

**Energetic Materials, Part 1: Decomposition, Crystal and Molecular Properties.** Edited by Peter A. Politzer and Jane S. Murray (University of New Orleans). From the series: *Theoretical and Computational Chemistry*, Volume 12. Elsevier: Amsterdam. 2003. xx + 466 pp. \$210.00. ISBN 0-444-51518-6.

In this book, the editors have compiled a selection of articles from that coterie of investigators who focus their research on explosives and propellants. The 16 chapters vary from a review of chemical behaviors to detailed discussion of computational results on a single system. Although a volume in a series devoted to theoretical and computational chemistry, this book deals more with experimental and computational chemistry and is devoid of any true theory. This appears to be the intent of the editors, as indicated by the title. There is no obvious structure to the sequence of chapters, making the connectivity between the topics minimal. The subjects of the chapters include an interesting historical review, the use of X-ray crystallography to obtain accurate electron densities, prediction of stable but, as yet, unmade materials, and, variously, molecular dynamics simulations, quantum chemical and density functional calculations of reaction paths, stabilities, heats of formation, mechanical properties, electronic structures, and optical properties. The quality of the articles varies, but a particularly fine exposition on the decomposition mechanism of FOX-7 is provided.

References are up-to-date, and several chapters have excellent and detailed bibliographies that will be of great use to those interested in entering the field. However, the references in some chapters are quite brief, self-referential, or both. This may be excusable since the subject matter is narrowly focused on a limited number of materials and involves a somewhat closed set of workers. The book is well produced, but its cost limits it largely to being archival material.

Much of the reported work is on free molecules, even though almost all applications involve condensed phases. The chapters treating solid-state behavior of these materials appear, with but few exceptions, to have little relationship to current (or even past) work in organic solids. For example, a calculation of the optical properties of selected energetic materials produces plots of the joint density of states of these molecular solids, a view useful for semiconductors but of limited benefit for molecular crystals. The choice to ignore decades of study of the optical properties of molecular crystals based on exciton theory, which was extensively developed by chemists and chemical physicists, is not surprising because much of the work on the physical chemistry of energetic materials is done by non-chemists. On the other hand, it is rather startling to read about conclusions drawn, largely by chemists, from calculations that claim to predict the very complex behavior of the reactions of energetic materials that are solids (many polymorphic), since, as re-emphasized recently by Gavezzotti, it is not yet even possible to predict, a priori, the crystal structure a given mole-

cule will assume, much less the number of polymorphs that will form.

Those familiar with organic solid-state chemistry should not expect to find discussions cast in terms of the topological postulate, reaction cavities, steric compression, mechanical susceptibilities, Zimmerman's calculative approaches, and other concepts that have been developed since Schmidt initiated his seminal studies on the reactivity of organic solids. Indeed, it can be argued that most of these ideas are not applicable to these materials. Chemists interested in the problems posed by these extremely complex and interesting systems may find that reading these reports will pique their curiosity, challenge their understanding of organic solid-state chemistry, and suggest new avenues of research.

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**Oxazoles: Synthesis, Reactions, and Spectroscopy, Part B. The Chemistry of Heterocyclic Compounds, Volume 60.** Edited by David C. Palmer (Johnson & Johnson Pharmaceutical Research & Development, L. L. C., Raritan, NJ). John Wiley & Sons, Inc.: Hoboken, NJ. 2004. xxii + 692 pp. \$325. ISBN 0-471-21925-8.

This book, the second part of Volume 60 in *The Chemistry of Heterocyclic Compounds* series, mainly focuses on the chemistry of oxazolones and oxazolines. Oxazoles were reviewed previously in Volume 45 of this series in 1986 as well as in Part A of this volume; the material in Part B largely covers developments from the late 1980s through 2001. The citations are thorough, including references to reviews, journal articles, and the patent literature.

An excellent feature of this volume is its organization. Each chapter is subdivided by structural type, and under each subtype is a section on chemical synthesis arranged by starting material, followed by a section describing characteristic chemical reactions. Most chapters contain an addendum listing the most recent developments in the field. This organization allows the reader to locate a specific area of interest easily. The text is well written and understandable. In addition, the chapters have many synthetic schemes and extensive tables that are helpful in understanding the scope and limitations of various chemical transformations. Mechanistic schemes are also included where appropriate.

Another hallmark of this book is that the chapters are very comprehensive and cover synthetic methodology as well as applications to natural product synthesis, medicinal chemistry, and, to a limited extent, polymer chemistry. Chapters 8 and 9 are devoted to 2-oxazolines and bis(oxazolines), which have a crucial role in asymmetric synthesis because they are readily derived from optically pure  $\alpha$ -amino acids.

This book should be useful for novice organic chemists who are unfamiliar with the chemistry of oxazolones and oxazolines. However, by virtue of its organization and thoroughness, it should also serve as an important reference for experienced researchers who are interested in specific information regarding either the synthesis or reactions of these heterocycles. In summary, while the magnitude of this work precludes the

inclusion of references much beyond the year 2001, it should be a valuable resource for organic chemists.

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