

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

each subsection to differentiate between important statements, exercises, or programs in the text or on the CD-ROM, which is thought to give the book a didactically appealing quality. But enough “smalltalk” for now.

Chapters 1–6 lay down the physical basis for the quantitative description of nuclear and electron spin magnetic resonance. In these chapters, classes and objects in Hilbert and Liouville space are defined. Chapter 7 describes spin–spin interactions for nuclei and electrons, and quadrupolar and chemical shift interactions, together with their Hamiltonians and representative one-dimensional spectra. The principle of magic angle spinning (MAS) is also explained. At the end of the chapter the transition from a defined sample rotation to random molecular reorientation is made in order to describe relaxation. This topic is then discussed in detail in Chapter 8.

A detailed analysis of spin echo sequences such as the well-known Hahn echo is given in Chapter 9. Furthermore, rotary, driven, stimulated, quadrupolar, solid, and magic echoes are discussed. These echoes are nowadays used as building blocks in many pulse programs. A thorough understanding of these elementary concepts is essential for the design of any new pulse sequence. The authors devote almost 60 pages to this topic, an investment that is certainly well justified.

Double resonance experiments such as ENDOR, DNP, SEDOR, and CP are treated in Chapter 10. The concept of these experiments is first explained for a three-level system, then later extended to multilevel systems, and finally discussed from the standpoint of spin temperature. The main emphasis here is on the discussion of double resonance experiments where electronic transitions are involved.

The next chapter (11) deals with multiple pulse sequences and the prob-

lems of homonuclear decoupling. Sequences such as CPMG, WAHUHA, LG, and their derivatives MREV-8 and BR-24 are discussed. Chapter 12 gives an introduction to multiple-quantum spectroscopy. Unfortunately, some important experimental concepts, such as MQ-MAS or double quantum local field separated spectroscopy are not discussed. In Chapter 13 the basic principles of two-dimensional spectroscopy are briefly explained for completeness.

Recently NMR spectroscopy has received a lot of attention since it can potentially be used as a kind of quantum computer. The memory of such computers consists of quantum states which can be regarded as superpositions of many different numbers at once. By performing a computation on these quantum states, then convoluting the results to get a single answer, a quantum computer has the potential to be much more powerful than a classical computer of the same size. The principles of quantum computing are discussed in Chapter 14, thus bridging the gap between object-oriented computer programming and programming of NMR pulse sequences.

The last chapter outlines analytical and numerical methods which are indispensable for a quantitative description of any experiment. This chapter includes a brief overview of the Floquet approach, perturbation theory, and secular averaging.

In addition, the book provides an introduction to numerical simulation programs for magnetic resonance phenomena. The corresponding object-oriented numerical simulation software packages GAMMA and NMRMAT are supplied on CD-ROM for easy access, together with examples of a few simulation programs. This is a very good idea, since many solid-state NMR spectroscopic experiments require numerical tools in order to properly describe the experimental spectra in a multispin environment.

The first author of the book, Michael Mehring, also wrote *High Resolution NMR in Solids* (2nd edition, Springer-Verlag, 1983), which unfortunately is now out of print. In comparison to that earlier work, the authors of the present book have added a rigorous treatment of the quantum-chemical nature of the spins, a longer chapter on relaxation, and chapters on spin echoes and quantum spin computing. However, that has been achieved at the cost of sacrificing some of the clarity and intuition of the earlier book. Also, the chapter on magnetic shielding tensors that discussed practical aspects and examples of chemical shift anisotropy has been left out. Also, unfortunately, some developments that have been introduced more recently (after 1985) are not covered in the new book (except for quantum computing). In general, too much attention is paid to the formalism, which might be frustrating for the reader who is more interested in applications. For example, the reader will look in vain for a chapter discussing recoupling phenomena in the solid state. Since decoupling and recoupling are very closely related, this would have fitted very well into Chapter 11 where homonuclear decoupling is discussed. Also, a chapter describing applications to polymers or biomolecules would have been helpful. Of course, it is probably not possible to cover all interesting topics in one book.

The book can be recommended for everybody who is interested in the physical principles of nuclear and electron spin magnetic resonance. This is definitely a book which should be in the library of every hardcore NMR spectroscopist.

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