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1,7-Bis(diphenylphosphino)-1,7-dicarba-*closo*-dodecaborane

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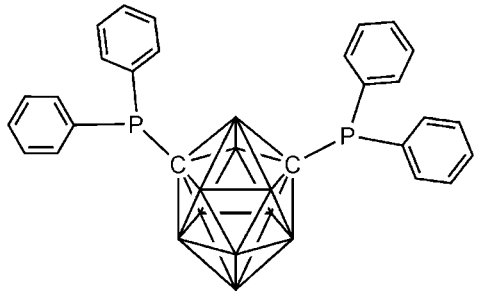
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.143; data-to-parameter ratio = 14.4.

In the title compound, $C_{26}H_{30}B_{10}P_2$, the carborane cage has the expected near-icosahedral geometry. The dihedral angles between the phenyl ring pairs attached to the pendant P atoms are 57.11 (17) and 64.22 (17)°.

Related literature

For details of the synthesis, see: Alexander & Schroeder (1963). For an isomeric structure, see: Zhang *et al.* (2006).



Experimental

Crystal data

$C_{26}H_{30}B_{10}P_2$
M_r = 512.54
Monoclinic, $P2_1/n$
a = 9.783 (5) Å
b = 18.069 (9) Å
c = 16.373 (8) Å
β = 104.399 (6)°
V = 2803 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 298 (2) K
0.55 × 0.53 × 0.50 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.911, T_{max} = 0.919
14413 measured reflections
4925 independent reflections
3134 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.143
S = 1.07
4925 reflections
343 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 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); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: HB2667).

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Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Zhang, D.-P., Dou, J.-M., Li, D.-C. & Wang, D.-Q. (2006). *Acta Cryst.* E**62**, o418–o419.

  doi:10.1107/S1600536807061843

supplementary materials

Acta Cryst. (2007). E**63**, o4918 [**doi:10.1107/S1600536807061843**]

1,7-Bis(diphenylphosphino)-1,7-dicarba-*closo*-dodecaborane

Q. Wang, D. Li and D. Wang

Comment

A number of 1,2-bis(diphenylphosphino)-1,2-dicarba-*closo*-dodecaborane derivatives have been investigated (*e.g.* Zhang *et al.*, 2006). However, only a few studies base on the 1,7-dicarba-*closo*-dodecaborane askeleton have been reported. We now report the structure of the title compound, (I), (Fig. 1), the derivative 1,7-(PPh_2)-1,7-$C_2B_{10}H_{10}$. Its synthesis was reported over 40 years ago (Alexander & Schroeder, 1963).

The molecule is composed of an icosahedral carborane skeleton with –PPh_2 groups bonded to two interphase cage carbon atoms. The carborane cage has the expected near-icosahedral geometry, the lengths of the C—B bonds are in the range 1.702 (4)–1.733 (4)Å and that of B—B bonds are in the range 1.751 (5)–1.780 (6) Å. The P1—C1 and P2—C7 distances in (I) are 1.821 (3) and 1.882 (3) Å, respectively, which are in agreement with those [1.889 (3) and 1.880 (3) Å] for the isomeric 1,2-(PPh_2)-1,2-$C_2B_{10}H_{10}$ (Zhang *et al.*, 2006). The dihedral angles between the phenyl ring pairs attached to the pendant P atoms are 57.11 (17)° and 64.22 (17)° for the C2 + C9 and C15 + C21 pairs, respectively.

Experimental

The title compound was synthesizd according to the literature procedure (Alexander & Schroeder, 1963). The white solid was dissolved in dichloromethane, and colourless blocks of (I) were obtained after partial evaporation (65.2%, m.p. 373 K). FTIR (KBr) v (cm^{-1}): 2930, 2845 (C–H); 2639, 2624, 2593, 2580 (B–H); 1081(P–C).

