Computer Software Reviews*

Chem Master. Version 3.2. Envirogenics Inc., P.O. Box 596, St. Marys, PA 15857. List Price $950.00–$4950.00 depending on version and features.

Chem Master is a computer application for preparing, maintaining, and reporting on chemical information including identity and hazards associated with these chemicals. It permits the generation of reports to satisfy the requirements of Community Right to Know under SARA Title III. The application also permits the printing of labels.

The application package reviewed required an IBM PC/XT, PC/AT, or PS/2, or 100% compatible. A minimum of 640K Ram and at least a 40 megabytes hard disk with at least 25 megabytes of space available is required. MS-DOS 3.3 or above is required to run the application. The software package is available in the single user or multi-user packages.

The application comes with an installation routine that makes quick work of the installation. The reviewed version included a database of approximately 4700 chemicals. The indexing of this database appears slow but is well worth the wait because of the wealth of information that came with the database. The software comes prepackaged for a variety of printers including the Epson and IBM line of printers. The IBM Graphics selection is generic and should work with compatible printers. The selection of a printer is required at the initial startup of the program. Later changes are made from the System Parameter menu selection.

The application is easy to use after the initial setup of facilities and work areas. The tracking of multi-work areas is easily done with this application. The user environment consists of a series of menus that intuitively guide the user through the program. There is on-line help available with the touch of the F1 key. The help information provided is informative and easily understood. The application allows for easy entry of new chemicals to the master database. The program will check the CAS registry number for all new chemicals added to prevent the duplication of information already in the master database. The application allows for easy transfer of chemicals among work areas via the inventory transfer option. This is particularly useful where operations are relocated or chemicals are shared among related facilities as in an academic institution. The application provides worksheets to compute the releases of toxic chemicals to air, land, or offsite locations per EPA requirements.

The available reporting options are numerous. These include but are not limited to SARA Section 304 (Spill and Release analysis), SARA Section 312 Tier I Survey, SARA Section 313 Toxic Chemical release summary. One important criteria of OSHA HAZCOM is labeling. The application provides labels in large formats and small formats. The large format provides OSHA precautionary label information, Hazard Rating, and Emergency contact and Emergency Phone number. This makes the information available for employee or other concerned person. The small format label provides less information but gives vital information including the Hazard Rating and Target Organs of the chemical.

The application is a useful tool for preparing and maintaining chemical information, including their identities and hazards and related government regulation. The program is easy to learn. The accompanying manual is easy to follow. It is enhanced by the on-line help that is provided by the application. The application is also available in a multi-user version.

*Unsigned reviews are by the Computer Software Review Editor.

Book Reviews

Advances in Heterocyclic Natural Product Synthesis. Volume 2. Edited by William H. Pearson (University of Michigan). JAI Press: Greenwich, CT and London, England. 1992. xi + 400 pp. $90.25. ISBN 1-55938-333-X.

There are five chapters in this important and superbly written monograph on the synthesis of heterocyclic natural products. The first contribution is titled "Design, Synthesis and Evaluation of Functional Analogues of CC-1065 and the Duocarmycins: A Study of Structural Features Effecting DNA Binding Selectivity". In this chapter Bolger describes the design, preparation, and evaluation of functional analogues of (+)-CC-1065, the potent antitumor/antibiotic isolated from cultures of *Streptomyces zelensis*. The approach rests heavily on molecular modeling coupled with the initial studies on CC-1065 by the Hurley and Upjohn groups. A concise preparation of CDPI and its subsequent incorporation into oligomers is presented which employs the indole synthesis pioneered and developed by Hemetsbergen, Moody, and Rees, respectively. Because of the structural nature of CC-1065 analogues, this chapter is replete with modern methods for the regiospecific synthesis of indoles and indolines. In addition to efficient target-directed organic synthesis, this chapter also includes an analysis of the in vitro and in vivo cytotoxic activity of CC-1065 analogues and the duocarmycins. For example, a model for the duocarmycin DNA alkylation was constructed and illustrated for the single, high-affinity binding site within w794 DNA. The in vitro and in vivo activity are rationalized via this model which had been generated with MacroModel (Version 2.5 AMBER supplemented with parameters for duocarmycin derived from an X-ray crystal structure). The parameters employed for the molecular graphics, as well as color photos of the proposed DNA–analogue binding, are contained in the Appendices to this section.

This chapter serves to highlight the use of modern synthetic methods for the construction of indole-related natural products, but the contribution is much more profound. Simply put, it is the manner in which modern medicinal chemistry should be carried out. This book should be required reading for young students in medicinal chemistry as well as those actively engaged in the search for clinically important anticancer agents.

