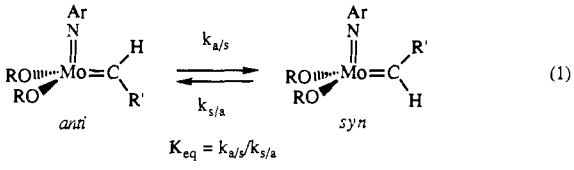
Additions and Corrections

Diphosphines with Natural Bite Angles near 120° Increase Selectivity for *n*-Aldehyde Formation in Rhodium-Catalyzed Hydroformylation [*J. Am. Chem. Soc.* **1992**, *114*, 5535–5543]. CHARLES P. CASEY,* GREGORY T. WHITEKER, MARGARET G. MELVILLE, LORI M. PETROVICH, JAMES A. GAVNEY, JR., and DOUGLAS R. POWELL

Page 5540, Table II: The turnover rate of hydroformylation in the presence of complex **1**, BISBI, should read 12.4 [moles aldehyde] × [moles Rh]$^{-1}$ h^{-1}, not 29.4 [moles aldehyde] × [moles Rh]$^{-1}$ h^{-1}. This correction does not change any of the conclusions of the paper.

Rate of Interconversion of Syn and Anti Rotamers of Mo(CHCMe$_2$Ph)(NAr)(OR)$_2$ and Relative Reactivity toward 2,3-Bis(trifluoromethyl)norbornadiene [*J. Am. Chem. Soc.* **1992**, *114*, 7588–7590]. JOHN H. OSKAM and RICHARD R. SCHROCK*

Page 7588: The equality for K_{eq} appeared incorrectly in the published version. Equation 1 should have appeared as follows:



(1)

$$K_{eq} = k_{a/s}/k_{s/a}$$

Computer Software Reviews

Autonom, Version 1.0. Springer-Verlag: 175 Fifth Avenue, New York, NY. List price $1980.00; educational discounted price $980.00.

Autonom, short for *auto*matic *nom*enclature, is a fully automatic computer program for the generation of IUPAC systematic names of organic compounds directly from structure diagrams. The software was developed by and is used at the Beilstein Institute and has been described in several recent journal articles.[1] Simply put, the user draws a structural diagram of a single organic compound using the mouse, menus, and keyboard and then asks the program to name the structure. While the program currently implements only a subset of the "Blue Book",[2] in particular sections A and B, nomenclature of chains and rings, the user's manual claims that Autonom 1.0 was able to correctly name better than 71% of over 1 million compounds from the recent literature. Structures are limited to 100 heavy atoms from a set of 20 currently supported non-hydrogen atoms and a maximum ring or chain size of 44 atoms. The most serious lack of this program is its current inability to handle three dimensional stereochemistry and generate stereochemical descriptors. Future expansions of the program's capabilities are promised in the manual. Discussions with Springer-Verlag revealed that both a PC batch version, which will not include the molecular editor but will be able to generate names from downloaded ROSDAL[3] files, and a mainframe version are both in the works at the Beilstein Institute.

Features: The program runs on an IBM PC or compatible with DOS 3.3 or higher, 640 KB RAM (500 KB free) and requires 4 MB of hard disk storage space for program files. The program supports a large number of graphics cards and printers, the latter including Postscript and several HP variations. A Microsoft mouse or compatible is also required. We tested Autonom on two platforms, a DELL 486D/50 with 32 MB RAM and super VGA monitor, and a DELL 320 N+ notebook with an 80387 coprocessor, 4 MB RAM and VGA monitor. Both systems were running DOS 5.0; in addition the 486 was running Windows 3.1 while the 386 was running Windows 3.0. The software was tested under DOS and Windows[4] as the operating environment on both machines even though the program does not require Windows, and it operated flawlessly in all cases. Installation of the software is trivially accomplished by the automatic install program.

