Crystal and Molecular Structure of *trans*-Dichlorobis(hexaborane-10)platinum(II)

By JAMES P. BRENNAN and RILEY SCHAEFFER*
(*Department of Chemistry, Indiana University, Bloomington, Indiana* 47401)
and A. DAVISON and S. S. WREFORD
(*Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts* 02139)

Summary $(B_6H_{10})_2PtCl_2$ is a *trans*-square-planar complex with the platinum bridge-bonded to the unique (4,5-position) basal boron atoms in each of the B_6H_{10} ligands; the bridged B–B bond is nearly perpendicular to the Cl–Pt–Cl axis.

DAVISON *et al.*[1] recently reported the synthesis of μ-$Fe(CO)_4$-B_6H_{10} and postulated a 4,5-bridged structure. Work at Indiana had given similar results but the crystals obtained proved to be crystallographically disordered.

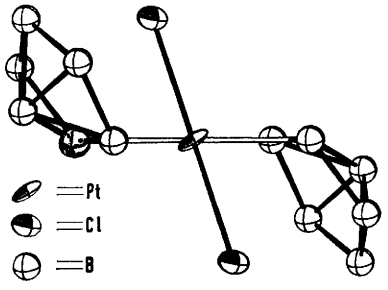

FIGURE. *Molecular structure of* $(B_6H_{10})_2PtCl_2$. Pt–Cl = 2·313 (3), Pt–B = 2·27(2) Å, *all* B–B *distances* = 1·82 ± 0·05 Å; *angles about boron* = 60 ± 2°; *internal angles of basal* B *atoms* = 108 ± 2°.

The structure of an analogue, $(B_6H_{10})_2PtCl_2$, has been determined by single-crystal *X*-ray techniques. The complex was prepared by the reaction of B_6H_{10} with $K[\eta$-$C_2H_4)PtCl_3]$ and formed yellow needles from (−20°) toluene–hexane (2:5 v/v). Although the crystals are unstable to air at room temperature a complete set of diffraction data was collected at −170° in a nitrogen-vapour cooling system.[2] The crystal showed no apparent damage from the *X*-ray beam and three orthogonal standards were constant to ±2.5%.

Crystal data: $B_6H_{10}PtCl_6$, monoclinic, space group $P2_1/_n$, $a = 8·095(2)$, $b = 11.144(2)$, $c = 7·796(2)$ Å, $\beta = 93·9(1)°$, $Z = 2$. Diffraction data were collected with a Picker FACS-I automated diffractometer using Mo-K_α radiation and a graphite monochromator. Absorption and LP corrections were applied and of the 2451 reflections collected with $2\theta \leqslant 60°$ 1036 out of a unique set of 2167 were judged significant $[I \geqslant 2·33\sigma(I)]$ and were used in the refinement, which has proceeded to a final *R* value of 4·26%.

The molecular structure is shown in the Figure. The two B_6 units are icosahedral, with platinum bridging the unique 4,5-position in both ligands. The boron atoms bonded to platinum are nearly perpendicular to the Cl—Pt–Cl axis. The structure is best viewed as *trans*-planar-co-ordination about Pt with the centres of the B(4)–B(5) vectors occupying two co-ordination sites.

Although the hydrogens have not been located, the Pt–B distances compare favourably to those found in $[Me_2PhP]_2PtB_3H_7$ (2·4–2·13 Å)[3] and $[Et_3P]_2Pt(H)B_9H_{10}$-S(2·20–2·25 Å).[4] Pt–H–B bonding is thus unlikely. The most noteworthy feature of the B_6 fragment is the lengthening of the unusually short (1·6 Å) B(4)–B(5) distance found[5] in uncomplexed B_6H_{10} to a value typical of B–B distances in triangulated polyhedral boranes.[6] Each set of basal borons is tilted toward a chlorine such that the molecule has idealized C_{2h} symmetry.

The authors acknowledge the support of the National Science Foundation.

(*Received, 2nd April* 1973; *Com.* 451.)

[1] A. Davison, D. D. Traficante, and S. S. Wreford, *J.C.S. Chem. Comm.*, 1972, 1155.
[2] J. C. Huffman, J. M. Mueller, W. E. Streib, unpublished work.
[3] L. J. Guggenberger, A. R. Kane, and E. L. Muetterties, *J. Amer. Chem. Soc.*, 1972, **94**, 5665.
[4] A. R. Kane, L. J. Guggenberger, and E. L. Muetterties, *J. Amer. Chem. Soc.*, 1970, **92**, 2571.
[5] K. Eriks, W. N. Lipscomb, and R. Schaeffer, *J. Chem. Phys.*, 1954, **22**, 754; F. L. Hirschfeld, K. Eriks, R. E. Dickerson, E. L. Lippert, jun., and W. N. Lipscomb, *ibid.*, 1958, **28**, 56.
[6] W. N. Lipscomb, 'Boron Hydrides,' Benjamin, New York, 1963.