

have isolated double bond character. Elemental chlorine adds to olefinic hydrocarbons by polar, nonradical, or radical pathways, and both types of addition can occur in a single system.¹³ Several experiments indicate participation of radical species in chlorinations of C₆₀. An ESR absorption with $g = 2.0027$ ($\Delta H = 15$ G) was observed for the solid product of a typical reaction of C₆₀ with liquid chlorine as well as for a dilute solution of C₆₀ and Cl₂ in *tert*-butylbenzene at -50 °C ($\Delta H = 11$ G). The ESR absorption of the solid was lost when it was dissolved in benzene at ambient temperature. Detection of these radicals does not rule out polar additions of Cl₂ to C₆₀ or to its partially chlorinated derivatives.

Broad featureless spectral data obtained on chlorinated C₆₀ are symptomatic of mixed species. In the Raman spectrum, the complete absence of sharp strong features from 1500 to 200 cm⁻¹ suggests that chlorination, under the conditions reported, extensively alters the normal mode structure of C₆₀, probably because, on average, large numbers of chlorine atoms are present in molecules of low symmetry.¹⁴ The ¹³C NMR spectrum of chlorinated C₆₀ (500 MHz, C₆D₆ or CDCl₃) is a broad featureless peak centered near 147 ppm which does not distinguish between chlorinated and non-chlorinated carbons.

Electrochemical data may provide insight into the chemical properties of C₆₀Cl_{11.6}. Its multielectron reduction at positive potentials (Figure 2) is more characteristic of compounds with highly electron withdrawing groups such as CCl₃NO₂ or CCl-

(NO₂)₃¹⁶ than of hydrocarbons with active chlorine in allylic and benzylic positions, which are typically reduced near -2 V.¹⁷ The ease of electrochemical reduction is consistent with rapid chemical reduction found with PPh₃ and may be related to the relatively facile reductive dechlorination above 200 °C.

In conclusion we report that C₆₀ treated with liquid chlorine near -35 °C is quantitatively converted to multiply chlorinated products whose structural identities are masked because they are mixtures of compounds of low symmetry. We have shown by chemical and electrochemical means that C₆₀ can be regenerated in good yield (50–80%) from its chlorinated products. We thus deduce that the integrity of the 60-carbon framework is largely maintained under the reported conditions of chlorination and dechlorination. The multielectron reduction process which takes place at relatively positive potentials sets this system apart from normal chlorinated hydrocarbons.

Note Added in Proof. In liquid bromine at ambient temperature over 6 days, C₆₀ is converted to yellowish microcrystals which contain about 28 bromine atoms/C₆₀. The simplicity of the Raman spectrum (intense lines at 132, 178, 538, and 840 cm⁻¹) is consistent with a molecule of high symmetry. Structural studies are in progress.

Acknowledgment. We thank B. A. Parkinson for initial electrochemical experiments; T. Berzins for quantitative analyses of Cl₂; E. W. Matthews for UV–vis spectra; F. J. Kitson, W. J. Simonsick, J. Lazar, and C. N. McEwen for MS data; G. S. Reddy for NMR spectra; R. J. Young, Jr., for technical assistance; and T. Fukunaga, T. V. Rajanbabu, J. I. Brauman, and F. Davidson for discussions.

(11) (a) Hawkins, J. M.; Meyer, A.; Lewis, T. A.; Loren, S.; Hollander, F. *J. Science* **1991**, 252, 312. (b) Fagan, P. J.; Calabrese, J. C.; Malone, B. *Science* **1991**, 252, 1160. (c) Fagan, P. J.; Calabrese, J. C.; Malone, B. *J. Am. Chem. Soc.* In press.

(12) See, for example: (a) Scuseria, G. E. *Chem. Phys. Lett.* **1991**, 176, 423. (b) Marynick, D. S.; Estreicher, S. *Chem. Phys. Lett.* **1986**, 132, 383. (c) Yannoni, C. S.; Bernier, P. P.; Bethune, D. S.; Meijer, G.; Salem, J. R. *J. Am. Chem. Soc.* **1991**, 113, 3190.

