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Book review

Mathematical® computer programs for physical chemistry

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Springer Verlag, Berlin, Heidelberg, New York, 1998, 265 pages with CD-ROM,
softcover US $42.00, SFR 71.00, GBP 30.00 ISBN 0-387-98337-6

One of the challenges in the instruction of physical chemistry is the fact that most of us learned the subject along fairly traditional lines; lectures, homework sets, and the dreaded exams. It is often tempting to take the path of least resistance and stick to teaching this type of course. However, the assessment that can be done in such a course is limited by construction to assessing how well students take tests. If you have it in mind that students may be able to learn something different about physical chemistry by carrying out computational projects, texts such as this one can be valuable resources

This particular text is an ambitious attempt to provide students and instructors of physical chemistry with enough raw power to tackle and analyze a number of complex examples without the need to debug a Mathematica program from scratch. It is not meant to stand on its own as a textbook but rather to be used as a supplement to a traditional physical chemistry text. The book is best described as summation of the important formulas used in the programs with worked examples, and a series of problems and projects to be worked through. It is well written and adequately referenced, the examples are helpful and the problems and projects are well conceived, requiring the student to modify the Mathematica programs included on the accompanying CD-ROM.

To tell the truth, if the codes supplied were trivial examples then I would not be able to recommend the use of such a text. There is certainly considerable pedagogical value in a student's struggle to get Mathematica to work and to debug a computer project; however many of the examples in this collection are anything but trivial, and so the overall result is satisfying and sound.

The CD-ROM contains approximately 140 Mathematica programs with separate files provided which are compatible with Mathematica versions 2.3 and 3.0. Five Monte Carlo programs written in QuickBASIC are also provided. I tested a number of the Mathematica programs on a Macintosh PowerPC (MacOS 8.1), running Mathematica 3.0. The programs functioned well, but I encountered a few technical problems before getting started. Although not explicitly mentioned on the jacket or in the text, the author implicitly assumes that the programs are being run on a Windows/DOS platform. When attempting to open files from within Mathematica, MacOS Finder errors resulted from the extremely large number of files in a single folder (over 800 files). It was necessary to copy all the files to a hard drive and separate them into folders because all the files on the CD-ROM reside in the topmost folder. This proved to be time-consuming and slightly difficult, because some programs depended on other files and required that they be located in the same folder as the program, and there was no documentation of data dependencies; it was necessary to read through each program to find out which files would be needed. Obviously these problems were easily overcome, but they cost me some time. If the editor had simply organized the files into two separate folders, one for each of the two versions, much time and effort would have been saved.

The book is especially strong in the much-neglected areas of chemical thermodynamics, kinetics, and polymer physics (macromolecules). An appropriate tone is set in Chapter 1, which reveals equations of state which are of gradually increasing complexity, ultimately arriving at the 55-parameter Keenan–Keyes–Hill–Moore equation for steam and liquid water. Comparisons are emphasized between the predictions made by the various equations of state and experiment. Clearly, it would not be a practical proposition for an undergraduate student to code up this last equation. Similarly nontrivial examples are introduced which illustrate the properties of non-ideal mixtures and the hydrodynamics of macromolecules. Electrode kinetics, oscillating reactions, and unimolecular kinetics are also nicely covered. Statistical thermodynamics is also extended beyond typical textbook treatments by the provision of programs to carry out corrections to quantum partition functions for vibration-rotation interactions, anharmonicity, and nonrigid rotations. There is a nice section on solids, liquids and surfaces which emphasizes diffraction methods. I would go so far as to say that some of the programs in these areas are so useful and powerful that some researchers will find this text useful as research tool, especially those who are a little rusty in thermodynamics.

However, I was somewhat disappointed by the sections on quantum mechanics. It seems to me that these sections missed a good opportunity to demonstrate the use of nondegenerate perturbation theory and the variational method. I was also surprised that no significant use was made of Mathematica's surface-plotting capabilities to display wavefunctions; however, the Hartree–Fock equations are nicely solved for a diatomic molecule with one electron. Also, the section on quantum vibration-rotation was unfortunately entitled "Molecular Mechanics". This phrase is commonly used to describe the use of empirical force fields to carry out conformational studies, and I feel that some undergraduates would find this confusing. Some of the spectroscopy section encompasses material which I believe is at a level beyond that of a typical undergraduate physical chemistry course. On the other hand, there are nicely conceived codes which predict the relative intensities of vibration-rotation absorption peaks, which include Boltzmann factors and isotope abundance. Overall, the relative weakness of these sections is more than made up for by the excellence of the rest of the text. This book represents a valuable contribution to the pedagogy of physical chemistry.

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