

technics (explosive materials that, unlike explosives or propellants, react at visibly observable rates with the formation of solid residues). The chapter deals with performance and composition for gun propellants (those designed to provide large quantities of gas, which is used to propel projectiles with high kinetic energies) and rocket propellants (those designed to burn uniformly and smoothly without detonation but burning less rapidly than gun propellants). Among the pyrotechnics dealt with are heat-producing, smoke-generating, light-generating, and noise-generating varieties.

Akhavan's book contains a few errors, but these are mostly in the spelling of names (e.g., Berthold Schwarz (not Schwartz), Johann Kunckel (not Kun- kel)). It includes 35 figures, 64 tables, and 95 numbered items (mathematical or chemical equations and structural formulas or reaction schemes—many consisting of multiple formulas or schemes). A two-page bibliography of 30 articles and books dating from 1958 to 1996 and a 13-page (two columns per page) subject index conclude the volume.

The book is intended primarily for students at the British A-level (equivalent to advanced placement in U.S. high schools) and undergraduate or graduate students, all with no previous knowledge of explosive materials. As a volume in the RSC Paperbacks series, it is an "inexpensive text suitable for teachers and students and ... a clear, readable introduction to selected topics in chemistry." It should also be useful for experienced chemists in the explosives industry or for anyone looking for concise information on the subject.

George B. Kauffman
California State University
Fresno, California (USA)

Protein Structure Prediction. Methods and Protocols (Methods in Molecular Biology, volume 143). Edited by David M. Webster. Humana Press, Totowa 2000. 422 pp., hardcover \$ 89.50.—ISBN 0-89603-637-5

The avalanche of genomic DNA sequences received by the genetic databanks will constitute comprehensible

biological information only when proper links between genome sequence and protein (and possibly RNA) structure and function are established. This book, edited by David Webster, is concerned with the limiting step in the solution of this biological puzzle; namely, discovering (though not necessarily understanding) the connection between protein sequence and structure. To date, the joint SWISS-PROT-TrEMBL non-redundant database contains over 560 000 protein sequences. By contrast, only 7050 protein structures (with a maximum sequence homology of 95%) have been deposited in the Protein Data Bank (PDB). Whole genome sequencing of a number of organisms, including a working draft of the human genome (announced in June 2000), and subsequent efforts on genome annotation will yield an even larger gap between the number of known protein sequences and the number of solved three-dimensional structures. In the absence of an unprecedented revolution in experimental structure determination, theoretical methods are hoped to help fill this gap.

Protein Structure Prediction: Methods and Protocols covers the major topics in computational protein-structure prediction, with eighteen chapters contributed by experts in the field. The book is organised following a natural sequence in the process of structure prediction, from sequence analysis, through secondary and tertiary structure prediction, to molecular docking. In Chapter 1, D. G. Higgins and W. R. Taylor give a detailed introduction and practical guide with examples to their respective multiple sequence alignment programs. Unfortunately, the two programs presented are based on the same general type of alignment algorithm, a progressive global alignment, and no overview on other types of algorithms is provided, limiting the chapter's utility. W. R. Taylor has also written a chapter on protein-structure alignment, where he gives a brief outline of different methods and describes in some detail his own algorithm and program. In Chapter 3, I. Jonassen provides a nice introduction to sequence-pattern recognition, with special emphasis on pattern discovery from unaligned protein sequences. He surveys different algorithms and describes his own program in some more detail. The

chapter by C. P. Ponting and E. Birney addresses the identification of structural domains from the analysis of the protein's sequence. For this purpose they propose a protocol which combines a number of programs from different authors. The chapter on secondary-structure prediction has been contributed by B. Rost and C. Sander. They have written an excellent retrospective review, with practical discussions and extensive bibliography. In addition, some special attention is devoted to their own secondary-structure prediction program. With Chapter 6 the book enters the frontiers of protein-structure prediction: comparative modeling, fold recognition, and ab initio prediction. R. Sánchez and A. Šali introduce the reader to comparative modeling, and provide a number of practical examples using their own methods and program. D. Jones has written a concise, instructive introduction to protein-structure prediction, including a practical guide with examples aimed at exploiting the possibilities of different programs at each stage of the prediction process. B. A. Reva, A. V. Finkelstein, and J. Skolnick sign a chapter on the derivation and testing of effective energy functions for use in fold recognition, illustrated with the authors' own functions. Ab initio prediction is treated by S. Schulze-Kremer, who has written a rather detailed introduction to the use of genetic algorithms in protein-structure prediction, and by E. S. Huang, R. Samudrala, and B. H. Park who give a survey of effective energy functions in the context of different ab initio structure-prediction methods. In Chapter 11, R. E. Bruccoleri presents his program for ab initio loop modeling, illustrating its functioning with an example. Again, one misses some discussion on alternative algorithms. Next, M. De Maeyer, J. Desmet, and I. Lasters describe the dead-end elimination theorem and their implementation to the modeling of side-chains on a fixed main-chain template. In Chapter 13, R. B. Russell gives an introduction to the classification of protein folds, with a brief description of different classification approaches and their related databases. M. S. P. Sansom and L. Davison treat the difficult yet biomedically important problem of structure prediction of membrane proteins. They describe an approach to

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.

Xavier Daura

Laboratorium für Physikalische Chemie
Eidgenössische Technische Hochschule
Zürich (Switzerland)

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