Vital Statistics

Design and Analysis in Chemical Research. Edited by *Roy L. Tranter*. Sheffield Academic Press, Sheffield 2000. xviii+558 pp., hardcover £ 95.00.—ISBN 1-85075-994-4

It can be said right at the start that this book is a pleasure to read. Instead of a formal and dry description of the fundamentals, variants, and applications of statistical methods, the emphasis here is on "statistical thinking". In fact, that is the subject of Chapter 1, which attempts to answer questions of the "what should I do when …?" kind that are commonly asked by beginners in statistics or by those with no relevant knowledge at all. Statistics is the application of a wide variety of methods to tasks such as planning experiments, analyzing data, and establishing quantitative models. Statistical thinking, on the other hand, is much more than that: it includes not only the methods but, most importantly, the thought processes whereby we develop an understanding of a problem, and decide which approach to adopt and which method to use for analyzing the resulting data. It includes a recognition of the capabilities and limitations of the various methods, and rests on the general philosophy of analyzing and interpreting data in the most effective way.

This introduction is followed by chapters dealing with the collection and description of data, the selection of samples and of data, and the interpretation of experimental results based on statistical criteria, although still without using mathematical models. The section on robust nonparametric methods discusses error distributions, spread of data, and variance. Two chapters are then devoted to the statistical planning of experiments, which is important for ensuring that the analysis of the data yields meaningful information. These are followed by a chapter on the analysis of variance. The section on optimization and control is mainly concerned with graphical methods. There is then a large section on model development, which is subdivided into chapters on cluster analysis and pattern recognition, linear regression, and regression methods with latent variables (PCA, PCR, and PLS methods, etc.). The last chapter, on processing and transforming experimental data, seems rather unconnected with the rest.

The book leads the reader gently by the hand. Each chapter begins with a table listing important terms, with references to the relevant subsections. This excellent aid makes the book very clear and easy to use. The many carefully chosen examples illustrate the versatility of the individual methods. The text is enlivened by pithy phrases which guide the user onto the right path. For example, on the "outlier" problem we read: "A [data] point is never to be excluded on statistical grounds only", or on ANOVA (analysis of variance) tables: "Much of this table can and should be ignored." A remarkable wealth of subject matter is presented and discussed. Naturally one should not expect individual methods to be treated in great depth here, and therefore a more or less detailed list of references to specialized literature is provided at the end of each chapter, in some cases arranged under subject headings, sometimes also numbered and referred to in the text.

Mistakes in the text are rare. For example, on page 422 there is a cross-reference to "Section 11.4.3", which does not exist. Unfortunately Section 10.6.5 contains a statement that is completely wrong; the purpose of transforming biological data to a logarithmic scale is not to obtain a normal distribution curve, but to make the experimental errors conform approximately to a normal distribution (as correctly pointed out at the top of page 436). Also, regrettably, the subject index contains many faults, with keywords missing or in the wrong place. The authors have listed their keywords under general subject headings, and unfortunately these packages have not been subsequently broken down further. Thus, for example, the subject "D-optimal design" cannot be found under either D or O, but instead under "Experimental design" and "Response surface modelling", which are the relevant chapter headings. Under "Noise" one finds 29 different pages listed, which is not very helpful. The acronym ANOVA (analysis of variance, a commonly used method) appears frequently in the book, but is not in the index. It first appears on page 58, without explaining the acronym, and again later on page 175; that explanation is only to be found on page 142. There is no such explanation in Chapter 8 (pages 279 ff.), which is entirely devoted to variance analysis and where the term ANOVA appears often. All these are typical weaknesses of a multiauthor work in which the editor has not ensured the necessary consistency.

Despite that, the book is enthusiastically recommended for all analysts, planners of experiments, and budding statisticians. Also chemists, physicists, biologists, and other interested scientists should find the contents useful. Powerful suites of statistical programs are now available for non-statisticians to apply to their experimental planning and data analysis, and this book is a unique source of help in such work. To read and understand the discussions about the breadth of application of the methods and their limitations will in itself be an important and valuable experience. The

editor's recommendation that one should become competent in the use of just a few of the methods, rather than trying to cover all the many variants, is sensible. This book will not make the reader into a statistician, but will give him or her the knowledge to use the methods effectively. Statistical thinking and action, initially in planning experiments and later in analyzing the data and developing models, will enable one to reduce the number of experiments needed, while at the same time improving the quality and reliability of the results. That is the purpose for which the book was written, and it achieves it fully.

