

Table 2. Bond lengths (Å) and valency angles (°) with *e.s.d.*'s

	Molecule A	Molecule B		Molecule A	Molecule B		Molecule A	Molecule B
C(1)—C(2)	1.370 (9)	1.386 (9)	C(6)—C(7)	1.498 (9)	1.498 (9)	C(12)—C(13)	1.425 (9)	1.407 (9)
C(1)—C(10)	1.350 (9)	1.387 (8)	C(7)—C(8)	1.502 (9)	1.508 (9)	C(12)—C(17)	1.370 (8)	1.392 (9)
C(2)—C(3)	1.392 (10)	1.367 (9)	C(8)—C(9)	1.518 (10)	1.531 (10)	C(13)—C(14)	1.405 (9)	1.379 (9)
C(3)—C(4)	1.354 (10)	1.363 (9)	C(8)—C(11)	1.528 (10)	1.526 (10)	C(14)—C(15)	1.369 (10)	1.361 (10)
C(4)—C(5)	1.368 (9)	1.401 (9)	C(9)—C(10)	1.472 (9)	1.474 (9)	C(15)—C(16)	1.363 (10)	1.396 (10)
C(5)—C(6)	1.515 (9)	1.536 (9)	C(9)—C(11)	1.539 (10)	1.554 (9)	C(16)—C(17)	1.366 (9)	1.380 (9)
C(5)—C(10)	1.426 (9)	1.384 (9)	C(11)—C(12)	1.504 (9)	1.491 (9)			
C(2)—C(1)—C(10)	122.4 (8)	120.8 (8)	C(7)—C(8)—C(11)	120.7 (7)	122.2 (7)	C(9)—C(11)—C(12)	117.9 (7)	119.4 (7)
C(1)—C(2)—C(3)	120.0 (9)	121.2 (8)	C(9)—C(8)—C(11)	61.7 (6)	61.1 (5)	C(11)—C(12)—C(13)	117.4 (7)	119.2 (8)
C(2)—C(3)—C(4)	118.7 (9)	118.2 (9)	C(8)—C(9)—C(10)	119.9 (7)	117.8 (7)	C(11)—C(12)—C(17)	124.4 (7)	123.4 (8)
C(3)—C(4)—C(5)	121.8 (9)	122.1 (9)	C(8)—C(9)—C(11)	60.0 (5)	59.3 (5)	C(13)—C(12)—C(17)	118.2 (7)	117.4 (8)
C(4)—C(5)—C(6)	122.2 (8)	121.6 (8)	C(10)—C(9)—C(11)	121.6 (7)	118.4 (7)	C(12)—C(13)—C(14)	116.9 (7)	119.6 (8)
C(4)—C(5)—C(10)	119.6 (8)	119.4 (8)	C(1)—C(10)—C(5)	117.5 (8)	118.3 (8)	C(13)—C(14)—C(15)	122.8 (8)	122.2 (8)
C(6)—C(5)—C(10)	118.1 (8)	118.9 (8)	C(1)—C(10)—C(9)	121.7 (8)	119.6 (8)	C(14)—C(15)—C(16)	119.2 (9)	119.4 (9)
C(5)—C(6)—C(7)	115.3 (7)	114.2 (7)	C(5)—C(10)—C(9)	120.7 (8)	122.1 (7)	C(15)—C(16)—C(17)	119.8 (8)	118.8 (8)
C(6)—C(7)—C(8)	115.4 (7)	112.9 (7)	C(8)—C(11)—C(9)	59.3 (5)	59.6 (5)	C(12)—C(17)—C(16)	123.2 (8)	122.5 (8)
C(7)—C(8)—C(9)	116.7 (7)	117.2 (7)	C(8)—C(11)—C(12)	116.1 (7)	120.6 (7)			

-0.3 e \AA^{-3} . Molecular geometries were generated by the *GX* package (Mallinson & Muir, 1985).

Atomic coordinates are listed in Table 1, bond lengths and valency angles in Table 2.* The atomic arrangement is shown in Fig. 1.

