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Structure of 1a,2,3,7b-Tetrahydro-1-phenyl-1*H*-cyclopropa[*a*]naphthalene

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Abstract. $C_{17}H_{16}$, $M_r = 220{\cdot}3$, monoclinic, $P2_1/c$, $a = 10{\cdot}098\ (9)$, $b = 11{\cdot}315\ (10)$, $c = 22{\cdot}121\ (27)$ Å, $\beta = 90{\cdot}27\ (9)°$, $V = 2527{\cdot}5$ Å^3, $Z = 8$, $D_x = 1{\cdot}16$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}32$ cm^{-1}, $F(000) = 944$, $T = 293$ K, $R = 0{\cdot}079$ for 1710 observed reflexions. The two molecules of the asymmetric unit adopt similar conformations with the aromatic chromophores *trans* to the cyclopropane ring. In both molecules the C(7)—C(8)—C(11)—C(12) torsion angle is 146 (1)° but there is a small difference between the C(8)—C(11)—C(12) valency angles. The H atoms attached to C(6) and C(7) are β and α axial respectively.

Experimental. Colourless crystal, 0·50 × 0·40 × 0·20 mm. Nicolet *P*3 automated diffractometer, monochromated Mo $K\alpha$ radiation. Cell dimensions from setting angles of 12 independent reflexions with $2\theta \approx 20°$. Data corrected for Lorentz and polarization effects, absorption ignored. 4183 unique intensities measured with $\theta < 60°$ as θ–2θ scans; 1710 reflexions had $F > 5\sigma(F)$. Range of *hkl*: $-11 < h < 11$, $0 < k < 11$, $0 < l < 22$. Two reference reflexions monitored periodically showed no significant variation in intensity.

Structure was determined with *MITHRIL* (Gilmore, 1984) and all H atoms were observed in difference Fourier maps with *SHELX76* (Sheldrick, 1976). Full-matrix least-squares calculations on *F* with anisotropic thermal parameters for C atoms and isotropic thermal parameters for H atoms converged at *R* 0·079, *wR* 0·063. The cyclopropane H atoms were freely refined, the remaining H atoms were allowed to ride on their attached C atoms. Atomic scattering factors from *SHELX76*. Poor crystal quality resulted in high final *R* value. Final $w = 2{\cdot}68/\sigma^2(F_o)$, $\Delta/\sigma < 0{\cdot}01$, final $\Delta\rho_{max} = 0{\cdot}3$, $\Delta\rho_{min} =$