The second section deals with the synthesis of naphthyridinomycin authored by Tohru Fukuyama. This is not simply an excursion through the chemistry executed in the author's own laboratory at Rice but is a walk through the elegant approaches to naphthyridinomycin which have occupied the attention of several research groups including those of Evans, Danishefsky, Joule, and Garner. Both retrosynthetic analyses and careful descriptions of novel chemical reactions are included. The remainder of the chapter contains both the model studies and successful completion of the syntheses of (±)-cyanocycline A, (+)-cyanocycline A, and naphthyridinomycin by Fukuyama and co-workers. The strategy of the approach at Rice, as well as each reaction, is described in detail. The plethora of new reagents and novel reaction conditions make this chapter well worth reading for any organic chemist.

In the section titled "Bis-Heteroannulation: Total Synthesis of Furanoterpenes, Butenolides, Lactones and Related Materials", Jacobi clearly illustrates the versatility of the intramolecular Diels–Alder reaction of acetylenic oxazoles for the synthesis of important natural products. The regioselectivity of this process was employed in a highly efficient manner to prepare evodone, ligularone, petasalbine, gnididione, isognididione, paniculide-A, (−)-norsecurinine, and (+)-norsecurinine as well as to provide an approach to geigerin. The method has since been extended to thiazoles to provide synthetic routs to 7α-eremophilane, as well as the 7β-isomer. Since the precursor azoles are readily available from a variety of carboxylic acid derivatives, this bis-heteroannulation strategy should be applicable for the preparation of a wide range of natural products. As Jacobi illustrates time and time again, there is no ambiguity in the position of the furan or thiophene nucleus relative to other functionality present in the molecule, providing regiocontrol unavailable in other approaches to these systems.

Harring, Edstom, and Livinghouse have contributed a chapter which should be read by all those who plan to use episulfonium (ESI) and episelenonium (ESeI) ions in organic synthesis. The discussion begins with current myths which surround the chemistry of episulfonium ions and quickly goes to "reality" in this area. In regard to the intermediacy of ESIs and ESeIs in organic reactions, a review of both mechanistic and stereochemical experiments is included to provide the reader with an accurate picture of the chemistry of these two species, respectively. The generation of ESIs and ESeIs is discussed followed by attack of oxygen, nitrogen, carbon, and sulfur nucleophiles on these onium ions. The use of ESIs and ESeIs in the synthesis of (±)-retronecine (Kametani) and

the mitomycins (Danishefsky) and the elegant intramolecular cyclizations by the Livinghouse group are appropriately included. The section concludes with the total synthesis of racemic-nimbidiol, totarol, and totarolone.

Reviewed in the final chapter are the isolation, structure determination, biosynthesis, and synthesis of the marine alkaloids characterized by the pyrido[*k,l*]acridine skeleton. These bases of planar structure are found in a number of different marine animals. Moody and Thomas describe the cytotoxic activity of these alkaloids and correlate this biology with reference to recent results on the mode of action of intercalating drugs. The total synthesis of a number of these alkaloids including amphimedine, ascididemin, 2-bromoeptoclinidinone, and cystodytin, as well as routes to related compounds, is included. This short chapter is full of information of importance to scientists in this field. Although this book as a whole lacks a subject and author index, it should still be an important addition to the libraries of synthetic organic, natural products, and medicinal chemists.

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Advances in Solid-State Chemistry. Volume 2. Edited by C. R. A. Catlow (The Royal Institution, London). JAI Press: London and Greenwich, CT. 1991. ix + 393 pp. $78.50. ISBN 0-89232-954-8.

This volume has four chapters:

Chapter 1, The Growth and Characterization of Silicon Carbide and Diamond for Microelectronic Applications, by R. F. Davies and J. T. Glass contains 111 pages and 270 references. If silicon carbide and diamond could be prepared with the quality currently available for silicon, many exciting possibilities for microelectronic devices would be opened up. In this excellent article, some of the appalling difficulties in the way and the progress toward their solution are well described. There is much food for thought here for an "ivory tower" chemist. Questions such as the factors determining the composition and structure (and their inter-relationship) of "SiC" are far from being answered. The mechanism of the production of diamond by gas phase synthesis also offers some nice theoretical challenges. The history of this topic is also fascinating. Although gas phase diamond synthesis was clearly demonstrated in Russia in the early 70's, it has only recently been taken seriously. Now, as the authors state, "it appears that with a microwave oven or a welding torch and methane and hydrogen sources it is straightforward to prepare diamond films". Fullerene chemists take note.