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Chemical Topology. Applications and Techniques. (Mathematical Chemistry Series, Vol. 6.) Edited by *Daniel Bonchev* and *Dennis H. Rouvray*. Gordon and Breach Science Publishers, Amsterdam 2000. 350 pp., hardcover $ 125.00.—ISBN 90-5699-240-6

Chemists are usually reluctant to learn abstract new mathematics, or in extreme cases, any mathematics at all, and the theories of knots, links, and non-Euclidean geometry as featured in *Chemical Topology* may seem far from the realities of the laboratory. Nevertheless, familiarity with the Lewis Carroll world of flypes, writhes, tangles, and reticulations may soon be a required skill for the researcher in supramolecular, solid-state, or biological chemistry. As the review articles in this collection argue, the mathematical objects of topology have a surprisingly close correspondence to molecules and materials of current interest such as catenanes, artificial and natural DNA, zeolites, liquid crystals, and the new forms of carbon.

The latest in a series devoted to mathematical chemistry, and the second on chemical topology itself, this volume spans a variety of topics and approaches, from an austere discussion of topological chirality (Cerf), a beautifully illustrated 150-page survey of "hyperbolic crystallography" (Hyde and Ramsden), a more specialized treatment of the connections between symmetry groups, knots, and DNA topologies (Qiu), a review of topological and physical aspects of protein folding (Bohr and Bohr), to a modeling study of topological coding of polymer and protein structure (Karasev et al.). Overlaps between the articles do occur but they are mostly helpful. Mathematical prerequisites vary, but on the whole the authors begin at the beginning and make appropriately extensive use of illustration to introduce the more tricky concepts.

Although this volume contains a huge amount of specific information, its lasting value probably lies more in the convincing case that it makes for the overall relevance of topology to structure and dynamics in chemistry and biology. This is good for topology as well as for chemistry; given the incentive of applicability, chemists and biologists may soon be making the sort of contribution to this area of mathematics that chemists and physicists of the last century made to group theory and graph theory. Professional topologists watch out!

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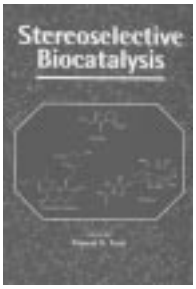
Stereoselective Biocatalysis. Edited by *Ramesh N. Patel*. Marcel Dekker, New York 1999. xiii+932 pp., hardcover $ 250.00.—ISBN 0-8247-8282-8

To be very straightforward: this is not a book that would immediately qualify for the category "love at first sight". The reader has to be very active, take notes, work through the material, flip the pages back and forth, in order to see the benefits of digging through 900 pages. *Stereoselective Biocatalysis* does not set out to be a textbook or dictionary on the topic; it is less structured as to the chemistry at which the enzymes are targeted. One should understand the book more as a reference for biocatalysis, in which experts in the field share their views with the readers.



It is the need for small chiral molecules in a wide range of industrial applications that drives the search for new chemistry to reach such targets. The organic branch of that discipline has been one of the most successful developments in the last 150 years, and it has come up with brilliant solutions to the problem of making chemical entities at will. In parallel with synthetic chemistry (often referred to as "classical"), biocatalytic transformations have been developed since the beginning of the last century. However, it has taken almost a hundred years to write concise accounts of that topic of a standard equal to that existing for organic transformations.

The 30 main chapters are equally balanced between enzyme classes and compound classes, with a short appendix of two chapters on enzyme technology (immobilization and new reaction media). The enzymes discussed here span almost all technically interesting classes of biocatalysts: a) hydrolytic enzymes cleaving the C–heteroatom bond to arrive at asymmetric compounds by resolving racemic mixtures; b) the formation of C–O bonds by mono- and dioxygenases and Baeyer–Villiger oxidations for the synthesis of chiral diols, epoxides, and esters. Chapters on aldolases and hydroxynitrile lyases cover C–C bond forming reactions.

Those chapters focusing on target compounds place more emphasis on the specific generation of functional groups in different chemical contexts. Central themes are the generation of enantiopure building blocks for drug synthesis, enzyme-mediated protecting group techniques, the synthesis of β-hydroxy acids and steroids, and terpene functionalization, to mention just a few.

It might be perceived as a drawback that some topics appear scattered throughout the book, with similar targets or enzymes being mentioned by several authors in their individual contributions. However, if one takes time to go through these different presentations, the advantages of having the topic illuminated from several angles become clear, as the reader gains a more "integrated" view of the subject.

