

Book Review

THERMOCHEMICAL DATA OF ORGANIC COMPOUNDS (Second edition)

J. B. Pedley, R. D. Naylor and S. P. Kirby

published by Chapman & Hall, May 1986 (Price £ 55)

To those who need to calculate thermochemical data for organic compounds and reactions, reference books such as this are an indispensable tool. The task of compiling such a volume is, however, something few would contemplate with equanimity!

The first edition of this particular work under the title "*NPL Computer Analysed Thermochemical Data: Organic and Organometallic Compounds*", by J. B. Pedley and J. Rylance was published by the University of Sussex in 1977. It has already established itself as a major reference work and this updated new enlarged edition published by Chapman & Hall should help to further establish its reputation and to bring it to the attention of a wider readership. In this new edition there is a greatly extended textual introduction (*ca.* 80 pp.). Most of this is concerned with a description and evaluation of a new "group additivity" method for calculating standard enthalpies of formation. This has been developed at the University of Sussex and claims advantages over similar but more established group additivity rules. For example, it includes a method for estimating uncertainties in the calculated values. The heart of the book, however, consists of two long tables of thermochemical data (total *ca.* 530 pp.). The first of these is of standard enthalpies of formation for about 3,000 organic compounds and the second is of *assessed* thermochemical data for their organic reactions (mostly enthalpies of combustion). The tables are produced by computer and are clear although the second (reactions) table has features which seem designed to help the computer rather than the general reader. Unnecessarily complex codes are used for the references, information on who abstracted each entry (which can be of little interest to most users) is included and most annoying of all a system is employed whereby only CNH formulae are given and isomeric compounds are distinguished by a number. To establish the structural formula for each compound or isomer the user has to refer back to the first table. The situation is partly redeemed by a good name and Chemical Abstracts Registry Number index. An advantage promised from the use of computer production is that as time passes it will be possible to update and supplement the tables. Indeed a supplement on organophosphorus compounds is already planned.

*John Wiley & Sons, Limited, Chichester
Akadémiai Kiadó, Budapest*

Some of the reference information is also to be made available through the CATCH (Computer Analysis of Thermochemical Data) search and retrieval system which as well as providing a data base has software for use in the prediction of standard enthalpies of formation. Although, as in other areas of data retrieval and manipulation, this is undoubtedly the way forward computer retrieval systems are always plagued by problems of cost and availability and the need for books such as this will remain.

Despite minor criticisms this is a thorough, carefully researched work that will prove useful to a wide range of practising chemists. Although the price will deter individual purchasers there is no doubt that it will find a deserved place in most well-founded scientific and technical libraries.

Dr. R. J. Bushby