Preparation and *X*-Ray Structure of the *N*-Benzyl Derivative of 10-Aza-7,8-dicarba-*nido*-undecaborane(11) (10-$PhCH_2$-10-N-7,8-$C_2B_8H_{10}$)

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Summary A *nido*-structure for the 10-aza-7,8-dicarba-*nido*-undecaborane(11) species has been confirmed by an *X*-ray crystal structure analysis of its *N*-benzyl derivative.

ALKYLATION of the heteroborane[1] $NC_2B_8H_{11}$ with $PhCH_2Br$ in Et_2O in the presence of KOH gives 10-$PhCH_2$-10-N-7,8-$C_2B_8H_{10}$ (I) in 50% yield, m.p. 58—59 °C, b.p. 110 °C at 10^{-2} Torr.

Crystal data: compound (I), $C_9H_{17}B_8N$, crystallizes in the non-centrosymmetric orthorhombic space-group $Pca2_1$ $a = 19{\cdot}23$, $b = 7{\cdot}25$, $c = 9{\cdot}23$ Å (at -160 °C), $Z = 4$. 1541 reflection intensities were collected by the θ–2θ scan technique using graphite-monochromated Mo-K_α radiation on a Picker FACS-1 automated diffractometer for a crystal grown and mounted in a nitrogen-cooled glass capillary. 1487 reflections were considered non-zero, and were used in the subsequent refinement. The N, C, and B atoms were located using direct methods and the H atoms were located using standard difference Fourier techniques.

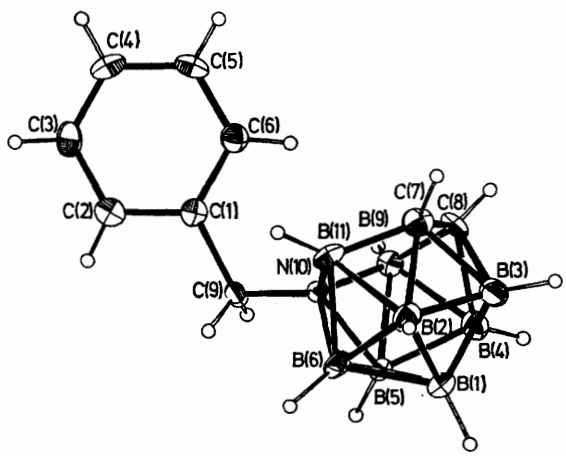

FIGURE. Structure of 10-$C_6H_5CH_2$-10-N-7,8-$C_2B_8H_{10}$

Anisotropic least squares refinement on the heavy atoms (isotropic refinement of H) gives an overall *R*-factor of 0·065.

The *X*-ray results confirm the proposed structure (Figure).[1,2] Plane 1 [B(2), B(3), B(4), B(5), B(6)] is, within experimental error, parallel to plane 2 [B(9), B(11), N(10), C(7), C(8)]. The crystal lacks a molecular plane of symmetry because of the torsional twist about the CH_2–N bond [torsion angle about C(1)–C(9)–N(10)–B(11) = 51·9°]. Plane 3 [C(1)–C(6)] is not perpendicular to plane 2 but forms an 101·9° angle with it and forms a 66·9° angle with the line joining C(7) and C(8). All bond distances and angles appear normal although the N–B(9) bond is 0·03 Å shorter than the N–B(11) bond, perhaps as a result of C(1) of the benzyl ring being closer (by 0·26 Å) to B(11) than B(9).

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