

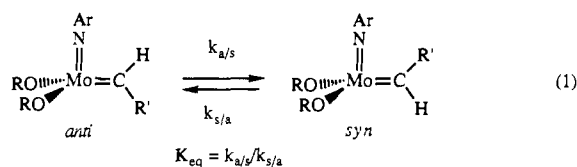
## Additions and Corrections

**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]<sup>-1</sup> h<sup>-1</sup>, not 29.4 [moles aldehyde] × [moles Rh]<sup>-1</sup> h<sup>-1</sup>. This correction does not change any of the conclusions of the paper.

**Rate of Interconversion of Syn and Anti Rotamers of Mo-(CHCMe<sub>2</sub>Ph)(NAr)(OR)<sub>2</sub> and Relative Reactivity toward 2,3-Bis(trifluoromethyl)norborene** [*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:



## 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 *automatic nomenclature*, 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.<sup>1</sup> 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",<sup>2</sup> 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<sup>3</sup> 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<sup>4</sup> 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