Additions and Corrections

A Remarkable Pericyclic Mechanism for Enzyme-Catalyzed P–C Bond Formation [*J. Am. Chem. Soc.* **1989**, *111*, 6885–6887]. MICHAEL S. MCQUENEY, SHENG-LIAN LEE, ELISE BOWMAN, PATRICK S. MARIANO,* and DEBRA DUNAWAY-MARIANO*

The configurational designations given to the CTPEP enantiomers shown in Scheme II and given in the text on page 6886 are incorrect since the priority order for groups should be S > enolpyruvyl > ^{18}O > ^{16}O. Thus (*S*)-CTPEP should read (*R*)-CTPEP and (*R*)-CTPEP should read (*S*)-CTPEP. This error has no effect upon the conclusions drawn.

However, it has recently come to our attention that the carboxylic acid function in phosphate esters of phosphoenolpyruvate serves as an intramolecular catalyst in hydrolysis reactions of these substances (Schray, K. J.; Benkovic, S. J. *J. Am. Chem. Soc.* **1971**, *93*, 2522–2529). If this type of catalysis, involving cyclization by carboxyl oxygen attack on phosphorus followed by P–O bond cleavage by water, were operating in the $H_2{}^{18}O$ hydrolysis of the phosphonamide enantiomers shown in Scheme II (page 6886), then the processes leading to ^{18}O-incorporation would have occurred with net retention of stereochemistry at phosphorus. In that event the configurational assignments to the CTPP enantiomers would be reversed. This would mean that the phosphomutase enzymatic process transforming CTPP to CTPEP involves retention of stereochemistry at phosphorus, a result that suggests the operation of a double displacement mechanism.

Nucleophilic Substitution within the Photoionized van der Waals Complex: Generation of $C_6H_5NH_3^+$ from $C_6H_5Cl{-}NH_3$ [*J. Am. Chem. Soc.* **1988**, *110*, 7238]. TOSHIHIKO MAEYAMA and NAOHIKO MIKAMI*

In writing this paper we were unaware of the previous work dealing with a similar process (Dimopoulou-Rademann, U.; Rademann, K.; Bisling, P.; Brutschy, B.; Baumgärtel, H. *Ber. Bunsenges. Phys. Chem.* **1984**, *88*, 215). We thank Dr. B. Brutschy for drawing this prior work to our attention.

Computer Software Reviews

Current Contents on Diskette (IBM Version). Institute for Scientific Information: 3501 Market Street, Philadelphia, PA 19104. List price $295 per year for the 600-publication Life Sciences series ($170 with a subscription to the printed version) or $495 per year for the 1200-publication Life Sciences series ($370 with a subscription to the printed version) and $345 per year for the Physical, Chemical and Earth Sciences edition ($220 with a subscription to the printed version).

As was reviewed in *J. Am. Chem. Soc.* **1989**, *111*, 2747–2748, Current Contents on Diskette makes available to the user the information found in the printed version of *Current Contents*. Where the earlier review reported on the Macintosh version, this version runs on an IBM or 100% compatible computer. The software is available on 5.25 in. 36 O KB discs, 5.25 in. 1.2 MB discs, or 3.5 in. 720KB discs. A hard disk is required as is a minimum of 512 KB RAM with 640 KB RAM desirable. Printed output is possible with either dot matrix or laser printers.

A single weekly issue, such as the one provided for the Life Sciences section of *Current Contents*, will occupy 1 MB of disk space for the version covering 600 journals and 1.5 MB of disk space for the 1200-journal version. Each week's edition of Current Contents on Diskette covers the journals in that week's printed edition of *Current Contents*. To conserve hard disk space, the program provides a convenient routine for erasing back issues. This procedure deletes all the files in the subdirectory where that issue was stored and then removes the subdirectory. The user guide supplied with the software is clearly written and easy to follow. Installation of the software and loading of the sample issue of Current Contents on Diskette required approximately 30 min. Opening each weekly issue takes considerably less time.

