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1,2-Bis(dicyclohexylphosphino)-1,2-dicarba-*closo*-dodecaborane

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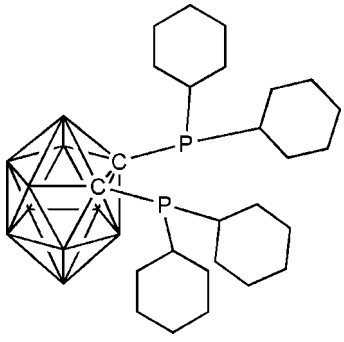
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.063; wR factor = 0.197; data-to-parameter ratio = 15.9.

The title compound, $C_{26}H_{54}B_{10}P_2$, was obtained by the reaction of 1,2-carborane, *n*-butyllithium and dicyclohexylchlorophosphine in diethyl ether. The molecule lies on a crystallographic twofold rotation axis through the mid-point of the C—C bond of the carborane. The P atoms of the dicyclohexylphosphine groups are bonded to the two C atoms in the 1,2-dicarbaborane cage with a unique P—C distance of 1.894 (3) Å.

Related literature

For synthesis see: Alexander & Schroeder (1963) and for related structures see: Zhang *et al.* (2006); Kivekäs *et al.* (1995).



Experimental

Crystal data

$C_{26}H_{54}B_{10}P_2$
M_r = 536.73
Monoclinic, $C2/c$
a = 21.507 (2) Å
b = 10.0350 (14) Å
c = 15.2976 (18) Å
β = 103.196 (2)°
V = 3214.4 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 298 (2) K
0.58 × 0.57 × 0.46 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.917, T_{max} = 0.934
6226 measured reflections
2743 independent reflections
1814 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.197
S = 1.00
2743 reflections
172 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2435).

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supplementary materials

Acta Cryst. (2007). E**63**, o3335 [**doi:10.1107/S1600536807030553**]

1,2-Bis(dicyclohexylphosphino)-1,2-dicarba-*closo*-dodecaborane

F.-F. Su, J.-M. Dou, D.-C. Li and D.-Q. Wang

Comment

The structure of 1,2-(PPh_2)-1,2-$C_2B_{10}H_{10}$ (Zhang *et al.*, 2006) has recently been reported and was synthesized by the method of Alexander & Schroeder (1963). In addition, 1,2-$(P^iPr_2)_2$-1,2-$C_2B_{10}H_{10}$ was synthesized and characterized by Kivekäs *et al.* (1995). Since then, many complexes containing the above two lignads have been reported. We are interested in phosphine derivatives of 1,2-dicarba-*closo*-dodecaborane. In this paper, we report the structure of 1,2-bis(dicyclohexylphosphino)-1,2-dicarba-*closo*-dodecaborane.

As shown in Fig. 1, the molecular structure of the title compound has crystallographic twofold rotation symmetry. The P atom of dicyclohexylphosphine group is bonded to C1. The P—C1 distance is 1.894 (3) Å, which is agreement well with the corresponding distance 1.894 (3)Å in 1,2-$(P^iPr_2)_2$-1,2-$C_2B_{10}H_{10}$ and 1.885Å in 1,2-(PPh_2)-1,2-$C_2B_{10}H_{10}$. The P—C1—$C1^i$ angle [symmetry code (i): $1-x, y, 1/2-z$] in 1,2-$(PCycl_2)$-1,2-$C_2B_{10}H_{10}$ is 113.48 (5)°. The corresponding angles in 1,2-(PPh_2)-1,2-$C_2B_{10}H_{10}$ (Zhang *et al.*, 2006) and 1,2-$(P^iPr_2)_2$-1,2-$C_2B_{10}H_{10}$ (Kivekäs *et al.*, 1995) are 116.6 (2),111.07 (19)° and 112.9 (2),112.3 (1)° respectively. The two phosphorus and two cage C atoms are almost coplanar with the torsion angle 10.9 (4)°, which is samller than that of 12.1 (2)° for 1,2-$(P^iPr_2)_2$-1,2-$C_2B_{10}H_{10}$ (Kivekäs *et al.*, 1995), and almost equal to that of 10.6 (3)° for 1,2-(PPh_2)-1,2-$C_2B_{10}H_{10}$ (Zhang *et al.*, 2006).