Autonom is not designed to use or take advantage of Microsoft Windows. Rather, the program's own graphical user interface contains a menu bar at the top of the screen, a command bar at the bottom, and a large central area including the structure editor screen and pop up menus. All program functions are chosen using the mouse, and further windows or menus may be displayed for user input. The keyboard is typically used only for entering text or file names. For anyone with experience with structure drawing programs, on-line structure searching, or even windows, the program is quite simple to learn. In fact, I found that I was able to draw, manipulate, and name structures from my own research within about 15 min without even reading the manual, although I kept it handy and referred to it several times. Freehand sketching of molecules accomplished using the left mouse button creates a carbon atom and a pop up menu containing the atom number, symbol, and lock symbol. At this point, the user may enter an alternative atomic symbol (this function is case insensitive, i.e., whether you type in upper or lower case the software recognizes the atomic symbol) or move the mouse to a new location. Moving the mouse causes the pop up menu to disappear and a bond to appear. The bond is terminated by another left click to generate the next atom. Atom types may be changed by clicking on an atom and then entering the new symbol via the keyboard. Bond types may be changed before drawing, after the bond has been drawn, or on the fly by typing a numeric key (i.e., 1, 2, or 3). Atom and bond deletions are done by double clicking the right mouse button. There is also a group template library containing 18 structures and a ring template library of 27 structures that considerably speed the drawing process. In addition, 48 functional groups are available through the keyboard or via the HELP SHORTCUTS selection in the menu bar. For ease of structure manipulation and drawing, the user can copy, move, and size fragments, groups, and the entire structure using the menu bar.

A total of five structure files are available to the user during program operation. In addition to group.tmp and rings.tmp template files, there is a user library file called trivial.lib and a working file called session.str. Users can add structures from all of these files, thus creating a customized version of Autonom for their particular use or type of chemistry. The fifth file, activated using the OTHERS menu choice, allows one to

load and save structures to any given filename. Wildcard operations are allowed in describing files when using OTHERS. Another useful function associated with files is the ability to document structures and queries using the TEXT menu. Since all structures are stored as ROSDAL[3] strings, files are in ASCII format and may be read and edited outside Autonom. Other Beilstein PC products such as MOLKICK or products from other software vendors that read ROSDAL can also interact with structures in these files. Conversely, Autonom can read ROSDAL structure files generated by other programs.

An interesting and very useful feature is the session history file kept by the program. This file contains a list of names of structures generated during the current session. Furthermore, the structures can be recalled to the structure editor for further manipulation. This history file can be saved to disk for recall and use in a later session.

Hard copy is obtained through the PRINT menu. The user may print either the query on the screen or structures in a file, a very useful option. We have an HP Deskjet 500 attached to the PC running the program, and we found that while print quality was very good, print speed was disappointingly slow (e.g. anthracene took almost 5 min to print). This may be because the printer driver supplied with the program is for an HP Deskjet rather than the Deskjet 500, since other software on our system prints graphics quite rapidly. We were unable to test the Postscript printer driver because the program does not currently allow one to print to a file rather than to an output device (i.e., LPT# or COM#). Because Autonom does not utilize Windows, printing ties up the PC for the duration of the printing process. One could avoid this problem by running Autonom using the MS-DOS prompt window rather than in full screen mode, but then the inherent slowness of graphics in a Windows 3.1 DOS prompt window makes the program unusable.

One of the best features of Autonom is the user's manual. This is one of the finest, most complete, and yet easiest to read documents I have gotten with software. In addition to a description of the software and operations, the manual includes a tutorial that runs the user through all of the basic program operations and a chapter called "Boundary Conditions of Version 1.0" which is devoted to describing the limitations of the program and extensive discussion of the IUPAC rules implemented in version 1.0. I found that using the program in conjunction with this explanation of the rules significantly increased my understanding of the various IUPAC rules for nomenclature. Thus, Autonom could serve as a very useful teaching tool in undergraduate organic chemistry (or as a refresher for those too long separated from nomenclature) in addition to its uses in research, such as data basing and cataloging and when reading and writing chemical literature, manuscripts, and patents. Also included in the manual is an appendix listing the twenty-five error and eight warning codes that may be generated by the program in response to a query as well as the causes and potential solutions to the errors. This feature makes the program much less black box, while extending the range of compounds that may be named. For example, one might get an error message and no name when a single ring system includes both fused and spiro elements. The manual suggests using the isolated fused and spiro systems as models and then working out the rest of the name manually. Finally, the help available by calling Springer-Verlag was excellent.

This is a unique and very good program that promises to get better. It should be useful to anyone who reads and writes for the chemical literature and should find significant use in many areas of research and teaching.

(1) Goebels, L.; Lawson, A. J.; Wisniewski, J. L. *J. Chem. Inf. Comput. Sci.* **1991**, *31*, 216. Wisniewski, J. L. *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 324.

(2) *Nomenclature of Organic Chemistry, Sections A–H*; Pergamon: Oxford, 1979.

(3) ROSDAL: Representation of Structure Description Arranged Linearly.