Related literature. A tentative assignment of the stereochemistry of the title compound (Heller & Morris, 1966) was made on the basis of the similarity of its UV spectrum to that of *trans*-1,2-diphenylcyclopropane (Curtin, Gruen, Hendrickson & Knipmeyer, 1961). This stereochemistry has been confirmed and may be compared with other cyclopropanaphthalenes such as dimethyl *cis*-1a,7b-dihydro-1,1-dimethyl-1*H*-cyclopropa[*a*]naphthalene-2,3-dicarboxylate (Noland & Kameswaran, 1981) and 1-carbamoyl-1a,7a-dihydro-1a-methyl-2,7-dioxo-1*H*-cyclopropa[*b*]naphthalene-1-carboxylic acid (Boyle, O'Mahony & Cardin, 1984).

* Lists of structure factors, anisotropic thermal parameters, H-atom positions and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51810 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

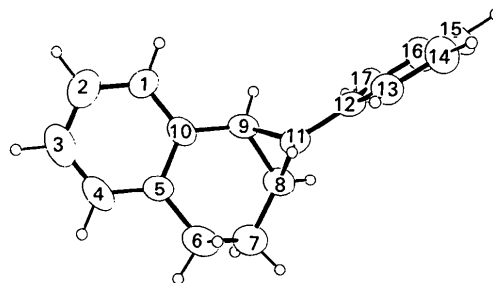


Fig. 1. The atomic arrangement in the molecules.

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Structure of the Dimeric Aldiminoborane (PhCH=NBMe₂)₂

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Abstract. Bis(μ -benzylideneamino)-tetramethyl-diborane(6), C₁₈H₂₄B₂N₂, *M_r* = 290.03, orthorhombic, *Pbca*, *a* = 9.15 (1), *b* = 18.26 (2), *c* = 10.37 (1) Å, *V* = 1732.6 Å³, *Z* = 4, *D_x* = 1.11 Mg m⁻³, $\mu(\text{Mo } K\alpha) = 0.33 \text{ mm}^{-1}$, *F*(000) =

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624, room temperature, *R* = 0.063 for 1172 diffractometer-measured intensities with *I* > 3 σ (*I*). The two halves of the molecule are related by a centre of symmetry, the phenyl rings lying in the same plane as the (BN)₂ ring. Each B atom has a distorted tetra-

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Table 1. Atomic positions ($\times 10^4$) and equivalent isotropic temperature factors ($\text{\AA}^2 \times 10^3$)

	x	y	z	U_{eq}^\dagger
B	5939 (3)	5016 (1)	9260 (3)	48 (1)
N	4480 (2)	4555 (1)	9465 (2)	44 (1)
C(1)	4042 (3)	4026 (1)	8788 (2)	47 (1)
C(2)	1659 (3)	3936 (1)	9840 (3)	59 (1)
C(3)	532 (3)	3203 (2)	9976 (3)	67 (2)
C(4)	513 (3)	2568 (2)	9286 (3)	68 (2)
C(5)	1586 (4)	2431 (2)	8424 (3)	71 (2)
C(6)	2711 (3)	2920 (1)	8258 (3)	59 (2)
C(7)	2767 (3)	3557 (1)	8973 (2)	46 (1)
C(8)	7315 (3)	4488 (2)	9418 (3)	63 (2)
C(9)	5830 (4)	5499 (2)	7988 (3)	68 (2)

$$\dagger U_{\text{eq}} = \frac{1}{3}(\sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j).$$

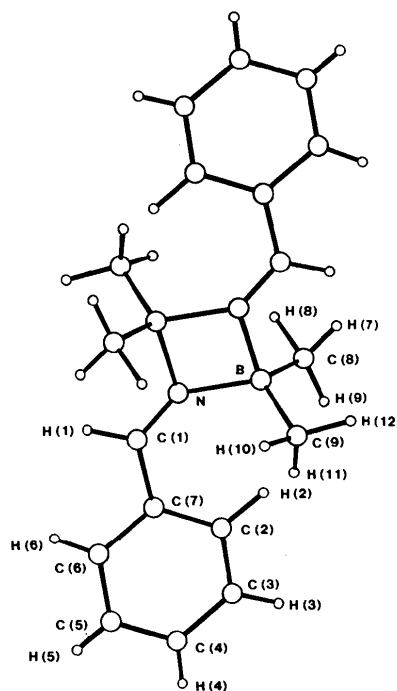
Table 2. Bond lengths (\AA) and bond angles ($^\circ$)