Experimental

The title compound was synthesizd according to the literature method (Alexander & Schroeder, 1963). But in our synthesis diphenylchorophosphine was substituted with dicyclohexylchorophosphine. A white solid was dissolved in dichloromethane, and crystals suitable for X-ray diffraction were obtained after partial evaporation (65.2%, m.p. 528–529 K). FTIR (KBr) v (cm-l): 2928,2850 (C–H); 2643,2622,2599,2555 (B–H).

Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms, with B—H 1.10, C—H 0.97 (methylene) C—H 0.98 Å (hypomethyl), with $U_{iso}(H) = 1.2U_{eq}(B,C)$.

Figures

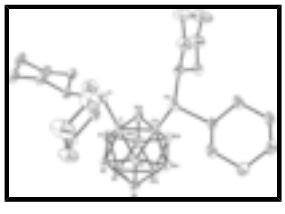

Fig. 1. The molecular structure with atom labels and 40% probability displacement ellipsoids for non-H atoms.

1,2-Bis(dicyclohexylphosphino)-1,2-dicarba-*closo*-dodecaborane

Crystal data

$C_{26}H_{54}B_{10}P_2$	F_{000} = 1160
M_r = 536.73	D_x = 1.109 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1912 reflections
a = 21.507 (2) Å	θ = 2.3–26.8º
b = 10.0350 (14) Å	μ = 0.15 mm^{-1}
c = 15.2976 (18) Å	*T* = 298 (2) K
β = 103.196 (2)º	Block, colorless
V = 3214.4 (7) Å^3	0.58 × 0.57 × 0.46 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	2743 independent reflections
Radiation source: fine-focus sealed tube	1814 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.081
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −25→19
T_{min} = 0.917, T_{max} = 0.934	*k* = −11→10
6226 measured reflections	*l* = −17→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.063	H-atom parameters constrained
$wR(F^2)$ = 0.197	$w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + 4.2002P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
2743 reflections	$\Delta\rho_{max}$ = 0.84 e Å^{-3}
172 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.42512 (4)	0.27894 (9)	0.24958 (6)	0.0338 (3)
B1	0.43839 (18)	0.5863 (4)	0.2987 (3)	0.0430 (10)
H1	0.3976	0.5852	0.3308	0.052*
B2	0.42621 (18)	0.5876 (4)	0.1819 (3)	0.0449 (10)
H2	0.3780	0.5879	0.1379	0.054*
B3	0.49093 (16)	0.4982 (4)	0.1542 (3)	0.0369 (9)
H3	0.4852	0.4392	0.0923	0.044*
B4	0.4907 (2)	0.6734 (4)	0.1540 (3)	0.0507 (11)
H4	0.4848	0.7297	0.0909	0.061*
B5	0.4581 (2)	0.7292 (4)	0.2444 (3)	0.0533 (12)
H5	0.4310	0.8228	0.2410	0.064*
C1	0.45992 (3)	0.4513 (3)	0.2439 (2)	0.0322 (7)
C2	0.34879 (14)	0.3209 (4)	0.2810 (2)	0.0376 (8)
H2A	0.3332	0.4063	0.2534	0.045*
C3	0.29691 (16)	0.2158 (4)	0.2520 (2)	0.0491 (10)
H3A	0.2880	0.2056	0.1872	0.059*
H3B	0.3121	0.1308	0.2788	0.059*
C4	0.23611 (17)	0.2539 (5)	0.2798 (3)	0.0585 (12)
H4A	0.2048	0.1837	0.2621	0.070*
H4B	0.2189	0.3346	0.2485	0.070*
C5	0.24694 (19)	0.2765 (5)	0.3802 (3)	0.0596 (11)
H5A	0.2079	0.3091	0.3943	0.071*
H5B	0.2581	0.1928	0.4116	0.071*
C6	0.30009 (18)	0.3768 (4)	0.4113 (3)	0.0579 (11)
H6A	0.3089	0.3847	0.4762	0.070*
H6B	0.2866	0.4634	0.3858	0.070*
C7	0.36042 (16)	0.3344 (4)	0.3831 (2)	0.0469 (9)
H7A	0.3750	0.2497	0.4110	0.056*
H7B	0.3937	0.3998	0.4040	0.056*
C8	0.40569 (16)	0.2213 (4)	0.1319 (2)	0.0411 (8)
H8	0.4456	0.2351	0.1124	0.049*
C9	0.35584 (16)	0.2903 (4)	0.0595 (2)	0.0421 (9)
H9A	0.3146	0.2842	0.0749	0.050*

