Additions and Corrections

Photochemical Hydrogen Abstraction by Singlet and Triplet $n\pi^*$ States of Aromatic Nitrogen: Fragmentation of 4-Alkylpyrimidines and 2-Alkylquinolines [*J. Am. Chem. Soc.* **1990**, *112*, 3940]. SREEDHARAN PRATHAPAN, SARAH LOFT, and WILLIAM C. AGOSTA*

Page 3941: Some values reported in Table I contained propagated errors. A corrected version of Table I is given below. The errors in (rel $1/\tau$) and (rel $1/\tau$ per H) were small and in no way affect statements or conclusions presented originally.

Table I. Quantum Yields, Relative Triplet Lifetimes, and Abstraction Selectivity for **1a–c**

		in water[a]					in acetone	
C–H bond	cmpd	Φ_5	rel Φ_5 per H	$k_q\tau$, M^{-1}	rel $1/\tau$	rel $1/\tau$ per H	$\Phi_5 \times 10^3$	rel Φ_5 per H
3°	**1a**	0.25	5.8	6.0	0.87	2.6	7.5	7.7
2°	**1b**	0.16	1.8	1.9	2.7	4.1	5.6	2.9
1°	**1c**	0.13	(1.0)	5.2	(1.0)	(1.0)	2.9	(1.0)

[a] Φ_5's in D_2O; $k_q\tau$'s in H_2O.

Asymmetric Induction in Reactions of Styrenes with 1,4-Benzoquinones Utilizing Chiral Ti(IV) Complexes [*J. Am. Chem. Soc.* **1991**, *113*, 5068]. THOMAS A. ENGLER,* MICHAEL A. LETAVIC, and JAYACHANDRA P. REDDY

Page 5069: In eqs 1 and 2, (−)-**4** should be (+)-**4**.

Decanuclear Homo- and Heterometallic Polypyridine Complexes: Syntheses, Absorption Spectra, Luminescence, Electrochemical Oxidation, and Intercomponent Energy Transfer [*J. Am. Chem. Soc.* **1992**, *114*, 2944]. GIANFRANCO DENTI,* SEBASTIANO CAMPAGNA,* SCOLASTICA SERRONI, MAURO CIANO, and VINCENZO BALZANI*

Page 2948, left column, line 38 of the Discussion: It was reported that preliminary ^{99}Ru and ^{1}H NMR data indicated that the complex $Ru(BL)_3^{2+}$ was obtained as a single species having a *mer* structure. Actually, a more careful analysis of the proton 2D-COSY 400-MHz spectrum that permitted a complete assignment of the signals has shown the presence of a small amount (8% of the purified material) of the *fac* isomer.

Computer Software Reviews

Pro-Cite for the Macintosh, Version 2.0.2, and Biblio-Link for the Macintosh. Personal Bibliographic Software, Inc.: P.O. Box 4250, Ann Arbor, MI 48106. Pro-Cite: $395.00. Biblio-Link: $195.00.

Pro-Cite for the Macintosh is a bibliographic program that allows the building and searching of a literature database. References can be entered into Pro-Cite manually in formats such as book, journal, conference proceedings, or dissertation; and fields in each format are available so that complete bibliographic information can be included for each record. References can also be input with Biblio-Links, a supplementary program that allows direct record transfer to Pro-Cite from BRS, Dialog, or Medlars. The records can be output in journal-acceptable formats, and the files generated can be copied directly into documents with word processors such as Microsoft Word. Version 2.0 has many substantial changes from Version 1.0, the most significant being the increased speed of searching large databases.

A hard disk is recommended, if not required, for the efficient use of Pro-Cite on the Macintosh. The application works on MacPlus computers with System 6.0.2 or better, according to the vendor. The authors have used Pro-Cite on a MacPlus or MacII with System 6.0.7 and with System 7.0.1 on a PowerBook 170. The disk space required for a database obviously depends on the number of records and the amount of data entered in each record. A database of 1600 chemical records that includes authors, journal information, a brief abstract, and keyword descriptors occupies about a megabyte of disk space. Version 2.0 Pro-Cite for the Macintosh creates a .KEY file for every database that is essentially an index the user can customize so that designated fields can be searched very rapidly. This .KEY file may, in some cases, double the disk space used by the database. Databases from Version 1.0 of Pro-Cite are automatically converted to Version 2.0 files when read by the application.