(4) This means that the program was run as a non-Windows application from within the Windows operating system. Thus the program was set up using the FILE PROPERTIES menu in the Program Manager.

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*Book Reviews**

Drying '92: Parts A and B. Edited by A. S. Mujumdar (McGill University). Elsevier: Amsterdam and New York. 1992. xxviii + 1954 pp. $437.00. ISBN 0-444-89393-8.

These two volumes contain the Proceedings of the 8th International Drying Symposium held in Montreal, August 2–5, 1992. The 197 papers, in typescript form, are organized under the following 15 sections: Part A: I. Plenary/Keynotes/Invited Lectures; II. Fundamental Studies in Drying; III. Modelling and Simulation; IV. Spray Drying; V. Dielectric Drying; VI. Infrared Drying; VII. Drying of Particulate Materials; VIII. Drying of Foods; Part B: IX. Drying of Paper; X. Drying of Wood; XI. Drying of Advanced Materials; XII. Industrial Drying; XIII. Drying of Agricultural Products; XIV. Novel Dryers; and XV. Miscellaneous Topics. There is an index of the contributors, but no subject index.

Structure & Function. Volume 1: Nucleic Acids. Volume 2: Proteins. Edited by R. H. Sarma and M. H. Sarma (State University of New York at Albany and National Foundation for Cancer Research). Adenine Press: Schenectady, New York. 1992. Volume 1: x + 276 pp. $95.00. ISBN 0-940030-37-3. Volume 2: x + 192 pp. $95.00. ISBN 0-940030-38-1. Two-volume set: $190.00. ISBN 0-940030-36-5.

These books contain the Proceedings of the Seventh Conversation in Biomolecular Stereodynamics held at the State University of New York at Albany, June 18–22, 1991, under the auspices of the Department of Chemistry and organized by the University's Institute of Biomolecular Stereodynamics. There are, in typescript form, 19 chapters in Volume 1 and 16 chapters in Volume 2. There are no indexes.

Biomembrane Structure & Function: The State of the Art. Edited by Bruce P. Gaber (Office of Naval Research, USA) and K. R. K. Easwaran (Indian Institute of Science). Adenine Press: Schenectady, New York. 1992. x + 386 pp. $95.00. ISBN 0-940030-35-7.

This book contains the Proceedings of the U.S.–India Workshop on Biomembrane Structure and Function under the auspices of the Office of Naval Research, USA, and the Dept. of Science and Technology, India, held in Bangalore, India, January 6–15, 1991. It consists of 27 papers organized under the following headings: Membrane Self-Assembly; Membrane Proteins; Membrane Lipids; Membrane Transport: Phospholipases; and Computers in Membrane Research. There are no indexes.

Elastomeric Polymer Networks. Edited by James E. Mark (University of Cincinnati) and Burak Erman (Bogazici University, Istanbul, Turkey). Prentice Hall: New Jersey. 1992. xiv + 354 pp. $72.00. ISBN 0-13-249483-3.

The *Polymer Science and Engineering Series* was introduced by Prentice Hall to make available a series of books covering current developments in the areas of polymer chemistry, physics, and engineering as well as applications of polymeric materials. In this volume of the series, the editors have assembled a collection of 23 papers as a memorial to Dr. Eugene Guth who died July 5, 1990 just prior to a planned 85th birthday celebration. Included in this volume are the recollections by Professor Herman Mark of his early collaborations with Dr. Guth.

The theory of rubber elasticity is one of the oldest in polymer science, although initially the interpretation of the behavior of rubber-like materials was qualitative. Theories became more quantitative with the development of the affine model of deformation and, later, the non-affine (or phantom network) model of chain deformation. The phantom network theories that were developed by Dr. Guth appeared to better explain the experimental results of rubber elasticity than did the affine theories. However, as the breadth of experimental and theoretical papers in this volume demonstrates, this is a very active field and further research is needed to develop a more encompassing theory that would help explain data such as those obtained by neutron scattering. Indeed, the affine and phantom network models may represent the limits between which most elastomers behave. The presentations in this volume are excellent in technical content as well as in giving the reader an insight into how these researchers modified and extended the concepts proposed by Dr. Guth. Thus, a newcomer to the field will be able to get an understanding of the current state-of-the-art of rubber elasticity as well as a perspective on the history of the development of these various concepts.

This book will be a useful addition to the researcher's library as well as for students majoring in polymer science and engineering.

Donald J. Lyman, *University of Utah*

*Unsigned book reviews are by the Book Review Editor.