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

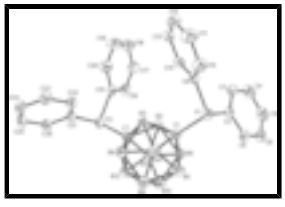
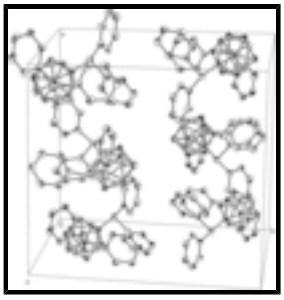


Fig. 1. The molecular structure with 40% probability displacement ellipsoids (H atoms omitted for clarity).



1,7-Bis(diphenylphosphino)-1,7-dicarba-*closo*-dodecaborane

Crystal data

$C_{26}H_{30}B_{10}P_2$	F_{000} = 1064
M_r = 512.54	D_x = 1.214 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3563 reflections
a = 9.783 (5) Å	θ = 2.3–22.2º
b = 18.069 (9) Å	μ = 0.17 mm^{-1}
c = 16.373 (8) Å	T = 298 (2) K
β = 104.399 (6)º	Block, colourless
V = 2803 (2) Å^3	0.55 × 0.53 × 0.50 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	4925 independent reflections
Radiation source: fine-focus sealed tube	3134 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 298(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	h = −11→11
T_{min} = 0.911, T_{max} = 0.919	k = −20→21
14413 measured reflections	l = −19→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.143	$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 1.4084P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001

4925 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
343 parameters	$\Delta\rho_{min} = -0.17$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.55217 (8)	0.22819 (5)	0.54071 (5)	0.0422 (2)
P2	1.14944 (8)	0.29856 (5)	0.52703 (5)	0.0448 (2)
C1	0.6907 (3)	0.28633 (15)	0.50867 (16)	0.0383 (7)
C7	0.9565 (3)	0.32104 (15)	0.50979 (17)	0.0396 (7)
B2	0.8322 (3)	0.25335 (19)	0.47661 (19)	0.0370 (8)
H2	0.8559	0.1942	0.4716	0.044*
B3	0.8539 (3)	0.29779 (18)	0.57592 (19)	0.0358 (7)
H3	0.8922	0.2675	0.6355	0.043*
B4	0.7249 (4)	0.36785 (19)	0.5644 (2)	0.0445 (9)
H4	0.6774	0.3827	0.6164	0.053*
B5	0.6246 (4)	0.3679 (2)	0.4582 (2)	0.0506 (9)
H5	0.5121	0.3828	0.4411	0.061*
B6	0.6921 (4)	0.2970 (2)	0.4040 (2)	0.0456 (9)
H6	0.6238	0.2661	0.3516	0.055*
B8	0.8999 (4)	0.39119 (19)	0.5651 (2)	0.0457 (9)
H8	0.9690	0.4219	0.6174	0.055*
B9	0.7583 (4)	0.4347 (2)	0.4930 (2)	0.0561 (10)
H9	0.7343	0.4937	0.4985	0.067*
B10	0.7368 (4)	0.3908 (2)	0.3935 (2)	0.0572 (11)
H10	0.6983	0.4214	0.3342	0.069*
B11	0.8664 (4)	0.31998 (19)	0.4050 (2)	0.0461 (9)
H11	0.9141	0.3045	0.3533	0.055*
B12	0.9087 (4)	0.4043 (2)	0.4594 (2)	0.0536 (10)
H12	0.9841	0.4432	0.4429	0.064*
C2	0.4947 (3)	0.16648 (17)	0.45081 (18)	0.0434 (7)
C3	0.3981 (3)	0.19668 (19)	0.3817 (2)	0.0569 (9)
H3A	0.3709	0.2459	0.3834	0.068*
C4	0.3424 (4)	0.1554 (2)	0.3112 (2)	0.0668 (10)

