

Two noteworthy tables are Table 3.1 and Table 3.2. These two tables provide information concerning theoretical and experimental parameters of selected bond potentials and about packing energies of selected organic molecules. Section 2 of this chapter is also particularly noteworthy in that it discusses thermodynamics. The discussion is brief but does touch upon the important points of thermodynamics as it relates to computer modeling of molecular systems.

The next three chapters, Chapter 4 written by B. Van Eijck, L. Kroon-Batenburg, and J. Kroon, Chapter 5 by L. Bartell, and Chapter 6 by R. Gdanitz, all cover various computational aspects of molecular simulations. Chapter 4 relates primarily to classical techniques of molecular simulations, i.e., Molecular Dynamics; Monte Carlo. Some of the computer codes briefly discussed and referenced are MM2/MM3, AMBER, GROMOS, ECEPP/UNICEPP, CHARMM, SYMBYL, and CFF91. Chapter 5 concerns the modeling of nucleation and phase transitions in molecular clusters. For those not familiar with experimental techniques used to study clusters, Chapter 5 is a good general review of some of these techniques. Chapter 6 discusses *ab initio* predictions of various molecular systems, but in particular how possible molecular crystal structures could be predicted. The author correctly points out that this is a very difficult area to simulate and also briefly review the many procedures used to perform modeling studies of crystal structure.

The final chapter of this book, Chapter 7 authored by G. Clydesdale, K. Roberts, and E. Walker, is primarily a summary of how and why the study and modeling of crystallization is important. It covers numerous crystalline materials, from both a simulation and experimental perspective. The computer program HABIT95 is discussed and is used in most of the simulations of the materials presented. It is pointed out that this program is used to aid in the morphological investigations of the various molecular materials.

In summary, this is a useful book, dealing primarily with computational modeling of molecular systems. It does concentrate its focus on the molecular solid state, but has very useful material concerning molecular modeling in general and the computer programs available to do this modeling. I recommend it to anyone who is interested in determining if molecular modeling is important to an understanding of how molecules interact and specifically how molecules coalesce into crystalline materials.

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**The Beilstein System: Strategies for Effective Searching.** Edited by Stephen R. Heller. ACS: Washington, DC. 1998. xiv + 208 pp. \$74.95 ISBN 0-8412-3523-6.

During the 1980s, the Beilstein Institute was a moribund operation, ploddingly producing a massive handbook series that few institutions could afford to buy, and even fewer cared to use. The antiquated *Handbuch* concept, which tried to codify the literature of organic chemistry and its cognate fields in systematic and timely fashion, had been unable to keep up with the rapid expansion of those fields since the 1960s. The venerable *Beilstein Handbook* was increasingly seen as an expensive, and expendable, anachronism. Then in the late 1980s Beilstein decided to re-invent itself as a database producer, to change its focus and image from a dusty, complicated handbook found only in libraries to a benchtop tool for chemists all over the world. Its success in doing so in only a few short years did not come without difficulty, but the transformation has been remarkable.

The metamorphosis began with the debut of Beilstein as an online database on the STN and Dialogue networks in 1988. User acceptance of this expensive pay-as-you-go access was minimal, however, especially in academic circles.

The subsequent and present incarnation, called Beilstein Crossfire, appeared in 1995. Crossfire is a powerful client-server database system

that can be either mounted locally or accessed remotely on the Internet. The database now contains information on over 7 million organic structures and 7 million reactions, drawn from the literature back to the 18th century. Coverage is now more up-to-date than was ever the case with the printed work (although Beilstein has nowhere near the currency or breadth of *Chemical Abstracts*). In addition to extraordinary speed in carrying out substructure searches, Crossfire boasts a hyper-linked data structure, allowing users to move seamlessly from substance to reaction to literature records just by clicking a mouse.

Its subtitle notwithstanding, *The Beilstein System: Strategies for Effective Searching*, is not really a how-to manual for Crossfire users. This monograph is rather a collection of chapters by twelve contributors (six of whom are current or former Beilstein staff) that outlines the history, content, structure, implementation, and uses of Beilstein Crossfire. One chapter, by J. Barnard and D. Walkowiak, explores in some detail the technical nuts and bolts of Beilstein's chemical structure-based search system. Chapters by A. Lawson and E. Zass give useful descriptions of the Reactions module of Crossfire, which is potentially the most powerful component of the new Beilstein system, in terms of providing new digital pathways for synthetic organic exploration. Comparisons to other commercial reaction databases are particularly enlightening. A chapter by K. Rouse and R. Beckman addresses Beilstein's evolution in the academic setting, culminating in the "Minerva" consortium that was established in late 1996, enabling U. S. research universities to gain affordable (for now) access to Crossfire. W. Warr offers a similar overview of Beilstein's implementation in industry. The book concludes with a description of AutoNom, a related software module that assigns IUPAC names to structures. Together, these contributions give the reader a thorough summation of what Beilstein is, how it works, and how it can be utilized.

Computer systems evolve very quickly, and if there is a drawback to a book such as this, it is that it can only present a snapshot of its subject at a certain point in time. *The Beilstein System* is nevertheless a good introduction to a complex tool, without being an overt marketing ploy. The book offers the kind of in-depth background that software documentation always lacks, and it will be useful to chemists and information specialists who use Beilstein to locate chemical data, and to decision-makers who are considering implementing it.

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**Specialist Periodical Reports. Nuclear Magnetic Resonance, Vol. 26.** By Senior Reporter G. A. Webb (University of Surrey). The Royal Society of Chemistry: Cambridge, U.K. 1997. xxii + 604 pp. \$407.00. ISBN 0-85404-312-8.

The periodical reports provide systematic and detailed review coverage in major areas of chemical research. Compiled by teams of leading authorities in the relevant specialist fields, the series creates a unique service for the active research chemist with regular critical in-depth accounts of progress in particular areas of chemistry.

Volume 26 of the SPR on NMR contains the familiar combination of annual and biennial reports which, taken together, attempt to provide a comprehensive coverage of the NMR literature. Current subject areas covered are Amino Acids, Peptides and Proteins, Carbohydrate Chemistry, Catalysis, Electron Spin Resonance, Nuclear Magnetic Resonance, Organometallic Chemistry, Organophosphorus Chemistry, Photochemistry, and Spectroscopic Properties of Inorganic and Organometallic Compounds.

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