As mentioned in the earlier review of this software package, one of the most useful features of Current Contents on Diskette is the ability to search the current volume by any of nine different indexing terms including title keywords, author, and journal. The volume may be searched employing the usual AND, OR, and NOT logic operators and employing either exact terms or truncated expressions. An additional feature of the program is a dictionary of terms that may be accessed during construction of the search statement to check spelling or the appropriateness of a given truncation.

If an EGA monitor is employed, the screen may be configured to display either 43 or 25 lines with the larger number of lines being especially useful when larger searcher profiles are developed. Additionally, the search profile may be stored and combined with other search profiles or employed when the next issue of Current Contents on Diskette arrives. Searches may be printed or exported to disk in any of four formats, with the Dialog format having the author's names in the standard ACS bibliographic style. Again as mentioned in the earlier review, printing of the popular "Request-A-Print" forms or requests for the "Genuine Article" from ISI from the results or a search are quite easy.

Several small discrepancies between the help screens and main menus were found. For example, the command for deletion of back issue of Current Contents on Diskette was listed as D in the main menu but E in the help menu. While this was initially disconcerting it otherwise had no identifiable effect on the execution of the program.

Current Contents on Diskette is an interesting addition to the available current awareness tools. The timeliness of the weekly issues is especially attractive. While browsing of Current Contents on Diskette is also possible and quite convenient it is the search function that makes this software so useful.

John T. Welch, *State University of New York at Albany*

Book Reviews

Annual Review of Computer Science. Volume 3, 1988. Edited by Joseph F. Traub (Columbia University) et al. Annual Reviews: Palo Alto. 1988. 423 pp. $45.00. ISBN 0-8243-3203-2.

When there is great activity near one's house, it is advisable that one learn the purpose of the activity. It is in this sense that the *1988 Annual Review of Computer Science* can be recommended to chemists. The book contains 13 chapters, each of which reviews a different subject area. The selection of subjects is quite eclectic; the subjects discussed are database security, expert systems, protein folding, algebraic geometry, image analysis, programming logics, the LISP language, common-sense physics, parallel algorithmic techniques, resolution theorem proving, algebraic complexity theory, computer applications in manufacturing, and computational geometry. Few of these are of current and immediate importance to many chemists, but others may become so in the not-too-distant future. The writing is generally accurate and authoritative, but the clarity is uneven. Some chapters, such as those on protein folding and image analysis, make easy and enjoyable reading while others, such as those dealing with database security and algebraic complexity, make few concessions to the reader. They exhibit a stubborn determination to avoid discussing concrete examples of the propositions at hand and are not at all "user-friendly". Outreach is a very desirable attribute in books of this sort; here it has been attempted very sporadically. In spite of this, the book contains enough excellent material and is sold at such an attractively low price that chemists should seriously consider spending some time with it.

G. W. A. Milne, *National Institutes of Health*

Organometallic Chemistry. An Overview. By John S. Thayer (University of Cincinnati). VCH: New York and Weinheim. 1988. xi + 170 pp. $35.00. ISBN 0-89573-121-5.

This book has been pitched at an unusual level and is intended to provide an introduction to organometallic chemistry intermediate between that available in standard inorganic texts and the more detailed coverage provided by monographs and graduate-level teaching texts. A successful book at this level would provide a useful introduction to organometallic chemistry for somebody with no previous exposure to the subject but with a reasonably good background in chemistry, and in many ways the present attempt succeeds in filling this niche. It does, for example, provide an introduction to the subject within a relatively short compass and at a reasonable price, but the author has complicated his task by choosing to define organometallic chemistry in the broadest conceivable sense. Thus, in addition to the transition-metal organometallic chemistry which provides the backbone of books such as those by Collman et al., he has included not only the very important area of main-group organometallic chemistry (which has been experiencing a resurgence of research interests) but (by defining an organometallic compound as any compound in which carbon is bonded to a more electropositive element) has also included molecules in which carbon is bonded to elements more commonly thought of as metalloids or even nonmetals, including As, P, Se, Te, and I.