H9B	0.3667	0.3839	0.0579	0.050*
C10	0.3510 (3)	0.2312 (5)	−0.0312 (3)	0.0753 (14)
H10A	0.3147	0.2705	−0.0727	0.090*
H10B	0.3891	0.2541	−0.0518	0.090*
C11	0.3436 (3)	0.0868 (6)	−0.0332 (3)	0.104 (2)
H11A	0.3444	0.0544	−0.0927	0.124*
H11B	0.3024	0.0642	−0.0216	0.124*
C12	0.3957 (3)	0.0175 (5)	0.0354 (3)	0.0798 (15)
H12A	0.4366	0.0311	0.0203	0.096*
H12B	0.3873	−0.0775	0.0346	0.096*
C13	0.3979 (2)	0.0735 (4)	0.1297 (3)	0.0677 (12)
H13A	0.3588	0.0504	0.1475	0.081*
H13B	0.4333	0.0333	0.1725	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0271 (4)	0.0393 (5)	0.0346 (5)	−0.0027 (3)	0.0062 (3)	0.0053 (4)
B1	0.0341 (19)	0.043 (2)	0.055 (3)	0.0033 (16)	0.0179 (17)	−0.006 (2)
B2	0.0306 (19)	0.047 (2)	0.059 (3)	0.0054 (17)	0.0147 (17)	0.013 (2)
B3	0.0304 (17)	0.043 (2)	0.040 (2)	0.0035 (16)	0.0118 (15)	0.0096 (17)
B4	0.045 (2)	0.041 (2)	0.070 (3)	0.0025 (19)	0.022 (2)	0.015 (2)
B5	0.046 (2)	0.040 (2)	0.079 (4)	0.0055 (19)	0.026 (2)	0.001 (2)
C1	0.0214 (15)	0.0375 (18)	0.0391 (19)	−0.0004 (13)	0.0103 (12)	0.0026 (14)
C2	0.0266 (15)	0.052 (2)	0.0353 (19)	−0.0063 (14)	0.0096 (13)	0.0050 (16)
C3	0.0410 (19)	0.069 (3)	0.040 (2)	−0.0186 (18)	0.0134 (15)	0.0007 (18)
C4	0.0346 (19)	0.093 (3)	0.051 (3)	−0.0203 (19)	0.0150 (17)	−0.003 (2)
C5	0.048 (2)	0.081 (3)	0.058 (3)	−0.015 (2)	0.0298 (18)	−0.003 (2)
C6	0.059 (2)	0.075 (3)	0.046 (2)	−0.016 (2)	0.0254 (18)	−0.008 (2)
C7	0.0398 (18)	0.062 (2)	0.038 (2)	−0.0123 (17)	0.0089 (15)	0.0043 (18)
C8	0.0354 (17)	0.048 (2)	0.040 (2)	0.0072 (15)	0.0083 (14)	0.0042 (16)
C9	0.0398 (18)	0.049 (2)	0.036 (2)	−0.0035 (16)	0.0053 (14)	0.0078 (16)
C10	0.091 (3)	0.082 (3)	0.047 (3)	0.007 (3)	0.003 (2)	−0.003 (2)
C11	0.157 (6)	0.081 (4)	0.055 (3)	−0.005 (4)	−0.013 (3)	−0.018 (3)
C12	0.111 (4)	0.056 (3)	0.066 (3)	0.007 (3)	0.007 (3)	−0.015 (2)
C13	0.076 (3)	0.054 (3)	0.071 (3)	−0.004 (2)	0.012 (2)	−0.003 (2)

Geometric parameters (Å, °)

P1—C8	1.845 (4)	C3—C4	1.514 (5)
P1—C2	1.861 (3)	C3—H3A	0.9700
P1—C1	1.894 (3)	C3—H3B	0.9700
B1—C1	1.712 (5)	C4—C5	1.517 (6)
B1—B2	1.747 (6)	C4—H4A	0.9700
B1—B5	1.757 (6)	C4—H4B	0.9700
B1—B4^{i}	1.762 (6)	C5—C6	1.516 (5)
B1—B3^{i}	1.764 (5)	C5—H5A	0.9700
B1—H1	1.1000	C5—H5B	0.9700