Within a database, records can be accessed in several ways. A GO TO RECORD feature allows access to any record while buttons on the record display allow return to the previous record or previous selected record or advance to the next record or next selected record. A BROWSE feature allows three abbreviated records to be viewed simultaneously. Records can be readily modified with all Macintosh fonts in the cursor input mode or the record can be modified with standard Macintosh CUT, COPY, and PASTE commands. Utilities GLOBAL FIND/REPLACE and GLOBAL EDIT allow for all records in a database to be modified quickly. Data can be input into records from authority lists generated from the application's indexing feature. Authority lists can be easily created from an existing database. An author authority file can be generated, for example, by selecting the author fields from the database and indexing all authors in the database to a list file. This file can be edited and used as a basis for automatically entering new records into the database. Similar authority lists for keyword descriptors, journal titles, etc. can be created, allowing speed of record input and minimizing errors in the database.

There are several search features. A full-text search scans every character in a field from beginning to end. This can be a slow procedure, a simple author search of our 1600 record chemical database took about 30 s on a PowerBook 170. A QuickSearch of the same database that utilizes the .KEY file was essentially instantaneous and found the same number of records. Records selected by a search strategy can be saved as a Results Set and this set can be searched further. Standard logic search strings can be generated and abbreviated roots of search words can be used to provide a more global search. For example, a descriptor index search using the term DIAST* would find records indexed with descriptors "diastereotopic" or "diastereomer", etc. Results sets can be printed directly in a specified format or they can be exported and saved as a separate database.

There are several ways to generate a Bibliography. As noted, a Results Set can be output to a disk file using a punctuation format of the users choice. Several standard formats are already established in the application and the user simply chooses the format of choice from the menu. In the Chemistry Punctuation Files folder that comes with the program, standard American Chemical Society (ACS), as well as *Canadian Journal of Chemistry*, *Biochimica et Biophysica Acta*, and *Biochemistry* formats are found. Punctuation formats that are not included with the program can be customized as TEXT files. A punctuation file for *Tetrahedron Letters* or *Angewandte Chemie* can be readily generated, for example, by modifying an existing punctuation TEXT file and saving the new file under a different name. Operations such as the creation of a new punctuation file require the use of the manual and the HELP feature is of limited use here. However, the HELP feature is useful for many other questions that arise during use of the application. It should be noted that all calls to the vendor's customer service department have been returned and the information received was always helpful and offered in a friendly, courteous way.

Individual records or multiple selected records can be PREVIEWED in the designated punctuation format and the selected records can be saved to disk in the designated format. The file saved can be opened as MacWrite or Microsoft Word files. A feature deleted from Version 1.0 is the "Format Current Record" option which creates a Text File, and references can be added to that file in the designated format. However, a "command-option-C" sequence copies the current record to the Clipboard which in turn can be pasted into a word processor document in the default font. This procedure does not bring reference numbers along with the formatted record.

Bibliographics can also be created from a manuscript. In this mode, Pro-Cite scans a document for imbedded references and generates a set of selected records which are matched to the database and make up the bibliography for the manuscript. This goal is undoubtedly a worthy one and scientists would welcome an easy procedure for generating bibliographies in this way. The Pro-Cite procedure may become easy with practice but the first time we attempted to use this feature, we found it to be extremely frustrating. Implementation is more difficult and demanding than other features of the program and even extensive reading of the manual did not solve all the problems of generating bibliographies by this strategy. This part of the program could definitely be improved in terms of "ease of use". The vendor has indicated that Version 2.0 is a vast improvement from the comparable feature in Version 1.0 but there still is room for development before the Mac user can avoid an extensive experimentation period with this part of the program.

Another feature that takes some experimenting is the Biblio-Link auxiliary program. We were able to download records from a Dialog-Science Citation Index search using the tagged version of the program. It took a few tries before this was successful, however. One serious limitation of the Biblio-Link application is the fact that no STN Link is now available for the Macintosh version. Downloading Chemical Abstracts searches is therefore not possible for academic users who use STN because of the academic discount rates. The vendor has indicated that the STN version of Biblio-Link will be available at some time in the future as will all Biblio-Links currently offered in the IBM format.

