Quantum Mechanics on a Microcomputer

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The Quantum Chemistry Program Exchange (QPCE, Creative Arts Buikding 181, Indiana University, Bloomington, IN 47405) has recently announced the availability of a compiled version of the Fortran-77 MOPAC Version 6.0 quantum chemistry package that will run on IBM/clone 386 and 486 microcomputers with math coprocessors. The price is only $125 for the compressed program on two 750KB 3 1/2-inch diskettes. Additional requirements for running the compiled version of MOPAC include 8MB of RAM, 10MB of disk space and the Phar Lap Dos Extender (Par Lap Software, Inc, 60 Aberdeen Avenue, Cambridge, MA 12138, $495). As delivered, the executable file will handle structures with up to 25 heavy (non hydrogen) atoms and 25 light atoms. (The normal workstation version of MOPAC is set for 40 heavy and 40 light atoms.) If the source files have to be recompiled for use with larger molecules, the NDP-Fortran compiler (MicroWay, Inc., P. O. Box 79, Kingston, MA, 02364, the 386 version is $695.; the 486 version is $995.) is required. Compilation for forty light atoms and forty heavy atoms will require 20MB of RAM.

In order to make the best use of MOPAC 6.0 a front-end program is uselful to prepare MOPAC input files by drawing on the computer screen, and to view and manipulate MOPAC output. PCMODEL Version 4.0 (Serena Software, Box 3076, Bloomington, IN 47402-3076) can be used to prepare MOPAC input files easily. MOBY Version 1.5 (Springer-Verlag NY, Inc., 175 Fifth Ave., New York, NY 10010), which will be available soon, will prepare input files for MOPAC, and also allow stereo viewing of the resulting structure with the ability to rotate the stereo view in real time. With the companion program, QC4MOBY, MOBY will display graphically (in motion) each vibration from the infrared spectra predicted by MOPAC and will also show graphical representations of the calculated molecular orbitals. (MOBY alone will run AM1 and MNDO calculations of molecules up to the size of glucose.)

Don't plan to do quantum chemistry on a microcomputer if you expect very fast calculations. A small molecule which can be run in less than a minute on an IBM RISC/6000 can take upwards of a half hour (using the AM1 PRECISE calculations).

I used a beta test copy of MOBY Version 1.5 this past summer in Organic Chemistry I, II. I found that students really enjoyed being able to construct and rotate stereoviews and to view infrared vibrations. After trhis experience, I am convinced that at least half of the students who currently pass organic chemistry do it without much of a sense of what an organic molecule looks like in three dimensions. This may explain why many students find organic chemistry so dfficult.

BOOK REVIEW COLUMN

by Harry E. Pence, Chemistry Department, SUNY-Oneonta, Oneonta, NY 13820

Many chemistry instructors are discovering that it's possible to do rather complex computer applications in their classes without expensive hardware or complicated software. A popular way of accomplishing this is to adapt commonly available spreadsheet programs for chemical problems. Most of the popular spreadsheets, like Lotus, Quattro, and Excel, include not only excellent graphing capabilities but also the mathematical functions that are needed for most types of chemical calculations. In addition, these programs are often available in inexpensive student editions and are relatively easy to learn.

Those who wish to pursue this approach need a textbook that teaches spreadsheet fundamentals using chemical examples. Such a book can both serve as a source of homework problems and also minimize the lecture time which an instructor must spend discussing how to use

the spreadsheet. The two books reviewed in this column provide exactly this type of support. It should also be noted that those instructors who use a computer during their lectures will find these books to be sources of simple, but effective computer simulations, which make a useful lecture supplement.

SPREADSHEET CHEMISTRY by O. Jerry Parker and Gary L. Breneman Prentice Hall, Englewood Cliffs, New Jersey, 1991 288 pages, softcover, $22.00

The book should be useful with a variety of the commonly encountered spreadsheets and/or general chemistry texts. The spreadsheets in the book are intended to be used with the DOS version of Microsoft Excel, and disks are available with the data in either the IBM or Macintosh versions of Excel. Beyond that, it shouldn't be too difficult to translate the instructions into one of the other commonly used software packages. The order of the topics is designed to correspond to that in Brown, LeMay, and Bursten's Chemistry: The Central Science, but it shouldn't create serious difficulty if the topics are rearranged to suit the sequence found in most standard General Chemistry textbooks.

The authors start with simple problem types that are commonly treated at the beginning of a general chemistry course, such as temperature conversions and density, and use these topics to introduce the student to basic spreadsheet techniques. The fundamentals of using Excel are also discussed in several appendices. As one proceeds through the book, the topics become more involved and the spreadsheet use also becomes more complex. Some support from the lecture and/or lab practice sessions should be enough to allow most students to develop reasonable facility with the software. The descriptions include both the command text to be placed in the cells as well as a copy showing what the resulting worksheet should look like. Each chapter concludes with a good selection of problems that can be best handled with a spreadsheet, and appendices are included that briefly discuss successive approximations and the Newton-Raphson Method.