B2—C1	1.727 (5)	C6—C7	1.519 (5)
B2—B5	1.762 (6)	C6—H6A	0.9700
B2—B4	1.766 (6)	C6—H6B	0.9700
B2—B3	1.786 (5)	C7—H7A	0.9700
B2—H2	1.1000	C7—H7B	0.9700
B3—C1	1.722 (5)	C8—C13	1.493 (6)
B3—C1^{i}	1.737 (5)	C8—C9	1.521 (5)
B3—B4	1.758 (6)	C8—H8	0.9800
B3—B1^{i}	1.764 (5)	C9—C10	1.491 (6)
B3—H3	1.1000	C9—H9A	0.9700
B4—B1^{i}	1.762 (6)	C9—H9B	0.9700
B4—B5^{i}	1.778 (7)	C10—C11	1.458 (7)
B4—B5	1.779 (7)	C10—H10A	0.9700
B4—H4	1.1000	C10—H10B	0.9700
B5—B5^{i}	1.771 (8)	C11—C12	1.517 (7)
B5—B4^{i}	1.778 (7)	C11—H11A	0.9700
B5—H5	1.1000	C11—H11B	0.9700
C1—C1^{i}	1.6911 (10)	C12—C13	1.539 (6)
C1—B3^{i}	1.737 (5)	C12—H12A	0.9700
C2—C3	1.526 (5)	C12—H12B	0.9700
C2—C7	1.530 (5)	C13—H13A	0.9700
C2—H2A	0.9800	C13—H13B	0.9700
C8—P1—C2	107.84 (15)	B3—C1—B2	62.4 (2)
C8—P1—C1	104.18 (15)	C1^{i}—C1—B3^{i}	60.30 (19)
C2—P1—C1	100.73 (13)	B1—C1—B3^{i}	61.5 (2)
C1—B1—B2	59.9 (2)	B3—C1—B3^{i}	112.0 (2)
C1—B1—B5	107.0 (3)	B2—C1—B3^{i}	111.8 (3)
B2—B1—B5	60.4 (2)	C1^{i}—C1—P1	113.48 (5)
C1—B1—B4^{i}	106.8 (2)	B1—C1—P1	123.10 (18)
B2—B1—B4^{i}	109.3 (3)	B3—C1—P1	121.0 (2)
B5—B1—B4^{i}	60.7 (3)	B2—C1—P1	128.88 (17)
C1—B1—B3^{i}	59.93 (19)	B3^{i}—C1—P1	111.8 (2)
B2—B1—B3^{i}	109.6 (3)	C3—C2—C7	107.3 (3)
B5—B1—B3^{i}	108.9 (3)	C3—C2—P1	113.4 (3)
B4^{i}—B1—B3^{i}	59.8 (2)	C7—C2—P1	109.6 (2)
C1—B1—H1	122.9	C3—C2—H2A	108.8
B2—B1—H1	120.6	C7—C2—H2A	108.8
B5—B1—H1	121.5	P1—C2—H2A	108.8
B4^{i}—B1—H1	121.7	C4—C3—C2	111.4 (3)
B3^{i}—B1—H1	121.0	C4—C3—H3A	109.4
C1—B2—B1	59.1 (2)	C2—C3—H3A	109.4
C1—B2—B5	106.1 (3)	C4—C3—H3B	109.4
B1—B2—B5	60.1 (2)	C2—C3—H3B	109.4
C1—B2—B4	105.3 (2)	H3A—C3—H3B	108.0