(13) Poutsma, M. L. *J. Am. Chem. Soc.* **1965**, 87, 2161.

(14) Studies of (Ph₃P)₂PtC₆₀^{11b} have shown that the Raman spectrum of C₆₀ is relatively unperturbed by bonding of a single platinum to two adjacent carbons.¹⁵

(15) Chase, D. B.; Fagan, P. J. *J. Am. Chem. Soc.* In press.

(16) (a) Armand, J. *Bull. Soc. Chim. Fr.* **1966**, 543. (b) Petrosyan, V. A.; Slovetskii, V. I.; Fainzil'berg, A. A. *Izv. Akad. Nauk SSSR, Ser. Khim.* **1973**, 2027.

(17) (a) Simonet, J.; Martinet, P.; Doupeux, H.; Bretelle, D. *Bull. Soc. Chim. Fr.* **1970**, 808. (b) Matsui, Y.; Soga, T.; Date, Y. *Bull. Chem. Soc. Jpn.* **1971**, 44, 513.

Additions and Corrections

Triangulanes: Stereoisomerism and General Method of Synthesis [*J. Am. Chem. Soc.* **1990**, 112, 7702]. NIKOLAI S. ZEFIROV,* SERGE I. KOZHUSHKOV, T. S. KUZNETSOVA, O. V. KOKOREVA, K. A. LUKIN, B. I. UGRAK, and SERGE S. TRATCH

Page 7703, right column: Line 1 should be deleted. Line 6 of paragraph 2 should read 4-tuples (1,2,3,4) and (2,3,4,5).

Page 7704, left column: In line 8 of paragraph 2, N should be N₂. In footnote 17a, line 4, 2ⁿ⁻³ should be replaced by 2ⁿ⁻³. Page 7704, right column: In footnote 22, line 7, 2.2^{(n-4)/2} should be replaced by 2 × 2^{(n-4)/2}.

Page 7705, left column: In line 7, **6a,b**; **6c,d**; **6e,h** should be **6a,b**; **6c,d**; **6e,f**; and **6g,h**. In line 11, **6h** → **8a** should be **6a** → **8a**. In paragraph 3, lines 9 and 10, N₄ and N₂ should be N₄' and N₂', respectively.

General Parameterized SCF Model for Free Energies of Solvation in Aqueous Solution [*J. Am. Chem. Soc.* **1991**, 113, 8305]. CHRISTOPHER J. CRAMER* and DONALD G. TRUHLAR*

Page 8308: In eq 13, r_{M+1} should be $(r_{M+1} - 0.5T_{M+1})^{-1}$. In

eq 14, r_k should be $\rho_k + 0.5T_1$.

Page 8309: In eq 17, $kk\phi$ should be kk' . In Table IV, the experimental values for F⁻, Cl⁻, Br⁻, and I⁻ should all be 2 kcal/mol more negative. The final experimental value in Table V is incorrect for the structure listed; no experimental value is available for N-protonated acetamide.

Page 8310: In Table VI, in the heading on the second column of numbers, G_S^0 should be G_{CD}^0 .

Page 8311: In the supplementary material, 1-butanol should be *t*-butanol.

Molecular Orbital Theory Calculations of Aqueous Solvation Effects on Chemical Equilibria [*J. Am. Chem. Soc.* **1991**, 113, 8552]. CHRISTOPHER J. CRAMER* and DONALD G. TRUHLAR*

Page 8552: In ref 7a, p 5129 should be p S129.

Page 8553: In Table I, rows 10–13 should read -3.3 , -7.7 ; 12.2 , 6.9 ; 4.7 , 1.6 ; 10.8 , 9.8 instead of 9.6 , 11.3 ; ..., 28.8 .