In summary, Pro-Cite for the Macintosh is an excellent bibliography application. Most of its features are intuitive and easy to use. Searches are easy and standard or custom punctuation formats allow preparation of a bibliography for any purpose. Version 2.0 is a dramatic improvement from Version 1.0 in terms of speed and this alone suggests that there is good value in the upgrade for those who already have used Pro-Cite.

Ned A. Porter and Katherine R. Porter, *Duke University*

ChemWindow. Version 2.0.1. SoftShell International, Ltd.: 715 Horizon Drive, Grand Junction, CO 81506. (303) 242-7502. List price: $499.00. Academic/faculty price: $399.00. Student price: $99.00.

ChemWindow is a chemical structure drawing program for producing typeset quality graphics with computers running Microsoft Windows 3.0 or 3.1. ChemWindow requires an IBM-PC or compatible computer with a 286, 386, or 486 CPU, 2MB RAM, hard disk drive, mouse, graphics display, Microsoft Windows 3.0 *and* Adobe Type Manager or Microsoft Windows 3.1, and a Microsoft Windows compatible printer. ChemWindow is not copy protected and is supplied on both a single 3.5-in. double-density disk and on a 5.15-in. high-density disk. Registered users receive a free structure album containing more than 300 chemical structures. Registered users who purchase ChemWindow after March 1, 1992 will receive ChemWindow Version 3 at no cost when it becomes available (expected by fall 1992).

Installation is automatic and can be performed from the DOS prompt or from within Windows. The documentation consists of a 125 page loose leaf style manual. Numerous graphical examples are use to illustrate how to draw, edit, and manipulate complicated chemical structures. Structures can be drawn using the seven bond-drawing tools or the ten ring-drawing tools. The bond-drawing tools include the following: standard (single, double, triple), hashed, wedge, dashed, wavy, Bēzier curve, and bold. Both bond lengths and bond angles can be constrained by the user to aid in drawing accuracy. The ring-drawing tools include three-, four-, five- (two types), size- (hexagonal, chair, boat), seven- and eight-membered rings as well as a tool to add an aromatic circle to a ring.

There are four arrow tools used to draw reaction, resonance, equilibrium, and dashed arrows. Arrows can be drawn curved by using one of the arc tools and they can be used as bonds. The arc tools are used to draw circles and ellipses or their fragments. There is a Bēzier curve tool which is used to draw smooth curves at any angle or direction. Other entities that can be added to structures include orbitals, electron dots, and charges.

Multiple objects can be grouped together to make them easier to work with. Groups can be nested making complicated reaction schemes easier to draw. The various manipulation tools allow for rotation, flipping, and alignment. The editing tools include cut, paste, and copy. Text may be entered as atomic labels which become part of the molecular structure or as captions. ChemWindow can use any fonts that are available through Windows (thus the necessity to have either Adobe Type Manager or Microsoft Windows 3.1). The kerning of character pairs can be changed by the user to fine tune the typset quality of text.

Two additional tools that ChemWindow uses to help reduce the number of times a commonly used structure needs to be redrawn are the template tool and the album tool. The template tool allows the user to add custom-made structures to a pop-up template so that molecules or fragments can easily be retrieved and reused. Template structures however may only contain bonds, straight arrows, and rings. Captions, labels, and circles cannot be saved in a template. The album tool can store anything that can be drawn or pasted into ChemWindow. Once an album is loaded, all of its contents are just a mouse click away. Between the template and album tools, it should never be necessary to draw the same thing twice.

ChemWindow can import graphics from the Windows Clipboard as Windows Metafiles or from other software as long as the software saves the graphics as Placeable Windows Metafiles as defined by Aldus (Pagemaker). ChemWindow can export graphics as Word Perfect Graphic (WPG), Windows Metafile (WMF), and Encapsulated Postscript (EPS).

