

modeling transmembrane helix bundles by restrained molecular dynamics simulation. In Chapter 15, D. E. Walters provides a brief introduction to the modeling of protein active sites from a series of known ligands, with emphasis on a program developed in his group. The last three chapters are devoted to molecular docking. J. Desmet, M. De Maeyer, J. Spriet, and I. Lasters describe their method for flexible docking of peptide ligands to proteins and its implementation. H. J. Wolfson and R. Nussinov present an overview of geometrical-docking algorithms, with special attention to their own methods. Finally, M. J. E. Sternberg, H. A. Gabb, R. M. Jackson, and G. Moont address a strategy developed in their laboratory for the prediction of protein-protein docking, which they put in context with other algorithms.

The different topics are treated skillfully, as one would expect from a group of renowned authors writing about their own areas of research. As a general rule, the use of programs is illustrated with examples. In some cases, the natural tendency to stress the merits and functionality of one's own methods and programs obscures the existence of alternative algorithms and drives the authors to excessive self-citation, but this is not a general trend in the book. Only a few small errors were noticeable to me, such as the confusion between the concepts of configurational space and phase space in Chapter 16, reminiscent of the fundamental difference between predicting protein structure and understanding protein folding. Inspection of the bibliographies suggests rather clearly that the original manuscripts were written toward the end of 1997. Only chapters 4 and 5 include a brief addendum to the original manuscript, and in a few cases a handful of references have been updated. Such a publication delay seems excessive in a field which is developing at good pace and has produced a vast amount of literature in the past three years. Note, for instance, that two new rounds of the CASP (Critical Assessment in Structure Prediction) experiment have been completed since the original manuscripts were written, shortly after CASP2. One of the conclusions of CASP3 (1998) was the remarkable progress made in the field of *ab initio*

structure prediction. It is precisely in this central topic that the book suffers most severely from a lack of references to recent developments. In general, while the contents of all chapters are perfectly valid today and the programs introduced in them are of current use, the reader will miss important literature from the last three years.

This criticism aside, the range of topics covered and the practical tone of each of the chapters will certainly make this book a useful working reference for both the newcomer to the field and the expert who wish for detailed information on particular methods in protein structure prediction.

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**Lubricants and Lubrication.** Edited by *Theo Mang* and *Wilfried Dresel*. Wiley-VCH, Weinheim 2001. xxxix + 759 pp., hardcover DM 328.00 (ca. € 167).—ISBN 3-527-29536-4

Lubricants, lubrication, friction, and wear form a very important and dynamic group of topics. The demands for energy savings, for conservation of resources, and for reduction of emissions require the development of new lubricants and the improvement of existing ones, including synthetic base oils and additives and new material combinations at interfaces. New requirements also arise in the development of tribological systems for special purposes like space travel or ultraclean room conditions, in semiconductor technology, or in situations of extreme loading arising through miniaturization of friction couples. Recently published monographs have emphasized different aspects of the above complex of topics, such as their chemistry (base oil and additive production and properties), physical chemistry (boundary lubrication), physics (friction and wear), and engineering (tribology as a system property). In accordance with these research and development activities, monographs which reflect the current state in the evolution and utilization of lubricants appear from time to time.

In this book, 17 authors cover the entire field of lubricated friction systems in 19 chapters, including metalworking fluids, forming lubricants, lubricating greases, and solid lubrication. In accordance with the aims of the book, the focus of attention throughout is the variety of mineral and synthetic base oils and additives for different applications, as lubricants for internal combustion engines (33pp.), gear lubrication oils (39pp.), hydraulic oils (55pp.), compressor oils (29pp.), turbine oils (16pp.), metal working fluids (135pp.), forming lubricants (18pp.), lubrication greases (43pp.), and solid lubricants (21pp.).

Further chapters are dedicated to lubricants in the environment (50pp.) and to the disposal of used lubricating oils. They describe how the particular legal regulations and requirements concerning the use of environmentally harmful constituents (identified by ecolabels) are handled in different countries. This includes transport regulations, requirements for restricting air and water pollution, protection from effects of oil, and the underlying national and ISO standards.

At the front of the book there is a very detailed table of contents occupying 23 pages. This is a valuable help to the reader for finding individual topics. On the other hand, the index of only 10 pages does not always enable one to find a subject quickly, considering the great abundance of material presented in the book.

There are some noticeable omissions concerning new types of friction systems, including ceramic materials. Compared to metallic abrading couples, these systems play only a technologically subordinate role, but it would have been worthwhile to include a chapter about ceramic materials.

The book provides a comprehensive introduction to all major lubricant applications. The authors are internationally recognized experts, mainly from industry. For that reason, there is a greater emphasis on applications-oriented aspects of the lubricants than on fundamental mechanisms. Newer ideas concerning the different mechanisms of various antioxidants are also not addressed. Moreover, the book does not include discussions of model substances as basic oils and additives, which would

give the researcher deeper insights into mechanisms. This is a shortcoming of the book, especially since new fundamental understanding of the effects and mechanisms of different classes of additives has been obtained by spectroscopic methods during the last few years.

