

To emphasize the electrophilic character of the reagent, some competitive experiments were also performed. When an equimolar mixture of 4-methylcyclohexanol acetate (**11**) and methyl cyclohexane were treated with the oxidative solution made from  $F_2$ , the latter reacted about 8 times faster. This is largely due to the difference in the tertiary CH electron density, which is lower in **11** because of the proximity of the electron-withdrawing group.<sup>5</sup> If the distance between such a group and the tertiary hydrogen

(10) The spectral properties as well as the microanalyses of the new compounds are in excellent agreement with the proposed structures.

(11) Fluorine is of course a strong oxidizer and a very corrosive material. An appropriate vacuum line made from copper or Monel in a well-ventilated area should be constructed for working with this element. The reactions themselves can be carried out in glass vessels. If elementary precautions are taken, work with fluorine is relatively simple, and we have had no bad experiences working with it.

increases as in the pair (4-*tert*-butylcyclohexyl)methyl acetate (**13**) and **7**, again, in accordance with the electrophilic nature of the reaction, the former reacts considerably faster.

Of some importance is the use of this reaction to introduce the  $^{18}O$  isotope into organic molecules. The most convenient source for this isotope is  $H_2^{18}O$ , and since, unlike any other hydroxylation method, the oxygen in the above process comes from water, introducing  $^{18}O$  becomes a relatively simple task. For example, when adamantane is treated with the oxidizing solution originated from  $F_2/CH_3CN/H_2^{18}O$ , [ $^{18}O$ ]-1-hydroxyadamantane was obtained in higher than 80% yield.

We are thus hopeful that  $F_2$ , now accepted by many fluorine chemists as an important fluorinating reagent, will also be considered by the general chemical community as a reagent that can perform some uncommon reactions leading to fluorine-free and difficult to obtain derivatives.

## Additions and Corrections

**X-ray Structures of Cubylcubane and 2-*tert*-Butylcubylcubane: Short Cage-Cage Bonds** [*J. Am. Chem. Soc.* **1988**, *110*, 7232]. RICHARD GILARDI,\* MICHELE MAGGINI, and PHILIP E. EATON

Page 7232, second paragraph: the intercage bond length for *tert*-butylcubylcubane is misstated as 1.464 (5) Å. The correct intercage distance is 1.474 (5) Å as shown in Figure 2b.

**Nephelauxetic Effect in Paramagnetic Shielding of Transition-Metal Nuclei in Octahedral  $d^6$  Complexes** [*J. Am. Chem. Soc.* **1988**, *110*, 8341]. NENAD JURANIĆ

Page 8343: The last equation in the Appendix should read:

$$B(\zeta_i, \zeta_j) = 4180 \zeta_i a^2 \{ 1 - 2\zeta_j a^2 [ 1 - (1 + a^{-1})^{-2} ] + 5\zeta_j a (1 + a^{-1})^{-3} + \frac{1}{3} (1 + a^{-1})^{-4} [ 72 + 88(1 + a)^{-1} + 95(1 + a)^{-2} + 90(1 + a)^{-3} + 70(1 + a)^{-4} + 35(1 + a)^{-5} ] \}$$

**Multiphoton Ionization of Acetone Clusters: Metastable Unimolecular Decomposition of Acetone Cluster Ions and the Influence of Solvation on Intracuster Ion-Molecule Reactions** [*J. Am. Chem. Soc.* **1989**, *111*, 6035]. W. B. TZENG, S. WEI, and A. W. CASTLEMAN, JR.\*

Page 6039: The two sentences before the paragraph head (B) Studies of Metastable Processes, "When water is present... on site B in structure II. As a result, ... is quenched." should read "When

water is present in the system, it can bond to either site A or site B. However, the dehydration reaction of the protonated acetone cluster is quenched if the water molecule is bonded to site A in structure II."

**Ligand Oxidation in a Nickel Thiolate Complex** [*J. Am. Chem. Soc.* **1989**, *111*, 5974-5976]. MANOJ KUMAR, ROBERTA O. DAY, GERARD J. COLPAS, and MICHAEL J. MARONEY\*

Page 5975, Figure 1: In the figure caption the data refer to an oxidation (not a reduction) of **1** at -190 mV employing 0.1 M supporting electrolyte.

**Oxidation and Reaction of Trolox c, a Tocopherol Analogue, in Aqueous Solution. A Pulse-Radiolysis Study** [*J. Am. Chem. Soc.* **1989**, *111*, 3315]. MICHAEL J. THOMAS\* and BENON H. J. BIELSKI

Page 3316: The NMR and IR data for **5** and **6** are consistent with those previously reported by Cohen et al.<sup>1</sup> The melting point of **3** is identical with that reported by Cort et al.<sup>2</sup>

(1) Cohen, N.; Lopresti, R. J.; Saucy, G. *J. Am. Chem. Soc.* **1979**, *101*, 6710.

(2) Cort, W. M.; Scott, J. W.; Araujo, M.; Mergens, W. J.; Cannalunga, M. A.; Osadca, M.; Harley, H.; Parrish, D. R.; Pool, W. R. *J. Am. Oil Chem. Soc.* **1975**, *52*, 174.

## Computer Software Reviews

**MassSpec. A Graphics-Based Mass Spectrum Interpreter. Version 1.0.** Trinity Software: P.O. Box 960, Campton, NH. List Price \$60.00.

MassSpec is a utility designed to aid in interpretation of mass spectra by identifying potential fragments from a user-entered chemical structure of up to 255 atoms. The program is available in both MS-DOS and Macintosh versions, which offer identical options and results with the exception of slight differences in the main menu structure. The MS-DOS system requires 256K RAM, mouse, and graphics card (CGA, EGA, or HGA) and a math coprocessor is recommended. The Macintosh version requires 512 K RAM and an 800K disk drive. Each version is supplied on a single disk along with a 29-page User's Manual. The Macintosh version was evaluated for this review.

The MassSpec utility can be broken down into two main functions: a structure editor and a fragment generator/locator. After starting the program, the user is given a blank work area in which a structure can be created, loaded, or saved to disk. Structures are created using menu options that include Ring (3-10 member and benzene), Bond (single, double, triple, and  $\pi$  circle), and Group, which can be any combination of elements up to atomic number 94, deuterium, tritium, a + or - charge, or a radical center. Options are also included to allow modification of various portions of a structure. After a structure is created, the user can make use of the Generate option to produce and display potential fragments based on up to three simultaneous cleavages. Only single bonds are selected for cleavage except for aromatic compounds with a molecular