We feel that ChemWindow is a very powerful molecular structure drawing program and is competitively priced. The student discount makes ChemWindow by far the best buy in drawing software for the chemist. It is very flexible in both drawing and editing and produces very high quality graphics on 300dpi laser printers which can easily be imported into most word processing programs. SoftShell International has promised that one of the changes that will appear in Version 3 will be an increase in price but it will be offered at no cost to buyers of Version 2.0.1 after March 1, 1992. Version 3 will also include a syntax checker, built-in portfolio, chemical recognition, and new drawing tools. The syntax checker will check valences in both rings and character strings that represent atoms. Drawings will also be able to be checked against a table of structure configurations that can be updated by the user. The portfolio is an integrated archive facility that can be used to store structures and graphics allowing thousands of drawings to be saved in a database-like format. Chemical recognition will allow ChemWindow to import line drawings from other programs and convert them into chemical structures. ChemWindow 3 will also be able to share structure files with SoftShell's ChemIntosh 3 chemical structure drawing program for the Apple Macintosh.

David Gosztola and Michael R. Wasielewski, *Argonne National Laboratory*

Book Reviews[*]

Fossil Fuel Combustion: A Source Book. Edited by William Bartok (Energy and Environmental Research Corporation) and Adel F. Sarofim (Massachusetts Institute of Technology). John Wiley & Sons: New York. 1991. 866 pp. $99.95. ISBN 0-471-84779-8.

This is a book of ten chapters and an appendix written by twelve top-flight authors and billed as a "Source Book" on fossil fuel combustion. It is organized into three parts: I. Combustion Chemistry (five chapters); II. Flame Phenomena, Diffusional Processes, and Turbulent Reactive Flow (three chapters); and III. Heterogeneous Combustion (two chapters). The very useful appendix consists of data tables and graphs on fuel and combustion properties, although the publication *Technical Data on Fuel* (now in its seventh edition) is generally more complete.

The first eight chapters are in the realm of combustion science with only the last two dealing with combustion engineering. This shows a little imbalance for a "Source Book". If the timing had been right, this would otherwise have been a good companion to the Palmer/Beer book *Advances in Combustion Technology* (Academic Press, 1976) which better covers combustion engineering and identifies additional topics that one would expect to find in a complete source book on fossil fuel combustion. In addition, significant parts essentially have been taken right out of their own textbooks, notably Strehlow's Chapter 6, Lefebre's Chapter 9, and Smoot's Chapter 10. Consequently, for this and similar reasons, the outstanding question to me is why the book was written at all.

The origin of this book, according to the flyleaf, was that a number of eminent combustion scientists were asked "to conduct a state of the art course on the principles of flame properties". The demand for such information was driven by the increasing scarcity of fuel at that time. While true fifteen years ago, emission constraints appear to be the biggest driver at the moment. Most if not all of the chapters were written between 1980 and 1985, for example, 1981 for Chapters 2 and 3 and 1984 for Chapter 8. The book then has the aura of having been put together as an afterthought. The label "Source Book" in the title appears to reflect more a rhetorical flourish than a meaningful plan. There were later updates before going to press (apparently about 1987 with publication in 1991), but all the chapters suffer somewhat from being five to ten years out-of-date, although some have stood up very well with the passage of time, notably Chapters 2 (by Golden on Thermodynamic and Rate Parameters), 3 (by Dryer on Combustion Chemistry Modelling), and 9 (by Lefebre on Atomization and Spray Combustion).

