anyone interested in the chemistry of technetium. It is well illustrated with structures and data tables, and comprehensive lists of references (over 1000 in all). It is clearly a book that all good chemistry libraries should buy.

P. J. SADLER
University of Edinburgh, UK

Organic synthesis workbook

J. A. Gewert, J. Gorlitzer, S. Götze, J. Looft, P. Menningen, T. Nobel, H. Schirock and C. Wulff
Wiley–VCH, Weinheim, 2000
xii + 274 pages. £22.50 (paperback)
ISBN 3-527-30187-9

Intended primarily for use by postgraduates, although of benefit to a much wider audience, this is an excellent book. Sixteen recent total syntheses of natural products (allowing for one aglycone portion), some of which are alkaloids, others terpenes or macrocycles, but all carefully selected, are presented in the form of problems to be solved, in an order of more or less increasing complexity. Each synthesis is dealt with in the same format: a brief introduction outlining the significance of the compound and previous synthetic approaches (where applicable); the problem section (the overview) that comprises a sequence of steps in which some of the reagents or structures are omitted; a section entitled synthesis; a summary of the synthetic strategy; and lastly, a set of useful references that are cited within the body of the text.

In the overview section, the reader is invited to fill in the gaps. Each gap is discussed in the synthesis section that comprises a re-statement of the problem, followed by a section of tips, of increasing information and hinting towards the answer. One should then attempt the problem before looking at the third section, the solution. A discussion section is used in the relevant places to provide additional detail or background material of general importance. Having thus worked through all the steps (problems), one has considered the total synthesis of the target molecule.

The idea of using selected syntheses as a means of imparting both interest and understanding is not new, and was used to great effect in *Selected Organic Syntheses* (I. Fleming, Wiley, 1972) with which the present book has part of its format in common. In *Organic Synthesis Workbook*, the reader is confronted with how to perform key reactions, but is given useful tips for each problem. This is an effective way of helping one to reason towards the answer. In many cases, a good postgraduate will have some idea of the answer, and may well reflect: 'I should have known that', even when the answer is not completely obtained without recourse to the tips as prompts. In only a few cases are several steps conflated, thereby giving rise to too many possibilities to consider. At each stage along the synthetic pathway one is exposed to just the right amount of information, enabling a sound understanding to be gained in a short while. In this way, many essentials of modern organic synthesis are introduced with minimum effort, by seeing them in context; asymmetric reductions, epoxidations and dihydroxylations, together with modern carbon–carbon bond forming protocols, are but a few of the key reactions any of which could be relevant at technical interviews. The index proves most effective in locating key reagents, reactions and concepts, and one can then readily obtain greater detail by consulting the references provided. The brevity and clarity of style, and the clear layout all contribute to ready assimilation. Mechanisms are provided in a way that leads to a clear understanding of the major principles. As would be expected, issues of stereochemistry must be constantly addressed, but handling them is usually not a problem because of the clarity of the presentation. Any organic postgraduate student can gain much from this book, and should own a copy. The level of the problems is well pitched, with plenty to challenge the able postgraduate, although without a daunting complexity to which synthesis can be prone. For those seeking an understanding, rather than a detailed work of reference, this book succeeds admirably in explaining in context many important principles of contemporary organic synthesis. This book is reasonably priced and I recommend *Organic Synthesis Workbook* to you highly.

C. M. MARSON
University College London, UK

Modelling molecular structures

A. Hinchliffe 2nd edn.
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xviii + 336 pages. £34.95 (paperback)
ISBN 0-471-48993-X

Is experimental chemistry old hat? Couldn't we — shouldn't we — be doing it all by computer nowadays? Well, up to a point: it all depends of course what you want to find out. For small molecular systems, there is no doubt that a very wide range of properties can now be computed better in both accuracy and precision than they can be measured. Moreover, the computations can give insight into the behaviour of selected electronic and vibrational states rarely visited by experiment and, indeed, into chemical species not readily accessible synthetically. With larger systems then, as usual, the bigger the canvas, the broader the brush that is required.

The basic theoretical principles underlying such

methods were all in place half a century ago when 'the only difficulty which exists.…is the amount of computing necessary' (Boys, 1950). It is the enormous strides made in both the software and hardware departments over the past decade or so that have brought computational methods to the point where they can, and should, be used routinely as a standard item in the chemists' instrumental armoury; indeed for anyone active in this area before the days of the universal desktop PC, the present-day capabilities are a constant astonishment.

But how can a newcomer best begin? There is an enormously wide range of methods described in literature aimed primarily at professionals, and an equally extensive range of software packages readily available via the Web. *Modelling Molecular Structures* aims to guide the novice, as well as those with modest experience, through this maze to the point where he/she will be able to use computational techniques to answer real chemical questions and, at least as important, will know what he/she is doing, and why: these do not always go together.

The author's preferred packages are Gaussian98 and HyperChem5.1, and he makes extensive use of printed screen dumps for illustration. Another excellent feature widely used here is the reproduction at the appropriate points in the text of the abstracts of nearly all the key papers on particular methods: in this way the reader meets the original authors, in their own words written at the time of each advance. This book is not, however, just or even mainly an instruction manual for software packages. It also contains a richly detailed background, seriously mathematical in places, with copious references to the original literature. Users may well prefer to begin at Chapter 10, on *ab initio* packages, in order to get a quick start, and then to move outwards to whichever area of the background detail they require, whether it be on molecular mechanics, the Hartree–Fock model, electron correlation, density-functional theory, potential energy surfaces, or whatever.

In terms of the properties we can actually calculate, the author bases his discussion on the classification of Boys and Cook, who considered primary and derivative properties (including energies, charge distributions, force constants, etc.), induced properties (including polarizabilities and hyperpolarizabilities, important in nonlinear optics, and magnetizabilities, important in NMR) and, finally, interactions between systems. This last is the most intractable of all, and, apart from a brief discussion of the use of solvent boxes to model properties in aqueous solution, the author wisely steers well clear of it. An important application here lies in the packing of molecules into crystals, and, in recently published tests, no currently available method was able to provide correct predictions for all of a set of four known, but unpublished, crystal structures of simple molecular compounds. Clearly, Clementi's 1973 claim 'we can calculate everything' has some way to run yet.

Nonetheless, this excellent handbook should be on the desk of all interested in the use of computational methods in chemistry.

CHRISTOPHER GLIDEWEWELL
University of St Andrews, UK