B1—B2—B4	108.0 (3)	C3—C4—C5	112.3 (3)
B5—B2—B4	60.5 (3)	C3—C4—H4A	109.1
C1—B2—B3	58.67 (19)	C5—C4—H4A	109.1
B1—B2—B3	107.2 (3)	C3—C4—H4B	109.1
B5—B2—B3	107.8 (3)	C5—C4—H4B	109.1
B4—B2—B3	59.3 (2)	H4A—C4—H4B	107.9
C1—B2—H2	123.9	C6—C5—C4	110.4 (3)
B1—B2—H2	121.7	C6—C5—H5A	109.6
B5—B2—H2	121.7	C4—C5—H5A	109.6
B4—B2—H2	122.3	C6—C5—H5B	109.6
B3—B2—H2	122.3	C4—C5—H5B	109.6
C1—B3—C1^{i}	58.54 (13)	H5A—C5—H5B	108.1
C1—B3—B4	105.9 (3)	C5—C6—C7	110.9 (3)
C1^{i}—B3—B4	105.9 (3)	C5—C6—H6A	109.5
C1—B3—B1^{i}	105.4 (3)	C7—C6—H6A	109.5
C1^{i}—B3—B1^{i}	58.6 (2)	C5—C6—H6B	109.5
B4—B3—B1^{i}	60.1 (2)	C7—C6—H6B	109.5
C1—B3—B2	59.0 (2)	H6A—C6—H6B	108.1
C1^{i}—B3—B2	105.7 (3)	C6—C7—C2	111.3 (3)
B4—B3—B2	59.8 (2)	C6—C7—H7A	109.4
B1^{i}—B3—B2	107.3 (3)	C2—C7—H7A	109.4
C1—B3—H3	123.5	C6—C7—H7B	109.4
C1^{i}—B3—H3	123.5	C2—C7—H7B	109.4
B4—B3—H3	122.4	H7A—C7—H7B	108.0
B1^{i}—B3—H3	122.5	C13—C8—C9	112.3 (3)
B2—B3—H3	122.3	C13—C8—P1	109.4 (3)
B3—B4—B1^{i}	60.1 (2)	C9—C8—P1	122.2 (3)
B3—B4—B2	60.9 (2)	C13—C8—H8	103.6
B1^{i}—B4—B2	108.2 (3)	C9—C8—H8	103.6
B3—B4—B5^{i}	108.2 (3)	P1—C8—H8	103.6
B1^{i}—B4—B5^{i}	59.5 (2)	C10—C9—C8	112.7 (3)
B2—B4—B5^{i}	107.8 (3)	C10—C9—H9A	109.1
B3—B4—B5	108.3 (3)	C8—C9—H9A	109.1
B1^{i}—B4—B5	107.1 (3)	C10—C9—H9B	109.1
B2—B4—B5	59.6 (3)	C8—C9—H9B	109.1
B5^{i}—B4—B5	59.7 (3)	H9A—C9—H9B	107.8
B3—B4—H4	121.1	C11—C10—C9	113.5 (4)
B1^{i}—B4—H4	122.1	C11—C10—H10A	108.9
B2—B4—H4	121.5	C9—C10—H10A	108.9
B5^{i}—B4—H4	122.0	C11—C10—H10B	108.9
B5—B4—H4	122.2	C9—C10—H10B	108.9
B1—B5—B2	59.5 (2)	H10A—C10—H10B	107.7
B1—B5—B5^{i}	107.7 (3)	C10—C11—C12	112.5 (4)
B2—B5—B5^{i}	108.3 (3)	C10—C11—H11A	109.1
B1—B5—B4^{i}	59.8 (2)	C12—C11—H11A	109.1

B2—B5—B4^{i}	107.9 (3)	C10—C11—H11B	109.1
B5^{i}—B5—B4^{i}	60.2 (3)	C12—C11—H11B	109.1
B1—B5—B4	106.9 (3)	H11A—C11—H11B	107.8
B2—B5—B4	59.8 (2)	C11—C12—C13	110.0 (4)
B5^{i}—B5—B4	60.1 (3)	C11—C12—H12A	109.7
B4^{i}—B5—B4	107.8 (3)	C13—C12—H12A	109.7
B1—B5—H5	122.4	C11—C12—H12B	109.7
B2—B5—H5	121.7	C13—C12—H12B	109.7
B5^{i}—B5—H5	121.4	H12A—C12—H12B	108.2
B4^{i}—B5—H5	121.7	C8—C13—C12	111.3 (4)
B4—B5—H5	122.1	C8—C13—H13A	109.4
C1^{i}—C1—B1	109.19 (19)	C12—C13—H13A	109.4
C1^{i}—C1—B3	61.16 (19)	C8—C13—H13B	109.4
B1—C1—B3	111.8 (3)	C12—C13—H13B	109.4
C1^{i}—C1—B2	110.50 (19)	H13A—C13—H13B	108.0
B1—C1—B2	61.0 (2)		

Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2.

Fig. 1