B—N	1.592 (3)	N—B—N'	86.9 (2)
N—C(1)	1.259 (3)	B—N—B'	93.1 (2)
C(1)—C(7)	1.460 (3)	N—C(1)—C(7)	129.1 (2)
C(7)—C(2)	1.379 (4)	C(1)—C(7)—C(2)	124.4 (2)
C(2)—C(3)	1.376 (4)	C(7)—C(2)—C(3)	119.9 (3)
C(3)—C(4)	1.362 (5)	C(2)—C(3)—C(4)	120.8 (3)
C(4)—C(5)	1.351 (5)	C(3)—C(4)—C(5)	119.7 (3)
C(5)—C(6)	1.374 (4)	C(4)—C(5)—C(6)	120.5 (3)
C(6)—C(7)	1.380 (3)	C(5)—C(6)—C(7)	120.5 (3)
B—C(8)	1.593 (4)	C(6)—C(7)—C(1)	117.0 (2)
B—C(9)	1.590 (4)	C(1)—N—B	126.7 (2)
B...B'	2.305 (5)	N—B—C(8)	109.2 (2)
N...N'	2.186 (4)	N—B—C(9)	110.6 (2)
B—N'	1.584 (3)	C(8)—B—C(9)	118.0 (2)

Symmetry code: (') $-x, -y, -z$.

hedral coordination with B—N 1.592 (3), B—N' 1.584 (3), B—C(8) 1.593 (4) and B—C(9) 1.590 (4) \AA . The ring angles are N—B—N' 86.9 (2) and B—N—B' 93.1 (2) $^\circ$.

Experimental. The title compound was prepared from benzonitrile and tetramethyldiborane in 2:1 molar proportions and crystallized from cyclohexane (Jennings, Snaith, Mahmood, Wallwork, Bryan, Halfpenny, Petch & Wade, 1983). The density was not measured because of the solubility of the compound in the liquids available for flotation. Accurate cell dimensions were obtained from oscillation and Weissenberg photographs with Cu $K\alpha$ radiation ($\lambda = 1.542 \text{ \AA}$). 1932 reflections were measured on a Stoe Stadi-2 two-circle diffractometer with graphite-monochromatized Mo $K\alpha$ radiation; crystal $0.10 \times 0.03 \times 0.12 \text{ mm}$, layers l 0–10, h 0–12, k 0–25, maximum $(\sin \theta)/\lambda = 0.77 \text{ \AA}^{-1}$, separate standard for each layer measured every 10 reflections (intensity variation less than 1%). Of the 1782 unique reflections, 1172 with $I > 3\sigma(I)$ were used for the refinement. No absorption correction was applied. The structure was solved and refined with *SHELX76* (Sheldrick, 1976) using full-matrix least squares on F magnitudes. The H atoms were located from a difference map. All atoms except H were given isotropic U_{ij} . Individual scale factors for the data-collection layers were intro-

Fig. 1. View of one molecule of (PhCH=NBM_e)₂.

duced in the final cycles of refinement. Unit weights were used throughout. The largest shift-to-e.s.d. ratio was 0.018 (U of an H atom), $R = 0.063$ and the largest features on the final difference map were $\pm 0.22 e \text{ \AA}^{-3}$. Final atomic positions and U_{eq} values are given in Table 1, bond distances and angles in Table 2.* A view of one molecule showing the atom-numbering scheme is given in Fig. 1. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974).

Related literature. The relationship between the title compound and others containing the (BN)₂ ring is discussed in Jennings, Snaith, Mahmood, Wallwork, Bryan, Halfpenny, Petch & Wade (1983) and references therein.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51836 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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