H4A	0.2791	0.1768	0.2654	0.080*
C5	0.3796 (4)	0.0829 (2)	0.3080 (2)	0.0685 (11)
H5A	0.3423	0.0551	0.2598	0.082*
C6	0.4720 (4)	0.0506 (2)	0.3758 (2)	0.0671 (10)
H6A	0.4958	0.0009	0.3739	0.081*
C8	0.5295 (3)	0.09241 (18)	0.44683 (19)	0.0512 (8)
H8A	0.5924	0.0705	0.4925	0.061*
C9	0.6517 (3)	0.17128 (16)	0.62705 (18)	0.0422 (7)
C10	0.6028 (4)	0.17367 (19)	0.6994 (2)	0.0591 (9)
H10A	0.5231	0.2016	0.6999	0.071*
C11	0.6711 (5)	0.1350 (2)	0.7709 (2)	0.0755 (11)
H11A	0.6368	0.1372	0.8190	0.091*
C12	0.7868 (4)	0.0942 (2)	0.7716 (2)	0.0688 (11)
H12A	0.8317	0.0683	0.8199	0.083*
C13	0.8384 (4)	0.09080 (19)	0.7005 (2)	0.0607 (9)
H13	0.9187	0.0630	0.7009	0.073*
C14	0.7707 (3)	0.12866 (17)	0.6290 (2)	0.0497 (8)
H14	0.8052	0.1257	0.5811	0.060*
C15	1.2338 (3)	0.34047 (16)	0.62844 (17)	0.0413 (7)
C16	1.3554 (3)	0.37966 (16)	0.6286 (2)	0.0474 (8)
H16	1.3856	0.3837	0.5793	0.057*
C17	1.4318 (4)	0.41272 (19)	0.7013 (2)	0.0644 (10)
H17	1.5136	0.4388	0.7009	0.077*
C18	1.3882 (4)	0.4075 (2)	0.7741 (2)	0.0652 (10)
H18	1.4408	0.4297	0.8232	0.078*
C19	1.2675 (4)	0.36979 (18)	0.7751 (2)	0.0589 (9)
H19	1.2374	0.3670	0.8246	0.071*
C20	1.1907 (3)	0.33611 (18)	0.70329 (18)	0.0528 (8)
H20	1.1091	0.3101	0.7045	0.063*
C21	1.1562 (3)	0.19890 (17)	0.54844 (19)	0.0437 (7)
C22	1.1403 (3)	0.15312 (19)	0.4789 (2)	0.0558 (9)
H22	1.1199	0.1740	0.4253	0.067*
C23	1.1539 (4)	0.0777 (2)	0.4870 (2)	0.0639 (10)
H23	1.1422	0.0483	0.4392	0.077*
C24	1.1844 (4)	0.0457 (2)	0.5648 (2)	0.0680 (10)
H24	1.1933	−0.0054	0.5704	0.082*
C25	1.2020 (4)	0.0897 (2)	0.6344 (2)	0.0765 (11)
H25	1.2235	0.0683	0.6878	0.092*
C26	1.1881 (4)	0.1655 (2)	0.6266 (2)	0.0630 (10)
H26	1.2005	0.1946	0.6748	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0345 (4)	0.0460 (5)	0.0455 (5)	0.0009 (4)	0.0089 (3)	−0.0012 (4)
P2	0.0420 (5)	0.0533 (5)	0.0387 (5)	−0.0126 (4)	0.0096 (3)	−0.0036 (4)
C1	0.0406 (16)	0.0389 (17)	0.0333 (15)	0.0003 (13)	0.0054 (12)	−0.0011 (12)
C7	0.0430 (17)	0.0395 (17)	0.0346 (16)	−0.0082 (13)	0.0066 (13)	−0.0005 (13)

