

A gateway to the literature

Chemometrics and Species Identification (Topics in Current Chemistry 141), edited by M. J. S. Dewar et al., Springer-Verlag, 1987, DM 108 (VIII + 184 pages) ISBN 3-540-17308-0

'Chemometrics and species identification' is volume 141 in the series 'Topics in current chemistry' and contains five review-like papers concerning various aspects of chemometrics and species identification.

Vandeginste has written the opening paper entitled 'Chemometrics — general introduction and historical development'. He presents an interesting overview of the role and development of the area of chemometrics, 'the interface between analytical chemistry and mathematics'. This is followed by some examples of the application of chemometrical techniques, in particular optimisation, multivariate data processing and multivariate calibration.

Kateman is on his pet-subject when he discusses sampling strategies in the second paper of the book. He presents an overview of methods for dealing theoretically with sampling problems, depending on the object of study, the objective of the analysis and the available means.

Various aspects of signal and data analysis in chromatography are discussed by Smit and Van den Heuvel. Although not particularly familiar with this topic, I found their exposition clear and easily comprehensible.

In over fifty pages, Forina, Lanteri and Armanino discuss various applications of chemometrics in the area of food chemistry. In what I consider the best contribution in the book, they give a very clear account of the background and application of a great many chemometrical techniques. Emphasis is placed mainly on classification and modelling, both of which are, of course, of paramount importance in food chemistry.

In the final paper, Gardiner treats the identification of traces of inorganic species in biological materials. It was rather disappointing to find

that most emphasis in this paper is on experimental techniques, whereas the use of computer modelling in this area (which would have been more interesting from a chemometrical point of view) is only briefly touched upon. Also, I was surprised to find that the actual characterisation of species is discussed in only five lines of text.

Considering the title of the book, I would have expected a contribution concerning the use of chemometrical and other techniques for the identification of species based on molecular spectral data (e.g., by means of library searches, pattern recognition and artificial intelligence). Vandeginste mentions the subject briefly, but does not dwell on it.

I do have some reservations about this book. The least serious is the fact that the publisher obviously has not provided any linguistic support. There are quite a number of typographical and spelling errors and the English is terribly clumsy in places. In fact, some new words are even introduced into the English language (such as 'neglectable', where 'negligible' is meant).

Personally, I find titles in refer-

ences very useful when sorting out which papers are worth pursuing — especially in reviews! A more serious defect is that, in my opinion, the captions of a considerable number of figures have an information content that is too low, in particular for the less initiated.

The major flaw, however, is that I find it very difficult to define the category of scientists to whom this book could be useful. Clearly, for experts in the various fields the book represents no more than a reiteration (although this, in itself, may be useful). The nature of the book also does not make it an obvious choice if one is looking for a teaching aid. It should — by virtue of the wealth of references — be of some use to those seeking references to the primary literature concerning one of the topics covered in the book.

In my opinion, two separate volumes would have been more appropriate to present the advances in the area of chemometrics on the one hand, and that of species identification on the other.

GERARD J. KLEYWEGT

Gerard J. Kleywegt is at the Department of NMR Spectroscopy, University of Utrecht, Padualaan 8, 3584 CH Utrecht, The Netherlands.

The plot revealed

Experimental Design: A Chemometric Approach, by S. N. Deming and S. L. Morgan, Elsevier, 1987, Dfl 225.00 (294 pages) ISBN 0-444-42734-1

It is unfortunate that experimental design, whilst representing a well-developed area of analytical chemistry, is so often poorly understood and applied. One of the possible reasons for this is proposed by the authors in the introduction: because the subject is usually taught from a statistical view rather than as a tool for research and development. This book is intended to provide a different perspective and develop the statistics alongside

the experimental design to provide an integrated and complementary approach to the subject.

Somewhat unusually, the book is written rather like a novel: the plot gradually unfolds as you progress through the chapters. Indeed, the reader is explicitly directed to read through from Chapter 1 to Chapter 12, working through the numerous exercises presented at the conclusion of each chapter. This structure also serves to highlight the value of the book, which is as a teaching text, rather than a reference book, from which one can select particular subjects of interest since every chapter continues to build on material which precedes it.