It might be a very personal view that lipases and esterases, although industri-

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ally very important, seem overemphasized here, with the theme of chiral resolution almost beaten to death, whereas glycosidases, glycosyl transferases, and phosphatases (to name just a few) could have received more attention. The chapter on yeast appears unexpectedly out of the blue; it seems anomalous since it could qualify as an account of the topic by itself. It is a bit of a drawback that the contributions on the larger scale applications are limited, and the main focus is on academic examples. Therefore, it could be a good idea to fill this need by a second volume on technical enzymatic transformations.

Much of the material presented here has been reviewed earlier; however, having it here in one book with a more or less consistent layout has its advantages. It can serve as one reference source for the organic chemist in industry or academia who wants to make use of enantioselective reaction steps or who seeks a cheap and "green" synthetic step. This book is a welcome addition to the library of anyone who is working in the field or wishes to take an in-depth look at the very exciting new developments in this area.

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Semiconducting Polymers. Chemistry, Physics and Engineering. Edited by *Georges Hadziioannou* and *Paul F. van Hutten*. WILEY-VCH, Weinheim 2000. xxvi + 631 pp., hardcover DM 398.00.—ISBN 3-527-29507-0

The rapidly developing field of semiconducting polymers is attracting the interest of increasing numbers of physics, chemistry, and engineering research groups. Many postgraduate students are looking for a good book that can provide a quick and comprehensive introduction to the fundamentals of the subject, to help them begin research in this area. Such a book has now at last appeared. The 16 chapters of *Semiconducting Polymers*, edited by Georges Hadziioannou and Paul van Hutten, cover all the important aspects of the technology of this new class of materials. All the chapters have been written by well-recognized experts in their special areas, so that the list of authors reads like a "Who's Who" of the work groups that are active in the field.

The book treats the important classes of semiconducting polymers, namely the polyphenylenevinylenes, the polyphenylenes, their heteroatom analogues, and polyacetylene. Chapters 1, 2, and 16 cover the synthesis of the materials, excluding that of polyacetylene. Chapters 3 and 4 are devoted to the theory of conjugated polymers; of these Chapter 3, by J. Knoester and M. Mostovny, concentrates particularly on the soliton model for *trans*-polyacetylene. Next comes a chapter by M. Lögdlund and W. Salaneck on the electronic structures at metal–polymer interfaces. The following four chapters (Chaps. 6–9) are concerned with spectroscopic details and the related photophysics. Chapter 12 discusses charge transport in conjugated polymers. The rest of the chapters describe the many different applications of semiconducting polymers: organic light-emitting diodes (Chaps. 11 and 13), optically pumped polymer lasers (Chap. 10, by U. Lemmer et al.), organic field-effect transistors (Chap. 14, by G. Horowitz), and solar cells (Chap. 15, by C. Brabec and S. Sariciftci).

The book provides an excellent introduction to conjugated polymers and an extremely useful compilation of the sort of data that one is often looking for, although these tend to be somewhat hidden in some cases. Examples of this tendency include the table of structural formulas in Chapter 13 (J. C. Scott and G. Malliaras), which also contains some small-molecule compounds, and the survey in Chapter 11 (I. H. Campbell and D. L. Smith) of the types of metal electrodes used. Commonly used experimental techniques, such as photoelectron spectroscopy, arrangements for laser spectroscopy, and time-of-flight measurements, are described in short introductions within the individual chapters. Also, Chapter 14 contains an excellent and easily readable introduction to the theory of field-effect transistors.

In their preface the editors explain that they asked the authors to write only what they felt certain about, and to omit results that still belonged to the realm of speculation. It is pleasing to find that, thanks to that policy, the book is not just a collection of specialist articles but has almost the character of a monograph. However, one's pleasure is slightly diminished on noting that there has evidently been no proper coordination between the individual contributions. There is much redundant material, and often topics are touched on and explained only briefly, whereas elsewhere in the book they are treated in much more detail. For example, the charge-transport mechanism in organic semiconductors is discussed in detail by H. Bässler in Chapter 12, but is then explained again in Chapter 14. Or again, the field-effect transistor is described in Chapter 1, whereas all that was needed was a cross-reference to Chapter 14. Although this redundancy means that the individual chapters can be read independently without difficulty, the absence of any interconnections between the chapters becomes very obvious. A little coordination work by the editors would have greatly improved the clarity of the book and reduced the number of pages. That would perhaps have prevented situations such as the presentation and discussion of exactly the same figure (!) in two different places (Figs. 8–5 and 9–11). Another source of trouble for the user is that the index has not been carefully checked, with the result that an index entry often fails to list all the relevant text pages. Although it is praiseworthy to have provided a subject index, there is a duty to ensure that it is usable.