With these authoritative authors, one does not expect anything but solid, accurate work, and this is essentially what we get. I noted, however, a number of questionable, arguable, debatable, and missing items. What follows is a sampling. On page four of Longwell's opening chapter in Table one, there is a listing of energy consumption through 2000 AD, but the source was Hottel and Howard's book published in 1971. Since that data there has been an oil embargo and two stunning jumps in oil prices followed by the big collapse of the 1980's, all in parallel with development of just about anything that could conceivably generate energy. Was the Hottel and Howard book really the best source and would those authors agree on the predictions today? Two further chapters (Chapter 5 on soot by Haynes and Chapter 7 on diffusion flames by Gerstein) suffer badly from the timing of publication since these chapters have nothing on the developments since the mid-1980's (by Glassman and Wagner amongst others) investigating the inverse diffusion flame (IDF) in which there is a dramatic difference in soot formation between the NDF's and IDF's. Also unmentioned in Chapter 7, presumably for the same timing reason, is the introduction in 1986 of the Species Stream Function that permits tracking of individual species in diffusion flames. William's Chapter 8 does the expected excellent job of defining the nature of the turbulence problem both in terms of the descriptions of the physical models and in the organization of the different flow and reaction regimes with prospects for effective solution of problems of practical value in the future. It still, however, leaves open how to handle today's practical problems of the turbulent jet diffusion flames. Smoot's Chapter 10 presents some major problems, although it is the only one that tries to cover the complete range from science to engineering. It has to be carelessness that my 1981 article in the Chemistry of Coal Utilization (2nd Supplement) written under the auspices of the National Research Council for the Chemistry of Coal Utilization, which he includes as reference 71, is not included in Table 1, Summary of Selected Surveys, since at 150 pages and 565 references with a table of 15 pages of rate data on coal and carbon gas reactions it is the longest review of all. That aside, however, as a matter of more substance, I am at a loss to understand why the empirical n-th order rate kinetics is still being advocated (Smoot's eq 23), and none of the fundamental rate equations are even mentioned, although there are 75 years of history from Langmuir, through Hinshelwood and Eyring, to say with equations that the carbon–oxygen reaction is *two* step, not the one step used in the n-th order treatment.

To sum this up, as a source book, it is incomplete, particularly in the small coverage of combustion engineering, and it is somewhat uneven in what it does cover. However, for what it does cover, the material is mostly sound, but certainly dated. Although it is mostly available in other texts, it is still a convenience to have so much of the material written by such authorities in one volume. One might say that the book is valuable, but not significant, but that is a position that could now be rectified by a second edition.

Robert H. Essenhigh, *Ohio State University*

Studies in Inorganic Chemistry. Volume 11. Chemistry of the Platinum Group Metals. Recent Developments. Edited by Frank R. Hartley (Cranfield Institute of Technology). Elsevier Science Publishers B.V.: Amsterdam. 1991. 642 pp. $274.50. ISBN 0-444-88189-1.

This series of books presents chemistry of importance and current interest to the members of the chemical community. In this volume the editor notes that while it has been about twenty years since major definitive books on these important metals have been published, specific aspects of their chemistry, such as organometallic chemistry and coordination chemistry, have received attention more recently. Thus, it was not the aim of the book to present a comprehensive coverage of the platinum group metals, but rather to cover recent developments.

Emphasis in the present volume was given to the occurrence and extraction of the metals; to their use in catalysis, electrochemistry, energy, and electronics; to their use in homogeneous catalysis in solutions and melts; to recent developments in our understanding of the chemistry of their coordination compounds which occur in biochemistry; to the use of their coordination compounds in cancer therapy; and to compounds and chemistry of the metals in high oxidation states.

The seventeen chapters in the book were written by twenty-four contributors either from educational institutions or research centers in industry. The contents of the chapters reflect the varied interests of the contributors, but the editor was successful in coordinating the material in such a manner that the pure chemistry and the wide range of applications of the compounds of these metals were skillfully interwoven.

The book begins with a chapter written by the editor (22 pages, 43 references) on the occurrence, extraction, properties, and uses of platinum group metals. There is an enormous amount of useful material on the metals in the chapter, and it will serve as a valuable source for lecturers. The chemistry is limited to extraction processes and some selected uses, since a number of the following chapters are devoted to reactions, chemical preparations of classes of compounds, and the wide variety of applications of the compounds.

Five chapters emphasizing the applications of the platinum group metals follow. These all emphasize catalytic properties and incude a general introduction by G. C. Bond (26 pages, 12 references); a discussion of catalytic combustion by D. L. Tim (14 pages, 28 references); a chapter on the use of these substances for the synthesis of chemicals from synthesis gas by G. R. Steinmetz and J. R. Zoeller (30 pages, more than 301 references); a discussion of the use of these metal catalysts in the petrochemical industry by A. W. Parkins (17 pages, 199 references); and

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[*] Unsigned book reviews are by the Book Review Editor.