Book Reviews *

Atmospheric Chemistry and Physics: From Air Pollution to Climate Change. By John H. Seinfeld (California Institute of Technology) and Spyros N. Pandis (Carnegie Mellon University). Wiley-VCH: New York. 1997. $89.95. xxvii + 1326 pp. ISBN 0-471-17815-2.

In the foreword to their book *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change*, authors John H. Seinfeld and Spyros N. Pandis describe their massive new work as the successor to Seinfeld's *Atmospheric Chemistry and Physics of Air Pollution* (Wiley, 1986). That book quickly proved to be a very successful addition to the literature of air pollution and now occupies the shelves of researchers and academics worldwide. Of course, the body of knowledge loosely termed "atmospheric chemistry" has burgeoned since this book was published and an update to Seinfeld's classic has been expected.

This new book, however, has far greater aspirations than merely incorporating the past decade's advances into an updated air pollution textbook. Rather, the authors tackle another and much larger goal: providing a distillation of the physical science underpinning climate change. There is a strong basis of reasoning behind this approach. After all, as currently understood, the forcing mechanism behind climate change (at least anthropogenically induced climate change) derives from enhanced concentrations of certain atmospheric trace constituents resulting from human activity—in other words, air pollution. It seems reasonable to address both issues simultaneously given this substantial overlap in subject matter. Alas, it appears that the authors required almost twice as many pages to achieve this further goal. The heir to Seinfeld's 738-page text of 1986 is a 1326-page behemoth nearly seven cm thick. Either there is not so much overlap after all, or, as we suspect, the somewhat amorphous subject of climate change is vastly more complex than the subject of air pollution.

As befits a text on climate change (and in keeping with the current trend for a "systems approach"), Seinfeld and Pandis spend a good deal of time describing the atmosphere/climate system rather than immediately diving into the specifics of air pollution. Pedagogically this is a desirable approach, especially for students studying the field from the standpoint of applied chemistry. After this lucid introduction, the authors then plunge into the nitty-gritty aspects of atmospheric chemistry. Much of the earlier book's material still appears intact, interspersed with additional new topics as appropriate. There are now chapters devoted to processes specific to certain atmospheric regions (troposphere and stratosphere). The treatment of aerosols has been expanded and reorganized, with an entire chapter now given to nucleation (activation) of aerosols. Much of the material in this chapter could well be incorporated into a graduate course in cloud physics. Curiously, the discussion of cloud physics itself is deferred for several chapters. The radiative impact of aerosols, both direct and indirect (indirect referring to modification of cloud radiative and dynamical properties through modulation of aerosol spectra), appears near the end of the book.

This somewhat disjointed organization evinces the book's pedigree as an air pollution text and is an inevitable outcome of trying to cover several topics simultaneously. In general, the second half of the book, which is where most of the new climate material appears, seems to bounce about between air pollution and climate change, though the transitions are smooth and the approach methodical.

It is a curious fact that the more a book tries to cover, the more vulnerable it is to complaints of omission, and *Atmospheric Chemistry and Physics* is no exception. Perhaps most lacking is a more thorough and ongoing discussion of the constant interplay between the climate system as a whole and its constituent parts, specifically here chemical composition and anthropogenic forcing. The sections of the book dealing with numerical modeling have a decided air-pollution monitoring and prediction slant. It would have been extremely useful to have a full chapter devoted to current efforts to combine sophisticated coupled ocean-atmosphere general circulation models with advanced biosphere models. The strongest coupling between these two systems appears to be through biogeochemical cycling and, as such, a survey of the tremendous ongoing worldwide effort to understand this complex issue would seem to be an indispensable part of any comprehensive text on atmospheric chemistry and climate. Also missing is a discussion of the use (and often abuse) of isentropic trajectory models in determining source and sink regions of various anthropogenic pollutants.

The sheer size of this book will no doubt make students anxious, and it is perhaps less useful as a textbook than the previous version. On the other hand, topics are presented in a meticulous and rather complete manner, allowing the instructor to pick and choose chapters or sections as they suit a particular class. As in the earlier book, a useful set of problems, rated by difficulty, appear at the end of each chapter, along with the references for that chapter. The problems range from direct application of concepts found in the chapter to problems requiring original computer code to obtain the solution. The problems are generally of high quality, but no subset of answers is provided to allow students to monitor their mastery of the material. As far as we know, no instructor's manual is available either. For a book of this size and breadth there are remarkably few errors, although some notation could be rather confusing to the chemistry student. An example of this is a chemical reaction which the authors treat as an algebraic expression. By subtracting products from both sides of the chemical equation, they obtain the result that reactants minus products equals zero. While mathematically plausible, this will certainly raise a chemist's eyebrows!

All this being said, there is no doubt that, at $89.95, *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change* provides a lot of bang for the buck. This book is the most comprehensive and up-to-date single source on the subject of human impact on atmospheric composition and climate. It will remain one of the authoritative texts for years to come and, as such, we recommend that all atmospheric researchers acquire this book for their personal libraries.

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Theoretical Aspects and Computer Modeling of the Molecular Solid State. Edited by Angelo Gavezzotti (University of Milan, Italy). John Wiley & Sons: Chichester, New York, etc. 1997. x + 237 pp. $70.00. ISBN 0-471-96187-6.

The book *Theoretical Aspects and Computer Modeling of the Molecular Solid State*, is both a very informative book as well as a comprehensive book on the subject of the various techniques available in computer modeling of the molecular solid state, at least in a summary manner. The book also makes a very useful introduction to molecular modeling in general.

The first chapter in this work was written by the editor himself, A. Gavezzotti, and covers the subject of crystal symmetry and molecular recognition. Although it is not a comprehensive treatment of symmetry, which of course it cannot be, it does provide the reader with a good overall treatment of symmetry especially as it relates to the crystal state of matter. Also, for someone who does not spend a great deal of their time in this field but occasionally "dabbles" in it, Chapter 1 provides a good overall review. This chapter also provides a useful section, Section 2.5, which supplies references to related literature and suggestions for further reading.

Chapter 2, written by S. L. Price, presents a discussion of intermolecular forces in the molecular solid state. However, in reading this chapter, one realizes that it is applicable to a much more general class of systems than just the molecular solid state. It discusses all of the various types of intermolecular interactions. One very useful feature of this chapter is its discussion of several programs available for performing calculations on intermolecular interactions. One program in particular worth noting is DMAREL, a program written to simulate static crystals of molecules whose electrostatic interactions are represented by a distributed multipole model.

The next chapter, Chapter 3, authored by the editor A. Gavezzotti and G. Filippini, discusses the energetic aspects of crystal packing. It begins with a brief synopsis of computer modeling of organic solids.

*Unsigned book reviews are by the Book Review Editor.

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 hyperlinked 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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