Films, (11) Organic Molecular Beam Epitaxy (OMBE), (12) Scanning Tunneling Microscopy (STM), (13) Biological Membranes, (14) Biosensors, (15) Biomolecular Optoelectronics (mainly bacteriorhodopsin-based systems), and (16) Molecular Electronic Logic and Architectures.

One of the troublesome issues in the area of molecular electronics is simply the definition of "molecular electronics," since some authors refer to it as any organic-based system such as films, or crystals. Other authors have preferred to reserve the term "molecular electronics" for single molecule tasks, such as single molecule-based transistors. The authors here, in Chapter 1, clarify the terminology by defining two subcategories, namely "molecular materials for electronics" and "molecular scale electronics". These more precise definitions are welcome for clarification in the field. Chapter 1 continues with an overview of the usage and prospects for the two different subcategories of molecular electronics, which also provides a feel for the time of commercialization of such systems.

In general, the following chapters provide a concise explanation of the topics in a readable format. Since molecular electronics is so cross-disciplinary, one is unlikely to be an expert of wide breadth in the area; therefore, everyone interested has something to learn from the presentation. Moreover, there is a useful index that could provide a rapid method for key term searches. Such indexes are not always provided in books with multiple authors. One could certainly find several dedicated volumes on any one of the covered subtopics, yet this book provides the needed background and overview.

Whether discussing molecular electronics in terms of molecular materials (bulk) or molecular scale electronics (single molecules), the field is moving at an enormous rate. Though the fundamentals evolve more slowly and older coverage remains helpful, any coverage could become rapidly outdated. *Introduction to Molecular Electronics* has a copyright date of 1995, but few references are beyond 1991. Thus many of the newest advances go unnoticed. The preface unabashedly states that, "This book is based on a series of short courses given in the University of Durham during the summers of 1987 to 1991." Thus several of the more recent developments in molecular electronics are not covered. For example, LB film techniques are adequately covered while self-assembled monolayer (SAM) techniques (other than OMBE) are only tangentially addressed. Through the 1990s, more than one user of LB techniques has traded in their troughs for beakers. Another deficiency, again possibly resulting from the somewhat out-of-date

coverage, is a basic physical analysis of molecular scale electronics. If one is to have molecular scale systems, will the conduction process be similar to tunneling, ohmic transport, ballistic transport, or hopping between localized states? Though there is presently no unified theory on the subject, a book entitled *Introduction to Molecular Electronics* should at least cover the present physical arguments along with some experimental attempts to address single molecules. The clock has moved faster than the compiling/publishing process making several recent advances, unfortunately, absent from the coverage in this book.

In summary, *Introduction to Molecular Electronics* does an adequate job of defining the field and outlining the current and future obstacles. However, the lack of timeliness has adversely affected the coverage.

James M. Tour, *University of South Carolina*

JA9552914

Organic Molecular Crystals: Interaction, Localization and Transport Phenomena. By Edgar A. Silinsh (Latvian Academy of Sciences) and Vladislav Capek (Charles University, Prague). American Institute of Physics: New York. 1994. xxiv + 402 pp. $60.00. ISBN 1-56396-069-9.

In spite of the scope implied by the first part of the title, this book is focused on charge transport in organic molecular crystals. The treatment is by two internationally recognized experts in the field, one an experimentalist and the other a theorist. The writing avoids the difficulties of reading a verbal and stylistic collage so common with multiauthor works. The style is friendly and conveys the desire of the authors to communicate their interest and fascination with the field. However, it is clear that their readers are expected to possess a relatively easy familiarity with mathematics and physics.

The approach is rather pedagogical and explanations are unusually clear with quite well-conceived drawings illustrative of more difficult concepts. The authors have been quite creative in this regard, and it would have been nice to have even more than the goodly number presented. Nevertheless, the written exposition suffices where figures are not given.

The book invites comparison with the earlier work of Silinsh, *Organic Molecular Crystals: Their Electronic States*, published nearly 14 years ago. Of course, the present tome is more current (references to 1994) and embodies all the advances made over the intervening years. The presence of the theorist coauthor gives a more encompassing and unified treatment than was conveyed by the earlier work. While this may also be attributed to the progress that has been made in the field, there is no question that the tone of the present volume reflects this influence.

The full range of current problems of charge transport in these systems is addressed and controversy is not avoided. Of particular interest to some will be the enlightening discussion of charge transfer states in organic molecular crystals. Additionally, the presentation of an energy level scheme for organic molecular crystals should be considered by all who are concerned with the electronic structure of these systems. Noteworthy is the treatment of carrier transport over a complete temperature range. The authors' polarization model employing their notion of the nearly small polaron is effective in providing a coherent conceptual framework for the treatment of the rather diverse phenomena associated with carriers in organic molecular crystals.

Since the formalisms for electron transport and excitons are the same, it is, of course, tempting to treat them together. But the handling of excitons and excitonic phenomena is much less complete than for the carriers. The involvement of excitons is mainly from the perspective of, and in service to, the understanding of charge transport, and there are aspects of excitonic states of optical interest (e.g., polaritons) that are ignored. With respect to the more limited subject matter of the book, however, the treatment of excitonic states is relevant and complete.

The first two chapters of the book, about 80 pages, serve as a fine general introduction to the properties of molecular crystals which could serve many who desire a concise, accurate, and coherent overview and introduction to collective interactions in molecular crystals. Beyond that, however, the book is of interest to the more limited audience of physicists and physical chemists concerned primarily with charge transport in organic molecular crystals. Many in this more circumscribed group will very likely want to have a copy on their bookshelves.

Craig J. Eckhardt, *University of Nebraska-Lincoln*

JA945159O

Nucleophilic Aromatic Substitution of Hydrogen. By Oleg N. Chupakhin and Valery N. Charushin (Urals State Technical University) and Henk C. van der Plas (Agricultural University, The Netherlands). Academic Press: San Diego, CA. 1994. x + 367 pp. $95.00. ISBN 0-12-174640-2.

The electrophilic removal of hydrogen from aromatic systems and the nucleophilic removal of a range of activating groups in aromatic systems have been extensively studied and reviewed and are well established. However, far less systematic attention has been devoted to S^H_N reactions, the nucleophilic aromatic substitution of hydrogen. The intention of the authors was to show "that the S^H_N reaction is an advanced field of chemistry by reviewing the material on S^H_N substitution reactions published in the literature up to 1993, showing the potential synthetic applications of S^H_N substitutions, and discussing the mechanism involved in these reactions." They have accomplished all of their objectives and have done so in a comprehensive and readable manner.

The book begins with an excellent introduction comparing and contrasting the entire range of S_N chemistry and setting the tone for the differences among various S_N reactions and the S^H_N reaction. The remainder of the book consists of just three chapters, but each is organized in a comprehensive manner. One chapter is devoted to Nucleophilic Substitution of Hydrogen in Arenes, including reaction of unactivated arenes, arene−metal complexes, nitroarenes, and electrochemical S^H_N reactions. A second chapter covers the Nucleophilic Substitution of Hydrogen in Heteroaromatics, with primary emphasis on reactions in azines and aza-aromatic substrates containing quaternary nitrogen. The final chapter is a thorough review of a variety of reactivity aspects and the mechanisms of the S^H_N reaction.

A useful and informative inclusion at the end of each chapter is the complete description of several typical experimental procedures for carrying out S^H_N reactions.

This is an excellent book that will prove useful for those interested in the chemistry of S_N reactions.

John P. Idoux, *Coastal Carolina University*

JA945154R