B2	0.0348 (18)	0.0392 (19)	0.0372 (19)	−0.0087 (15)	0.0091 (14)	−0.0069 (15)
B3	0.0363 (18)	0.0377 (19)	0.0323 (17)	−0.0048 (15)	0.0064 (14)	−0.0024 (14)
B4	0.049 (2)	0.040 (2)	0.040 (2)	0.0037 (17)	0.0028 (16)	−0.0065 (15)
B5	0.054 (2)	0.047 (2)	0.045 (2)	0.0089 (18)	0.0007 (17)	0.0056 (17)
B6	0.050 (2)	0.051 (2)	0.0314 (18)	−0.0049 (17)	0.0033 (15)	0.0006 (16)
B8	0.053 (2)	0.038 (2)	0.043 (2)	−0.0055 (16)	0.0048 (16)	−0.0057 (15)
B9	0.068 (3)	0.037 (2)	0.058 (2)	0.0041 (19)	0.005 (2)	0.0028 (18)
B10	0.065 (3)	0.054 (2)	0.045 (2)	−0.003 (2)	0.0011 (19)	0.0143 (18)
B11	0.053 (2)	0.048 (2)	0.0350 (19)	−0.0117 (17)	0.0060 (16)	0.0008 (16)
B12	0.065 (3)	0.042 (2)	0.049 (2)	−0.0145 (19)	0.0065 (18)	0.0091 (17)
C2	0.0337 (16)	0.0476 (19)	0.0472 (18)	−0.0061 (14)	0.0070 (13)	0.0014 (14)
C3	0.0455 (19)	0.054 (2)	0.064 (2)	−0.0050 (16)	−0.0010 (16)	0.0025 (17)
C4	0.064 (2)	0.074 (3)	0.052 (2)	−0.018 (2)	−0.0058 (17)	0.0045 (19)
C5	0.076 (3)	0.076 (3)	0.050 (2)	−0.028 (2)	0.0083 (19)	−0.013 (2)
C6	0.082 (3)	0.053 (2)	0.065 (2)	−0.014 (2)	0.016 (2)	−0.0116 (19)
C8	0.0515 (19)	0.050 (2)	0.0497 (19)	−0.0027 (16)	0.0078 (15)	0.0010 (16)
C9	0.0386 (17)	0.0448 (18)	0.0428 (18)	−0.0085 (14)	0.0096 (13)	−0.0032 (14)
C10	0.059 (2)	0.069 (2)	0.051 (2)	0.0007 (18)	0.0167 (17)	0.0004 (17)
C11	0.100 (3)	0.084 (3)	0.044 (2)	0.001 (3)	0.019 (2)	0.003 (2)
C12	0.084 (3)	0.063 (2)	0.048 (2)	−0.009 (2)	−0.006 (2)	0.0071 (18)
C13	0.049 (2)	0.055 (2)	0.071 (2)	−0.0026 (17)	0.0025 (18)	0.0106 (19)
C14	0.0477 (19)	0.048 (2)	0.054 (2)	−0.0024 (15)	0.0131 (15)	0.0105 (15)
C15	0.0370 (16)	0.0442 (18)	0.0404 (17)	−0.0036 (14)	0.0052 (13)	−0.0021 (14)
C16	0.0430 (18)	0.0408 (18)	0.058 (2)	−0.0020 (15)	0.0123 (15)	−0.0057 (15)
C17	0.050 (2)	0.057 (2)	0.081 (3)	−0.0156 (17)	0.0064 (19)	−0.022 (2)
C18	0.066 (2)	0.060 (2)	0.056 (2)	−0.0036 (19)	−0.0096 (19)	−0.0212 (18)
C19	0.070 (2)	0.058 (2)	0.0425 (19)	−0.0012 (19)	0.0027 (17)	−0.0041 (16)
C20	0.054 (2)	0.058 (2)	0.0425 (19)	−0.0131 (17)	0.0052 (15)	−0.0004 (16)
C21	0.0313 (16)	0.0534 (19)	0.0463 (18)	−0.0068 (14)	0.0097 (13)	−0.0060 (16)
C22	0.051 (2)	0.062 (2)	0.051 (2)	0.0029 (17)	0.0061 (15)	−0.0061 (17)
C23	0.063 (2)	0.058 (2)	0.066 (2)	0.0101 (19)	0.0074 (18)	−0.0148 (19)
C24	0.071 (3)	0.052 (2)	0.081 (3)	0.0091 (19)	0.018 (2)	0.000 (2)
C25	0.107 (3)	0.063 (3)	0.060 (2)	0.011 (2)	0.022 (2)	0.011 (2)
C26	0.084 (3)	0.057 (2)	0.047 (2)	−0.001 (2)	0.0163 (18)	−0.0022 (17)