This book is quite useful, both for learning spreadsheet techniques and also as a reference. The discussions are clear, there is an adequate index, and the many diagrams are a significant complement to the text. The discussion of the chemical background for each topic is brief, but it's more than adequate if a student needs a quick review of a specific point while working on the spreadsheet. It's a pleasure to recommend this book. DYNAMIC MODELS IN CHEMISTRY by Daniel E. Atkinson, et al.N. Simonson & Company, Marina del Rey, California, 1990,320 pages, softcover, $19.95

There are many similarities between this book and that which is reviewed above. Both are intended for students in the introductory chemistry course, can be used with a variety of spreadsheets, and invite the reader to order spreadsheet diskettes in either the MS DOS or Macintosh formats. This book doesn't follow the standard set of topics from freshman chemistry as closely as the book by Parker and Breneman. It omits some topics, such as atomic structure and orbitals, but does add some additional topics, such as fractional distillation and extraction, that may also be helpful.

Atkinson et al make extensive use of sidebars to highlight important ideas. For example, each chapter begins with a sidebar that briefly lists the prerequisite knowledge necessary for the upcoming exercises. Other sidebars discuss specific points of concern regarding the model discussed or show sample graphs of the resulting data. This approach, which lets the reader decide how much help is needed at a given point in the discussion, is welcome. On the other hand, it's regrettable to find that a book that will be used as a reference lacks an index.

It can be argued, and I believe that the authors of both of these books would probably agree, that the most important aspect of spreadsheet use is not just solving problems but rather building a model that can be used to explore a topic in much more detail than would be possible if each individual calculation must be done by hand. If students can be encouraged to interact with chemistry in this way, regardless of whether it's done in lecture or on their own, they will be much more likely to understand chemistry rather than simply memorizing a set of algorithms for commonly encountered problem types. This book includes a number of problems that invite this type of exploration, and this is one of its strengths.

Both of these books provides an excellent basis for eitherstudents or faculty who wish to explore spreadsheet applications in chemistry. This reviewer uses Parker and Breneman somewhat more, but both books are well worth owning.

A FINAL COMMENT

Since this column will be my last as the book review editor for "The Newsletter," I wish to take this opportunity to express my thanks to everyone who has helped with reviews and suggestions during the past few years. Even though I can't mention all of you by name, I do wish to offer a special word of appreciation to Don Rosenthal, who first invited me to undertake this job and has helped me so often. I welcome the new book review editor, Larry Julien from Michigan Technological University, and wish him good luck as he begins his new job.

——End—— BYE Harry.

INTEGRATING COMPUTERS INTO THE UNDERGRADUATE CHEMISTRY CURRICULUM

by Harry E. Pence, Department of Chemistry SUNY Oneonta, Oneonta, NY

The Committee on Computers in Chemical Education sponsored a one-day symposium titled "Integrating Computers into the Undergraduate Chemistry Curriculum" at the ACS National Meeting in Washington, DC this Fall. The symposium was organized by Tom O'Haver (Univ. of Maryland) and Harry Pence (SUNY Oneonta) in order to encourage chemistry instructors at all levels to share information on their progress in integrating the variety of available computer software and hardware into an environment that will be most conducive for learning. Both the number of papers submitted to the symposium as well as the attendance demonstrated the high level of interest in this topic.

As might be expected, the various presentations represented a broad spectrum of approaches and technology. These papers covered all levels from high school through the senior year in college, and even at the introductory levels the computer techniques used were often extremely powerful and sophisticated. It was, however, obvious that even modest financial resources were sufficient to create productive computer integration. Several speakers described how they had used inexpensive software, matching grants, and other avenues to develop innovative programs.

The presentations at this symposium demonstrated the wide variety of ways in which computers are being used in undergraduate chemistry courses. Individualized learning is supported not only as computer-assisted instruction, but also by providing each student in large classes with unique homework and quiz assignments. Computer-controlled, multimedia presentation systems ("hyperbooks") will soon be widely available for lecture and self-study. Strategies for electronic literature searches are becoming a routine part of the instructional program. The increasing availability of resource rooms for chemical computing allows students to share their knowledge and participate in applications that go beyond those discussed in class.

It may be unfair to single out one development that was most exciting, but the frequent mention of programs that allow students to visualize chemical systems was especially impressive. Even though such methods have only recently obtained wide acceptance at the research level, several papers described their use in introductory classes. A broad range of software is capable of supporting molecular modelling and visualization, ranging from share-ware like MacMolecule to very elegant and expensive packages, like the CAChe system. These systems allow students at all levels to interact with molecules with a facility that's impossible with models. Allowing students to manipulate molecular systems in this way not only captures their imaginations, but it also seems likely that those who learn three-dimensional visualization in this way will develop a new understanding of chemistry and chemical reactions.

This symposium gave an exciting look at one of the more active areas of innovation in chemical education. No one seriously expects that computers will solve all problems in chemical education, but if these papers are an accurate indication, computers have an important role to play in whatever form the actual solutions may take.

INFORMAL NOTES ON PROGRAMMING-LANGUAGES

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This is a follow-on from Part One (Comp. Chem. Educ. Newsletter, Fall, 1991), which covered the 'classical' languages