Table 1. *Fractional coordinates with e.s.d.'s and equivalent values of the anisotropic temperature factor coefficients*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	U_{eq}(Å^2)
Molecule *A*				
C(1)	0·3542 (7)	0·2166 (7)	1·0274 (4)	0·047 (5)
C(2)	0·3694 (7)	0·3367 (8)	1·0239 (4)	0·062 (6)
C(3)	0·3690 (7)	0·3924 (8)	0·9677 (5)	0·062 (6)
C(4)	0·3525 (8)	0·3256 (8)	0·9174 (4)	0·057 (6)
C(5)	0·3377 (7)	0·2056 (8)	0·9204 (3)	0·044 (5)
C(6)	0·3149 (8)	0·1305 (8)	0·8646 (3)	0·070 (6)
C(7)	0·3725 (8)	0·0091 (8)	0·8672 (3)	0·064 (6)
C(8)	0·3514 (8)	−0·0562 (7)	0·9255 (4)	0·050 (6)
C(9)	0·3356 (8)	0·0184 (7)	0·9820 (3)	0·043 (5)
C(10)	0·3403 (7)	0·1481 (7)	0·9778 (4)	0·040 (5)
C(11)	0·2173 (7)	−0·0527 (7)	0·9571 (3)	0·042 (5)
C(12)	0·1776 (8)	−0·1632 (7)	0·9902 (3)	0·042 (5)
C(13)	0·0400 (7)	−0·1906 (7)	0·9923 (3)	0·048 (5)
C(14)	0·0043 (8)	−0·2958 (8)	1·0219 (4)	0·070 (6)
C(15)	0·0953 (10)	−0·3696 (8)	1·0481 (3)	0·068 (6)
C(16)	0·2263 (9)	−0·3413 (7)	1·0454 (3)	0·056 (5)
C(17)	0·2647 (8)	−0·2393 (7)	1·0176 (3)	0·048 (5)
Molecule *B*				
C(1)	0·1328 (7)	0·0001 (7)	0·3324 (3)	0·047 (5)
C(2)	0·1414 (7)	−0·1036 (8)	0·3655 (3)	0·055 (6)
C(3)	0·1701 (8)	−0·2089 (8)	0·3383 (4)	0·062 (6)
C(4)	0·1874 (7)	−0·2100 (8)	0·2773 (4)	0·056 (5)
C(5)	0·1787 (7)	−0·1069 (8)	0·2424 (3)	0·046 (5)
C(6)	0·2045 (8)	−0·1081 (7)	0·1740 (3)	0·069 (7)
C(7)	0·1298 (8)	−0·0157 (7)	0·1394 (3)	0·065 (6)
C(8)	0·1402 (8)	0·1054 (8)	0·1675 (3)	0·047 (6)
C(9)	0·1453 (7)	0·1119 (7)	0·2366 (3)	0·043 (5)
C(10)	0·1518 (7)	−0·0003 (7)	0·2704 (3)	0·039 (5)
C(11)	0·2668 (8)	0·1488 (7)	0·1981 (3)	0·044 (5)
C(12)	0·3052 (8)	0·2759 (7)	0·1951 (3)	0·045 (5)
C(13)	0·4403 (8)	0·3064 (7)	0·1959 (3)	0·050 (5)
C(14)	0·4768 (8)	0·4237 (8)	0·1926 (3)	0·058 (6)
C(15)	0·3860 (9)	0·5126 (8)	0·1906 (3)	0·067 (6)
C(16)	0·2513 (9)	0·4850 (8)	0·1902 (3)	0·062 (6)
C(17)	0·2138 (8)	0·3678 (7)	0·1925 (3)	0·054 (5)

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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)			

$-0{\cdot}3\,e\,Å^{-3}$. 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-la-methyl-2,7-dioxo-1*H*-cyclopropa[*b*]naphthalene-1-carboxylic acid (Boyle, O'Mahony & Cardin, 1984).

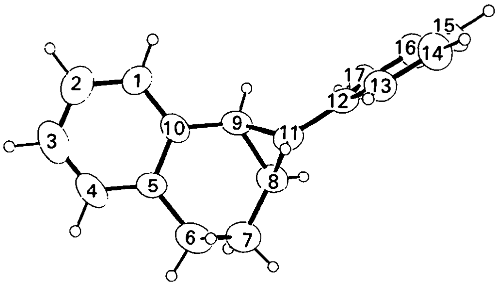

Fig. 1. The atomic arrangement in the molecules.

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* 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.

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Structure of the Dimeric Aldiminoborane $(PhCH{=}NBMe_2)_2$

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Abstract. Bis(μ-benzylideneamino)-tetramethyldiborane(6), $C_{18}H_{24}B_2N_2$, $M_r = 290{\cdot}03$, orthorhombic, *Pbca*, $a = 9{\cdot}15\,(1)$, $b = 18{\cdot}26\,(2)$, $c = 10{\cdot}37\,(1)$ Å, $V = 1732{\cdot}6$ Å^3, $Z = 4$, $D_x = 1{\cdot}11$ Mg m^{-3}, $\mu(\text{Mo}\ K\alpha) = 0{\cdot}33$ mm^{-1}, $F(000) = 624$, room temperature, $R = 0{\cdot}063$ for 1172 diffractometer-measured intensities with $I > 3\sigma(I)$. 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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