

replaced to advantage by others on areas of glycochemistry and glycobiology that have not been discussed at all. For example, I would have liked to find a separate contribution on carbohydrate analysis, as many of the results described would not have been possible without the remarkable developments that have occurred in NMR spectroscopy and mass spectrometry.

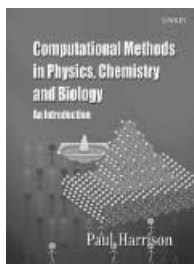
For readers who are not very familiar with glycochemistry the book offers a good way of quickly gaining a sound appreciation of the many different aspects of the field. As already mentioned, the amount of experimental detail in some chapters is probably too much for that purpose, but despite that I recommend the book to those readers, and therefore I answer yes to the above question. On the other hand, of course, the book does not go far enough for specialist readers. Their general needs are better served by other (mainly multi-volume) works that are already available. Also, in cases where a specific area of development is described in a short article in this book, the specialist reader will instead go to a relevant monograph where the topic is treated more thoroughly. Therefore, for those readers the answer to the question must be no.

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Computational Methods in Physics, Chemistry and Biology. By *Paul Harrison*. John Wiley & Sons, Inc., New York 2001. 201 pp., softcover £ 24.95.—ISBN 0-471-49563-8

Numerical experimentation, that is, the computational modeling of physical phenomena, has become established as a third pillar, next to laboratory experiment and theory, in the investigation of the natural world. The present book attempts to provide undergraduate students in physics, chemistry, biology, and related areas



with the basic techniques underlying many of the computational models used in these numerical experiments. The nine chapters cover topics such as numerical and approximate solutions for the Schrödinger equation (e.g., perturbation methods and the variational principle), technical applications such as matrix methods and the use of basis sets to expand state functions, deterministic and stochastic simulation techniques, percolation theory, evolutionary methods and genetic algorithms, and finally molecular dynamics.

The fundamental physics which the various numerical methods attempt to model is introduced in a very brief and often superficial manner. Constructs such as the Kronecker δ or divergence are used with no further explanation. Without solid prior knowledge the reader will certainly have difficulties in understanding this important background information. The numerical techniques themselves are explained in more detail, and are accompanied by examples of the use of the corresponding algorithms in computer programs written in C (one example in Fortran is also included). All chapters end with a summary and a set of tasks and projects. The source code examples, as well as hints and outline answers to the problems, are available through the Internet from the author's website.

As the title suggests, the author defines the audience of this book as computational physicists, chemists, mathematicians, and biologists. However, the examples and the overall style of treatment are strongly biased towards physics. Chemistry and biology related aspects are only very rarely touched upon. This becomes evident, for example, when Monte Carlo simulations are introduced with the words: "Monte Carlo simulations are usually associated with electron scattering processes in semiconductors". While this mirrors the author's background in quantum electronics and semiconductor physics, it completely neglects the important role of these techniques in other areas. For example, Monte Carlo methods have important applications in chemistry and are used for molecular mechanics simulations, an aspect which is not mentioned at all in the book. Similarly, the chapter on molecular dynamics focuses almost

exclusively on applications in solid-state physics. The great importance of these methods in many areas of chemistry is noted only very briefly, even though molecular dynamics simulations are nowadays frequently used in many academic and industrial laboratories for the prediction of properties of reagents, potential new drugs, and other chemicals. Moreover, some of the information regarding chemical aspects is even incorrect, for example in Figure 8.12 where C–H and H–H bonds are shown as being weaker than a C–C single bond.

To sum up, this book is certainly of value for students interested in computational physics. On the other hand, chemists, and probably also biologists, will find it less suitable because much physical background knowledge is required, and direct ties to applications in these disciplines are missing.

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Handbook of Modern Pharmaceutical Analysis. By *Satinder Ahuja* and *Stephen Scypinski*. Academic Press, San Diego 2001. 566 pp., hardcover \$ 124.95.—ISBN 0-12-045555-2

Pharmaceutical analysis can be considered from several aspects: the analytical methods that are available, the areas of application, and the regulatory requirements. The structure of a book on pharmaceutical analysis is determined essentially by the kinds of readers for whom it is intended. In the case of the *Handbook of Modern Pharmaceutical Analysis* those readers are analysts working in industry. Accordingly, the book places the areas of application and the regulatory aspects in the foreground, whereas the reader is assumed to be already largely familiar with the analytical methods.

