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A Review of "Organic Crystal Engineering: Frontiers in Crystal Engineering"

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Book Review

Organic Crystal Engineering: Frontiers in Crystal Engineering, 2010, edited by Edward R.T. Tiekink, Jagadees J. Vittal, and Michael J. Zaworotko, John Wiley & Sons, New York, NY, 336 pp., \$260.00, ISBN 978-0-470-31990-1

Crystal engineering has now progressed to a mature discipline by the concerted effort of its practitioners over several decades of study. The organizational power of molecular crystals continues to offer in-depth access to important structural principles less accessible from other material phases. The development of crystal engineering can be measured by the overall increase in literature contributions (e.g., articles, reviews, and journals dedicated to the field). However, a potentially more important indication of its contribution to the scientific community is in its recent application toward untangling high-impact scientific challenges. In this book, editors Tiekink, Vittal, and Zaworotko have assembled a timely review that encompasses a variety of crystal engineering topics. The first volume of this series by a similar name (*Frontiers in Crystal Engineering*, 2006) explored a collection of topics ranging from the fundamental aspects of crystal/supramolecular motifs to the design and practical aspects of pharmaceutical co-crystals. This previous work provided a valuable resource that has now been updated and extended by a fresh volume and a new group of chapter contributors.

The book opens with two chapters dedicated to computer-assisted crystal structure assessment. The first shows the utility of the Cambridge Structural Database (CSD) in crystal engineering by offering a summary of the principal application areas. The strength of this contribution rests with its treatment of new tools for database research as well as the more recognizable features such as structure validation and retrieval methods for the CSD. Chapter 2 presents a perspective on computational crystal structure prediction and includes two sections aimed at the methods employed for screening structures and the current capability and future directions of crystal structure prediction.

The next two chapters explore pharmaceutical co-crystals. The first of these introduces key topics related to the discovery and development processes of active pharmaceutical ingredients (APIs). An abundant supply of literature examples offers practical connections to many celebrated pharmaceuticals, with an emphasis on drug formulation challenges and improving bioavailability via co-crystal formation. In the next chapter, co-crystals constructed from surfactant and aromatic components provide an additional view, *albeit* more loosely connected, of APIs. The structure and common packing modes are addressed for many compounds with additional insights into engineering desired properties of APIs and perfumes.

As the preface to the book points out, modifying crystal structures to meet the need of specific applications requires exquisite control of the building blocks and, thus, an intimate

understanding of crystal cohesion. The remaining portion of the book is divided into chapters (4–8) based on functional group associations via hydrogen bonds. These groups include amides, alcohols, pyridines, thiocarbamides, and thioureas/ureas. Understanding the structural boundaries of supramolecular motifs constructed from non-bonded contacts supplies the greater part of these discussions. While such fundamental studies are essential to understanding the grammar of crystal engineering, the lack of current examples (moving beyond structural investigations) of functional materials other than solid-state pharmaceuticals is somewhat disappointing.

The coverage of the literature is not comprehensive, nor is it meant to be. The authors of the individual chapters have selected a range of examples, with an emphasis on motif and crystal structure prediction. Most chapters include citations to quite recent work, and the book is thoroughly indexed and well organized.

Given its extensive treatment of literature examples and practical emphasis, this book should make a valuable addition to the novice's library or those entrenched in the crystal engineering discipline. Institutional libraries should certainly include this on their acquisition list.

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