The book is essentially divided into four major sections; the first of which comprises introductory chapters on the development of organometallic chemistry, methods of synthesis of metal–carbon bonds, ionic metal–carbon bonds, and electron deficient metal–carbon bonds. These are followed by a series of three chapters on the metal–carbon σ bond, which focus on the reactive metals, the heavy metals, and the metalloids, respectively. The section on metal–carbon σ bonds is followed by a section on metal–carbon synergistic bonds, subdivided according to the type of ligands involved. Chapter 8 discusses mononuclear compounds of divalent carbon, Chapter 9 covers mononuclear complexes of unsaturated hydrocarbons, and Chapter 10 is a very brief introduction to polynuclear compounds.

The final section of the book is a series of three chapters on organometallic compounds in biology, which cover respectively medicinal and biochemical uses, toxicological and biocidal aspects, and environmental occurrence and transformation. I felt that these chapters form a highlight of the book and provide a useful introduction to the biological aspects of organometallic chemistry, and I know no other source that discusses the biological uses and impact of the whole spectrum of organometallic compounds.

Given the very ambitious breadth of coverage it is inevitable that the depth of coverage in this book will be somewhat frustrating to anybody with a significant background in any of the areas surveyed, and I certainly found the coverage of transition-metal organometallics to be somewhat naive and superficial. I must, however, admit that I learned something about main-group organometallics and enjoyed the three survey chapters on the role of organometallic compounds in biology. The limited depth of the coverage somewhat mars the impact of this book, since it is at a level where it is too superficial for a graduate course focusing on organometallic chemistry but is probably too ambitious in scope to do more than form a supplementary resource for most undergraduate courses.

N. John Cooper, *University of Pittsburgh*

Theory and Methods of Calculation of Molecular Spectra. By L. A. Gribov (USSR Academy of Sciences) and W. J. Orville-Thomas (University of Salford). John Wiley and Sons: New York. 1988. xvii + 636 pp. $186.00. ISBN 0471-91882-2.

It is stated in the preface that "this book gives an account of how computers can be used to supplement, and in some cases to replace, experimental spectroscopic studies in the identifications of molecular substances and to provide detailed information on their geometrical and electronic structure. ...The central problem of molecular spectroscopy is not only to identify a structural formula for a molecule but to obtain detailed information on its geometrical and electronic structure—ideally in the ground and excited electronic states." The book, based heavily on the research accomplishments and previous writings of L. A. Gribov and his associates in the USSR, surveys the theory of vibrational and electronic spectroscopy and the approach to solving the inverse spectral problem with the help of computed molecular parameters, or with the use of a library of stored experimental data. The results of illustrative computer calculations are frequently displayed but details of software or hardware are not included in this volume devoted predominantly to the theory of molecular spectroscopy.

Because of the authors' primary concern with the properties of large molecules in condensed phases, the book does not consider overall molecular rotation. Discussions of the vibrational and electronic properties of molecules are given in mathematical detail; this is not a book for beginners or for those primarily interested in nonmathematical descriptions. It begins with the Born–Oppenheimer approximation and the Franck–Condon principle and moves on to consider nonadiabatic approximations for the energy states and the Herzberg–Teller approximation for transition intensities. Approximate solutions to the Schroedinger equation for electrons moving in the field of fixed nuclei are considered at the ab initio level because of the usefulness of these results for estimating and correlating molecular geometries, isomers, vibrational force fields, and molecular charge distributions. The authors stress the power provided by the computer to yield results for increasingly detailed theoretical models and many of these models are therefore described in the book. The presentation goes well beyond considerations of the harmonic approximation for molecular vibrations or discussion of characteristic vibrational group frequencies. Some examples are the computation of vibrational anharmonicity by variational methods, the computation of transition intensities for overtone and combination modes, and the computation of Raman scattering intensities. General isotope product and sum rules are considered, and isotope effects on the intensities of nominal group frequencies, and the possibility of obtaining the permanent electric dipole moment of a molecule from analysis of isotopic infrared frequency and intensity measurements. The formal Boolean logic behind their computer codes for identifying spectroscopic unknowns from data banks is discussed. The coverage of vibrational energies, transition intensities, and ancillary topics is more extensive than the corresponding coverage of vibronic transitions.