After an introductory chapter giving a good overview of the main areas of



application of pharmaceutical analysis, Chapter 2 describes the role of combinatorial chemistry in searching for and synthesizing pharmacologically active compounds. The latest technologies and the most advanced methods of investigation are explained, with many literature references. Chapter 3 deals with the analysis of solid pharmaceutical formulations. A distinction is made between methods that give information at the molecular level (spectroscopic methods), at the particle level (optical and thermal techniques), and at the bulk level (physical measurements). Chapter 4 discusses impurities and decomposition products in medicines, and Chapter 5 deals with preformulation studies. Both these chapters are very comprehensive and practically oriented. The excellent graphics help the reader to grasp quickly the more difficult concepts, and the appendices to Chapter 5 are very useful. It is good to find that the authors have not hesitated to compare and evaluate the different methods, and in so doing have avoided the common mistake of always favoring the most modern methods that require sophisticated and expensive equipment.

The next three chapters are concerned with the different types of formulations. Here the authors do not give enough information about analytical aspects, especially when discussing modern therapeutic systems. There then follow chapters dealing with regulatory aspects, such as the setting of specifications, validation, method transfer, and documentation. In between the treatments of these aspects there are also chapters on method development (Chapter 10) and stability studies (Chapter 13). The final chapter departs from the plan of the preceding chapters in being devoted to a specific analytical method, electrophoretic microchip technology.

The underlying concept of this book, whereby it is structured according to areas of application, has resulted in a good deal of repetition between the chapters. Therefore each chapter can be read on its own (the idea of a handbook), but on the other hand reading several chapters one after another becomes boring. For the pharmaceutical analyst it is appropriate, and indeed essential, to view his or her work as it relates to that of the synthetic chemist

and the formulation specialist or technologist, and therefore I find the idea of this book very good and worthwhile. Nevertheless, it seems to me that some of the chapters contain too much information that is unconnected to analysis. Thus, Chapter 8 is completely dominated by pharmaceutical technology, and contains no mention of the special analytical problems presented by dosage forms such as aerosol sprays or suppositories, for example. The list of contents is detailed and informative, reliably directing one to the sections on a desired topic. On the other hand, the subject index, which needs to be as comprehensive as possible, especially in a handbook, is not entirely satisfactory. In cases where a term occurs in several different places, the index usually lists only one of them. Also the lack of a glossary of abbreviations is a serious shortcoming. There are many other small defects (for example, in the discussion of accuracy there is no mention of traceability), but it would not be helpful to list them here.

The book will certainly be very useful for readers beginning work in the pharmaceutical industry, and for all libraries concerned with the field. Old hands too are likely to find in it some stimulating ideas and new information.

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Object-Oriented Magnetic Resonance. Classes and Objects, Calculations and Computations. By Michael Mehring and Volker A. Weiberruß. Academic Press, San Diego 2001. 555 pp., hardcover and CD-Rom, \$ 79.95.—ISBN 0-127-40620-4

Michael Mehring and Volker A. Weiberruß, the authors of the book *Object-Oriented Magnetic Resonance* published by Academic Press in 2001, provide the reader with the quantum-mechanical principles of nuclear and electron spin resonance which are the basis for understanding and inventing new nuclear magnetic resonance (NMR) experiments and algorithms. The book covers

a wide range of topics, from the fundamentals of spin quantum mechanics to advanced topics such as Liouville space evolutions. These concepts are then applied to multiple-pulse, multiple-quantum, and multidimensional spectroscopy, as well as quantum computing. The book introduces the basic principles of NMR, especially for solid-state NMR, as well as EPR/ENDOR spectroscopy.

For many years there has been an urgent need for a book giving an introduction to the rapidly evolving field of solid-state NMR spectroscopy. Especially in recent years, methods and hardware for solid-state NMR experiments are developing at a rapid pace. Books that not only provide a thorough introduction to the field of solid-state NMR spectroscopy but also give expert advice are rare. According to the authors, this book is intended for scientists and graduate students working on the applications of NMR or ESR in biology, chemistry, materials, physics, and medicine. However, the physical language used in the book makes it particularly attractive for physical chemists or people who have a background in quantum mechanics.

The authors have chosen an appealing title for their book and relate it to object-oriented programming in computer science. Indeed, most pulse sequence elements can be employed as modular elements in many applications. Object-oriented programming is all about objects. In the case of NMR spectroscopy (according to the authors of the book), the objects are operators of spin physics such as spherical tensor operators, density operators, etc. Classes are defined as the ensemble of spin operators, propagators, etc. In computer programming, objects are treated as "black boxes" that contain code (the NMR pulse sequence) and data (the quantum-mechanical spin system under investigation), and can receive and send messages (which are the structural questions about the spin system). A primary rule of object-oriented programming is that the user of an object should never peek inside the black box. However, this is just what the authors want from their readers: they describe in detail all the objects and classes that are used in NMR spectroscopy. In addition to the mathematical, theoretical, and numerical object levels, a list of graphical symbols is added at