This book offers the following readers a quick introduction to this field of work: laboratory technicians involved in monitoring and evaluating lubricants, plant maintenance people for whom lubricants are an element in process technology, research and development people who have to deal with friction and wear, engineers for whom lubricants are functional elements and factors influencing the service life of machinery etc., and (increasingly important) safety and environmental protection officers who are responsible for workplace safety, for economical use of resources, and for the reduction or avoidance of emissions and wastes.

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**Self-Assembly in Supramolecular Systems.** By Leonard F. Lindoy and Ian M. Atkinson. (Series: Monographs in Supramolecular Chemistry; series editor: J. Fraser Stoddart.) Royal Society of Chemistry, Cambridge 2000. x + 224 pp., hardcover £ 69.50.—ISBN 0-85404-512-0

To cut a long story short: the new monograph *Self-Assembly in Supramolecular Systems*, by Lindoy and Atkinson, is a crude mixture of examples from this fascinating area, rather than the survey of highlights claimed by the authors in the preface. At first sight, the table of contents seems promising: the first chapter, "Self-Assembly: What Does it Mean?", comes with a philosophical touch, and leads the reader to expect a thorough definition. Unfortunately, no distinction is made between "self-assembly" and "self-organization", and there is no proper introduction to central concepts such as preorganization, templates, or cooperativity, even though these terms are used later in the

text. Furthermore, a precise discussion of entropy (only one entry in the index) and enthalpy would have been valuable, but is absent.

In contrast, the second chapter with its short but informative introduction to the different types of intermolecular forces is certainly worth reading by anyone seeking a brief overview. However, in view of the extensive discussion of metal-containing systems in the last two chapters, it would have been useful to include a discussion of metal–ligand bonds and their different geometries, allowing one to compare the bond strengths with other forces.

Unfortunately, with the third chapter and those that follow, the authors depart from their hitherto logical concept. Chapter 3 on "Hydrogen-Bonded and  $\pi$ -Stacked Systems" is concerned with the type of interaction, whereas Chapters 4 ("Rotaxanes") and 5 ("Catenanes") are organized according to topology, and Chapter 6 ("Metal-Directed Synthesis") deals with synthetic aspects. Some of the most important examples relating to the latter topic, namely the metallomacrocycles and capsules studied by Fujita, Stang, and Raymond, have been shifted to the final chapter. Its title, "Further Metal-Containing Systems", relegates them to the lesser importance of any "miscellaneous" chapter. The distinction of hydrogen-bridged and  $\pi$ -bonded assemblies of Chapter 3 is similarly inconsistent: self-replicating systems, which are defined by a functional property, comes at the end of the structure-based organization into simple, cyclic, cylindrical, and spherical assemblies. This section would fit better into the one-paragraph Section 3.2.2 "Molecular Assembly as Reaction Template". The only examples of self-replication cited are from the older work by Rebek, ignoring the artificial minimum models from the Kiedrowski group, Ghadiri's self-replicating peptides, and Orgel's pioneering ideas.

The third chapter also contains some annoying mistakes: the Rebek capsules **28** and **31** (pp. 38 and 40) are identical with the exception of the solubilizing side-chains, which are of minor importance for assembly. A similar unnecessary duplication occurs for the softball **30/33b**; as can be seen easily from computer models, both structures repre-

sent the same molecule—shown with two different formulas that are both wrong, due to missing double bonds in the middle of one and the omission of a nitrogen atom in the other. It is unclear to me why the two MM2-optimized structures differ at all. Certainly, the length of the hydrogen bonds in **33** is not reasonable. The text also contains repetitive passages on the softballs, leaving the impression of a lack of care during the preparation of the book.

Mechanically bound molecules, i.e., rotaxanes, catenanes, and knots, are distributed diffusely through Chapters 4 and 5, with their somewhat imbalanced focus on Stoddart's work, as well as in 6.2 and 6.7. The book would surely benefit from a consistent organization according to the various template effects used in synthesizing rotaxanes and catenanes. Treating rotaxanes and catenanes of the same types together would also have avoided repetitions, saving space for a more precise and in-depth discussion.

The authors hope to reach a broad readership, from senior undergraduates and newcomers to the field to experienced supramolecular chemists. Although seemingly easy to read, the book implicitly demands too much for understanding by undergraduate students, so that they will either find it difficult to extract the information, or will form only a superficial view of the highly interesting chemistry presented here. The newcomer may make use of the many references including literature up to the end of 1998 (a few reviews from early 1999 have also been included). The authors should have updated the references immediately before the book went into print. Finally, the expert will not learn much from the book, since the basic ideas lack thorough discussion.

Although I was at first enthusiastic about a new book with a focus on self-assembly, I have considerable reservations about recommending it. Many passages lack the care without which the book will not be a joy to read. The more I studied the text, the greater my disappointment. What a pity about the missed opportunity!

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