Chapter 2, Molecular Dynamics of Ionic Crystals, by P. M. W. Jacobs, Z. A. Rycerz, and J. Mościński contains 73 pages and 228 references. This article starts out with a forthright general review of the technique of molecular dynamics and its strengths and weaknesses when applied to ionic crystals. A number of results particularly with respect to ionic motion in solid electrolytes are then succinctly described and their implications discussed.

Chapter 3, Mössbauer Effect, Magnetic and Structural Studies of Wüstite, $Fe_{1-x}O$, by G. J. Long and F. Grandejean contains 35 pages and 96 references. The study of the defect structure of wüstite has played an important role in the development of solid state chemistry. The authors describe recent progress on this difficult topic, which is still far from closed.

Chapter 4, Ab-Initio Calculations of Inter-Ionic Potentials and the Cohesive Properties of Ionic Solids, by N. C. Piper contains 170 pages and 310 references. The theoretical methods used successfully for calculating the properties of covalent crystals such as silicon are less easily adapted to ionic crystals. This very detailed review discusses the methods applied to simple materials with the rock salt and fluorite structures "which are taken to be fully ionic and contain ions of closed electronic configuration". Particular emphasis is put on the relativistic methods necessary to properly treat compounds (such as PbF_2) of the heavier elements. The reader will learn that, although considerable progress has been made, much more will be necessary before properties such as elastic constants and lattice dynamics can be successfully predicted or the methods extended to lower-symmetry crystals.

My assessment is that the first article should appeal to a wide audience but that the other three are addressed to more specialist groups. The book is well produced and almost free of misprints. References generally cut off at 1988 but a few from early 1989 are included. Each chapter is preceded by a table of contents, but there are no indices.

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Thermodynamics of Solvation: Solution & Dissolution; Ions & Solvents; Structure & Energetics. G. A. Krestov, E. R. Myasnikov (Translator), and John Burgess (Translation Editor). Ellis Horwood: Englewood Cliffs, NJ. 1991. 284 pp. $62.00. ISBN 0-13-915042-0.

The book deals with a vast and a complicated subject. To do it full justice, several such volumes would be necessary. Naturally, the author selected topics which are of the most interest to him and to his research. Unfortunately there is no author's preface in which he could have discussed his reasons, plans, and intentions for writing this volume.

Six chapters of the book provide a thorough discussion of basic thermodynamics of ion–solvent interactions. They contain a vast amount of thermodynamic data on free energies, enthalpies, entropies, and heat capacities of many electrolytes and of some individual ions in different solvents and at different temperatures. A large fraction of these data appeared in Russian monographs and review papers which are obtainable with difficulty (if at all) outside Russia. It is one of the major merits of this book that these data now become available to non-Russian scientists. It should be noted, however, that the thermodynamic data for individual ions have been obtained, of necessity, on the basis of some extrathermodynamic assumptions, of which there are many and whose validity is somewhat controversial.

Thus this monograph describes in detail important Russian work in the field of ionic solvation and, in particular, work carried out at the Ivanovo Institute of Nonaqueous Solutions. By the same token, however, it is somewhat parochial, since many important foreign studies are omitted. It is also somewhat lax in the discussion of recent advances in the field. For example, out of 344 citations (many of which are multiple), there are only 33 post-1980 references, of which 18 are monographs or reviews. Of the remaining 15 citations, only 4 refer to non-Russian papers.

Incidentally, it is quite an inconvenience that in many citations of Russian journals the pagination of the Russian editions is used. Nearly all of these journals exist in English translation and since the book is inteded for English-speaking chemists, it would have been much more helpful if the monograph used pagination of the English editions.

Among the topics which seem important to this reviewer but which are either omitted or discussed very briefly are solvation thermodynamics in molecular solutions, the role of activities in ion–solvent equilibria (and the discussion of the Debye–Huckel treatment), the influence of donor and/or acceptor properties of solvents on the thermodynamics of ionic solvation, and a discussion of the influence of solvation on ion–ion interactions in solutions. Moreover, there is no mention of the thermodynamic data on ionic solvation obtained by various spectroscopic techniques. Clearly, the book will be useful to workers in the field, but it does not provide a comprehensive and critical review of the thermodynamics of solvation.

Finally, it should be mentioned that the translation is very good. There are no obvious errors; text is smooth and in good English. It is never necessary to mentally retranslate a sentence from English back into Russian (as is sometimes the case with other translations) in order to understand it.

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