BOOK REVIEWS

Computers in Analytical Chemistry. By Philip G. Barker (Teeside, Polytechnic). Pergamon Press, New York, 1983. ix + 453 pp.

"Computers in Analytical Chemistry" is an overview exposing the reader to the vocabulary involved in the application of a variety of computers to the analytical function. They range from embedded microcomputers, through specially interfaced stand-alone computers, to large data base system installations. In this one volume each subject cannot be addressed in depth; however, the vocabulary and philosophy of the plethora of areas involved in laboratory automation is serviced. Computer architecture, languages, analogue to digital conversion, interfacing, data manipulation, communication concepts, peripheral operation, networking, and data management are all explored. In some cases the coverage is in depth and in others superficial. In some cases the information is very current, while in others it is dated.

However, the bibliography is very extensive. This suggests that the book would be well-suited to a quick but broad introduction to the topic with the understanding that the exposure would not be altogether current or uniform. The book thus provides a good platform for further growth.

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Data Processing in Chemistry. By Z. Hippe (Ed.) (I. Lukasiewicz Technical University). Elsevier Scientific Publishing Company, New York. 1981. x + 287 pp. $70.00.

Frequently a collection of scientific papers in a single volume results in a disjointed, relatively unreadable book. However, this collection of papers presented at the Data Processing in Chemistry Summer School at Rzeszow, Poland, has been grouped very effectively into four categories (calculational, morphological, and semantic models, plus a final grouping of various topics) by Professor Hippe, and the result is a smoothly flowing, very readable book.

"The main aim of the DPC-School was to initiate discussion on research devoted to specialized, high-level software for chemistry" (p v). This aim is achieved, but it means that the vast majority of the 18 chapters are directed toward the computer chemistry expert, rather than the novice. This distinction should be considered when deciding on whether or not to purchase the book.

Although lack of space prevents comment on each chapter in this review, I have selected several to discuss briefly. The inaugural chapter by Sadlej reviews a complex subject, computational quantum chemistry, in a manner that should prove interesting to all computer chemists, whether or not quantum chemistry is their speciality. He emphasizes that the availability of many programs through the Quantum Chemistry Program Exchange and other programs on minicomputers will probably result in even more extensive use of ab initio calculations for chemical purposes. A somewhat different view is presented in a chapter by Gribov, who feels the complexity of theoretical methods as applied to molecular spectroscopy plus a world-wide shortage of workers have contributed to slowing growth in this field.

The semantic model section describes various approaches to computerizing chemical synthesis problems. Hippe states that whether the approach is based on "known chemistry" and uses data bases of synthetic pathways or based on mathematical models, the 1980s will end with these computerized syntheses being used routinely in research and education. I must confess to a degree of skepticism that this prediction will come true. It will at least be an enormous challenge.

Morphological models include techniques based on searching data bases. Clerc presents an interesting detailed analysis of the spectral interpretation process. His concluding remarks should be heeded by all workers in this area. It is improper to overemphasize the importance of the number of spectra in a data base. The quality of spectra is a far more critical commodity than the quantity of spectra. Heller had an unenviable task of describing a well-known package, the NIH/EPA Chemical Information System, without sounding repetitive since descriptions of this system have appeared in numerous places. I believe he succeeds admirably by giving a fresh approach to the description of the system design and development and the computer facilities of CIS.

This book certainly meets the goal of having an international flavor as nine countries are represented among the 30 contributing authors. Considering that English is not the native language of the vast majority of the contributors, the clear readability is most impressive, and the authors and editor are to be commended. There are an unfortunately large number of typographical errors and misspellings (e.g., maid rather than made) that some readers might find distracting.

Much of the material presented in this book is available in scientific journals, but having this wealth of information available in a single volume makes it a worthwhile investment for most libraries.

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LETTERS TO THE EDITOR

NUMBER OF RINGS AND CODING DIFFICULTY

Dear Sir:

The ring structure of a chemical graph may be defined as the collection of all that graph's rings plus the paths connecting them. Consider those vertices (we can call them "pivotal") in the chemical graph of degree greater than two in the ring structure. If in a graph of more than one ring each of these vertices has a unique label, then the graph is unambiguously coded by iterative refinement, such as in the algorithm of Schubert and Ugi.[1] This happens because every ring in such a graph contains at least one of the uniquely labeled vertices.

If r is the number of rings (cycle rank) of a chemical graph, then that graph can have at most $2r - 2$ pivotal vertices. These can then be uniquely labeled in at most $(2r - 2)!$ ways. The Schubert–Ugi algorithm yields unique codes for acyclic and single-ringed structures, so it is easy to see that a chemical graph with r or fewer rings is codeable in at most $(2r - 2)!$ times the speed of Schubert–Ugi. This suggests that the difficulty of coding a chemical graph is a function of that graph's number of rings. Efficiency in coding a chemical graph might be achieved by using an algorithm just powerful enough to yield unique codes for that graph's particular value of r.

(1) Schubert, W.; Ugi, I. "Constitutional Symmetry and Unique Descriptors of Molecules". *J. Am. Chem. Soc.* **1978**, *100*, 37–41.

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