spectroscopy in solution and by an X-ray crystal structure determination in the solid state.<sup>7</sup> 3 has an unexceptional 3-legged piano-stool structure with normal bond lengths and bond angles.

As shown in eq 2, the formation of 3 appears to indicate that the *initial* species formed in the reaction of 1 with PhCH<sub>2</sub>X was

CpFe(COD)(CH<sub>2</sub>Ph), 4. In the presence of DIPHOS, 3 was formed from 4 by ligand replacement. However, in the absence of a strongly coordinating ligand, 4 underwent disproportionation and reacted with TMEDA to form 2 and Cp<sub>2</sub>Fe (eq 1).

Finally, the coupling product, PhCH<sub>2</sub>CH<sub>2</sub>Ph, was formed in minutes upon the addition of excess PhCH<sub>2</sub>X to a solution of 2 at 25 °C. This clearly established the intermediacy of 2 in the coupling of benzyl halides by 1.

**Registry No. 1**, 69393-63-1; **1**-Cp- $d_5$ , 112440-11-6; **2**, 112440-07-0; **3**, 64827-29-8; (TMEDA)<sub>x</sub>FeCl<sub>2</sub>, 112440-08-1; PhCH<sub>2</sub>Cl, 100-44-7; PhCH<sub>2</sub>Br, 100-39-0; PhCH<sub>2</sub>Li, 766-04-1; PhCH<sub>2</sub>CH<sub>2</sub>Ph, 103-29-7; benzyl- $d_7$  chloride, 59502-05-5; benzyl- $\alpha$ ,  $\alpha$ - $d_2$  bromide, 51271-29-5; benzyl- $\alpha$ - $d_1$  bromide, 66343-88-2; benzyl-2, 3, 4, 5, 6- $d_5$  chloride, 68661-11-0; benzyl-3- $d_1$  chloride, 112440-09-2.

## Additions and Corrections

Secohexaprismane [J. Am. Chem. Soc. 1987, 109, 2212-2213]. GOVERDHAN MEHTA\* and S. PADMA

Page 2213: Structures 15 and 21 are missing one Cl atom each and the correct structures are as follows:

Page 2213, Scheme II, footnotes: Reagents and yields: (q) HgO-CH<sub>2</sub>Cl<sub>2</sub> should read HgO-CH<sub>2</sub>Br<sub>2</sub>.

## Computer Software Reviews

FORTRAN Package 2. Lektor, Inc.: P.O. Box 6713, Kennewick, WA. 77-page manual.

Lektor FORTRAN Package 2 is a collection of FORTRAN subroutines for a variety of numerical methods. The software is intended to run on an IBM PC or compatible with at least 256Kb of memory and two disk drives. A math co-processor is recommended. The software requires a FORTRAN compiler. Lektor suggests the IBM FORTRAN compiler, Version 2, or the IBM Professional FORTRAN compiler. These compilers require DOS, Version 2.00 or higher. The software is not copy protected; backing up the package is recommended by the vendor. The software consists of 34 source subroutines, as well as associated support routines and libraries.

The specific routines comprising the system perform the following functions: solutions to linear and nonlinear simultaneous and differential equations; numerical integration; interpolation; random number generation; special functions such as the error and  $\gamma$  functions and the exponential integral; the discrete Fourier transform; and an implementation of the Simplex algorithm. Since the software is distributed in source as well as object code, verification of the proper coding of the various algorithms can be accomplished by those wishing to do so.

The software is quite easy to use, as simple FORTRAN function calls are used, as

## CALL SIMPS(N,FUN,A,B,ANS)

The limitation, of course, is for those who do not program in the FOR-TRAN language.

Various functions of the software were tested and found to operate properly. Although this package does not address particular chemical

applications, it is a tool kit that can be readily applied to a number of problems of both industrial and academic interest. As with all numeric software, Lektor's caveat applies: "Because of the great variety of problems to which these service routines can be applied, no guarantee can be made... to the accuracy of any routine or its suitability for any particular application." For those in need of such FORTRAN software, this seems a complete and worthwhile package.

Brian J. McGrattan, The Perkin-Elmer Corporation

StatWorks. Cricket Software: 3508 Market St., Suite 206, Philadelphia, PA 19104. Retail price \$125.00.

StatWorks is a software package designed for the Macintosh personal computer to provide an easy-to-use statistical analysis. Although the range of statistical procedures found in StatWorks is not as wide as that in a main frame environment, the procedures available are more than adequate for any statistical analysis or graphical representation which I have found necessary in my work as a chemist.

It is quite true, as is claimed in the Introduction to StatWorks, that statistical analysis on a personal computer often required wending one's way through a sea of often cryptic documentation or learning new higher level languages. This package contrasts dramatically from such procedures in that it can be easily addressed by anyone familiar with the simplest programs designed for the Macintosh (e.g., MacWrite or MacPaint). The philosophical goal of automatically taking the user through several stages to a complete statistical analysis without the requirement of creation of dummy variables is surely achieved.

The options for graphical representation of the data handled by StatWorks are the easiest methods I have seen for generation of tabular

<sup>(9)</sup> Felkin, H.; Knowles, P. J.; Meunier, B. J. Organomet. Chem. 1978, 146, 151.