Despite this shortcoming with regard to the guidance of the user, the book is well on the way to becoming a standard work for everyone active in this field. Chemists using this book will probably have a formidable task in understanding the physical chapters, and physicists will have trouble with the chemical parts, but nevertheless this work has significantly reduced the gulf between the two disciplines. Therefore I can recommend the book, although I fear that the price of almost DM 400 may be an obstacle to its reaching its proper place, namely on the bookshelves of postgraduate students.

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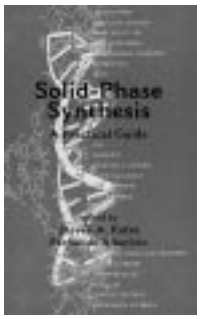
Solid-Phase Synthesis. A Practical Guide. Edited by *Steven A. Kates* and *Fernando Albericio*. Marcel Dekker, New York 2000. 848 pp., hardcover $ 250.00.—ISBN 0-8247-0359-6

In accordance with the authors' scientific background, this book is mainly concerned with individual disciplines in the area of the solid-phase chemistry of peptides. Readers who, on the basis of the title, expect to find in it also a detailed treatment of "classical" organic chemistry in the solid phase will unfortunately be disappointed, as that complex of topics receives only marginal attention. Regrettably, therefore, the title is misleading to that extent. Nevertheless, everyone involved in work on the synthesis of peptides, peptide mimetics, etc., will find here a comprehensive reference source, spanning the range from R. B. Merrifield's ground-breaking solid-phase synthesis of peptides to the latest advances in this broad field.



The various aspects of the subject are covered in 20 chapters, but the editors have not entirely succeeded in arranging the material in an orderly way. Also, as the chapters have all been written by different authors with different styles and layouts, the book has the disadvantage of not presenting a consistent appearance, and this may displease readers who are concerned with more than the actual content. Furthermore, it would have been helpful to provide a glossary of abbreviations, especially as there are so many in this area of chemistry.

Chapter 1 deals with solid supports (resins), and even includes laboratory procedures for preparing various types of polymeric supports, such as those based on polystyrene or polyacrylamide. I read this chapter with interest, but nevertheless I intend to continue using only commercially available resins, as the range of these with a wide choice of substituents has improved greatly in the last few years, so that it is now hardly ever necessary to consider preparing one's own.

Building on the above foundation, the following chapters deal with the various tools of solid-phase synthesis in detail, including linkers (Chap. 5), coupling reagents (Chap. 6), and protecting group strategies (Chaps. 2, 3, and 4). In the USA the Boc strategy is still preferred over the Fmoc strategy, so it comes as no surprise to European readers that the former receives so much attention in this book. The extensive lists of literature references in these chapters, as also in the later ones, are as detailed and comprehensive as one could wish.

Advances in the capabilities of solid-phase synthesis for peptides have opened up possibilities for more complex synthetic strategies. Therefore several chapters are devoted to syntheses of other structures derived from peptides, including cyclopeptides (Chaps. 7 and 8), and pseudopeptides or peptide mimetics (Chap. 16). Compared with normal linear peptides, these structures offer improved pharmacokinetic properties, and therefore are of great interest for pharmaceutical chemistry. Another chapter (Chap. 10) is devoted to phospho- and sulfopeptides.

The two-stage process in peptide chemistry (detachment of protecting groups followed by a coupling reaction) is gaining ground, and can be used for efficient syntheses of peptides with up to 30 amino acids. If one wishes to go beyond that, then, as in natural product synthesis, the fragment synthesis method can be effective. Chapter 9 discusses the principles of such syntheses in detail, and illustrates the strategy by discussing three representative highlights from the literature.

Chapters 11–13 review in turn developments in the synthesis of oligonucleotides, oligonucleotide–peptide conjugates, and peptide nucleic acids (PNAs), which are the analogues of (deoxy)-ribonucleic acids.

Chapter 14 contains an excellent review of the third main group of biopolymers, the oligosaccharides. As well as giving a general overview of the topic, the authors discuss in detail the key research projects of the last five years, which will very probably form the basis for new syntheses now being planned.

Chapter 15 is concerned with the solid-phase synthesis of heterocycles starting from amino acids and linear peptides. Considering the peptide background of the authors of this book, one can easily guess the origin of the examples chosen. However, in view of the many solid-phase heterocyclic syntheses that have been published in the last ten years, the choice of material seems rather arbitrary, and thus hardly serves to cover this broad field of research.

The book is completed by a look at progress in the automation of solid-phase syntheses, which includes a list of commercially available automated systems (Chap. 17), and by Chapters 18–20, which deal with the purification and analysis of peptides.

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