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*Crystallographic report*

# Dimethyl-2-phenylethan-2-olamine cyanoborane

**Khuloud Takrouri[1], Eli Shalom[1], Israel Goldberg[2], Jehoshua Katzhendler[1] and Morris Srebnik[1]***

[1]Department of Natural Products and Medicinal Chemistry, School of Pharmacy, Hebrew University in Jerusalem, Jerusalem 91120, Israel
[2]School of Chemistry, Sackler Faculty of Exact Science, Tel-Aviv University, Ramat-Aviv, Israel

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**The structure of the title compound reveals the geometry around the boron atom to be tetrahedral, and the B–C≡N moiety has a bent geometry. Copyright © 2005 John Wiley & Sons, Ltd.**

**KEYWORDS:** crystal structure; amine cyanoborane; dimethyl-2-phenylethan-2-olamine cyanoborane

## COMMENT

We have previously reported the synthesis of a new class of hydroxyl-containing amine cyanoboranes derived from trimethylamine cyanoborane by carbon-lithiation/alkylation.[1] In addition to being precursors to biological active boron analogs of $\alpha$-amino acids,[2,3] amine cyanoboranes also possess interesting biological activities, i.e. anti-inflammatory, anti-neoplastic and anti-hypolipidimic.[4,5] The structure of $C_{11}H_{17}BN_2O$, (**1**, Fig. 1) reveals that the geometry around the boron atom is tetrahedral and the B–C≡N moiety has a bent geometry, as indicated by the bond angle at carbon of 176.97(16)°. The B–N (1.611(2) Å), B–C (1.587(2) Å) and C–N (1.148(2) Å) distances in the $BH_2CN$ group are in accord with those found in other cyanoboranes.[6]

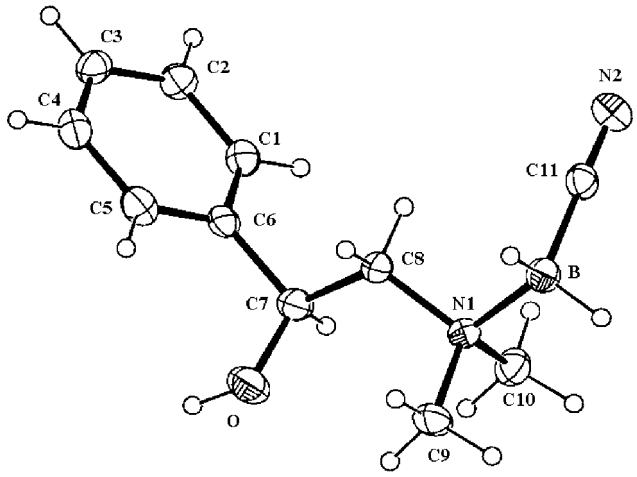


**Figure 1.** Molecular structure of $C_{11}H_{17}BN_2O$ (**1**). Selected bond distances and angles: O–C7 1.4143(19), N1–C8 1.5103(19), N1–C9 1.491(2), N2–C11 1.148(2), C1–C2 1.396(2), C7–C6 1.520(2), C7–C8 1.523(2), B–N1 1.611(2), B–C11 1.587(2) Å; N1–B–C11 109.99(13), N2–C11–B 176.97(16), B–N1–C8 108.4(12), N1–C8–C7 118.08(12), C1–C6–C7 121.34(14), C2–C1–C6 120.29(15), O–C7–C6 113.38(13), O–C7–C8 108.73(13)°.

## EXPERIMENTAL

**1** was prepared from trimethylamine cyanoborane via carbon-lithiation/alkylation method as described elsewhere.[1] Colorless single crystals were obtained from hot water. Nonius KappaCCD diffractometer, $T = 110(2)$ K. Crystal data for $C_{11}H_{17}BN_2O$: $M = 204.08$, monoclinic, space group $P2_1/c$, $a = 6.1780(3)$, $b = 18.1640(10)$, $c = 10.2910(4)$ Å, $\beta = 93.831(3)°$, $V = 1152.25$ Å$^3$, $Z = 4$, 2057 reflections with $I \geq 2\sigma(I)$. $R = 0.053$ (2057 data with $I \geq 2\sigma(I)$; $\theta_{max} = 27.9°$), $wR = 0.1271$ (all 9082 data). Programs used: SHELXL-97, Denzo, SIR-97. CCDC deposition number: 239390.

*Correspondence to: Morris Srebnik, Department of Natural Products and Medicinal Chemistry, School of Pharmacy, Hebrew University in Jerusalem, Jerusalem 91120, Israel.
E-mail: msrebni@md.huji.ac.il
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