Geometric parameters (Å, °)

P1—C2	1.821 (3)	B12—H12	1.1000
P1—C9	1.822 (3)	C2—C8	1.387 (4)
P1—C1	1.889 (3)	C2—C3	1.393 (4)
P2—C15	1.825 (3)	C3—C4	1.369 (4)
P2—C21	1.833 (3)	C3—H3A	0.9300
P2—C7	1.882 (3)	C4—C5	1.364 (5)
C1—B2	1.705 (4)	C4—H4A	0.9300
C1—B3	1.711 (4)	C5—C6	1.375 (5)
C1—B4	1.721 (4)	C5—H5A	0.9300
C1—B6	1.729 (4)	C6—C8	1.383 (4)
C1—B5	1.733 (4)	C6—H6A	0.9300
C7—B3	1.702 (4)	C8—H8A	0.9300

C7—B2	1.715 (4)	C9—C10	1.384 (4)
C7—B11	1.723 (4)	C9—C14	1.389 (4)
C7—B12	1.724 (5)	C10—C11	1.385 (5)
C7—B8	1.727 (4)	C10—H10A	0.9300
B2—B6	1.762 (5)	C11—C12	1.349 (5)
B2—B11	1.769 (5)	C11—H11A	0.9300
B2—B3	1.778 (4)	C12—C13	1.381 (5)
B2—H2	1.1000	C12—H12A	0.9300
B3—B4	1.764 (5)	C13—C14	1.375 (4)
B3—B8	1.767 (5)	C13—H13	0.9300
B3—H3	1.1000	C14—H14	0.9300
B4—B8	1.761 (5)	C15—C16	1.383 (4)
B4—B9	1.768 (5)	C15—C20	1.394 (4)
B4—B5	1.772 (5)	C16—C17	1.375 (4)
B4—H4	1.1000	C16—H16	0.9300
B5—B10	1.754 (6)	C17—C18	1.365 (5)
B5—B9	1.767 (5)	C17—H17	0.9300
B5—B6	1.776 (5)	C18—C19	1.367 (5)
B5—H5	1.1000	C18—H18	0.9300
B6—B11	1.751 (5)	C19—C20	1.371 (4)
B6—B10	1.768 (5)	C19—H19	0.9300
B6—H6	1.1000	C20—H20	0.9300
B8—B9	1.765 (5)	C21—C26	1.379 (4)
B8—B12	1.771 (5)	C21—C22	1.385 (4)
B8—H8	1.1000	C22—C23	1.372 (5)
B9—B10	1.777 (6)	C22—H22	0.9300
B9—B12	1.780 (6)	C23—C24	1.362 (5)
B9—H9	1.1000	C23—H23	0.9300
B10—B12	1.774 (5)	C24—C25	1.365 (5)
B10—B11	1.777 (6)	C24—H24	0.9300
B10—H10	1.1000	C25—C26	1.380 (5)
B11—B12	1.762 (5)	C25—H25	0.9300
B11—H11	1.1000	C26—H26	0.9300
C2—P1—C9	106.24 (14)	B8—B9—B10	108.0 (3)
C2—P1—C1	102.41 (13)	B5—B9—B10	59.3 (2)
C9—P1—C1	104.31 (13)	B4—B9—B10	107.6 (3)
C15—P2—C21	104.31 (14)	B8—B9—B12	59.9 (2)
C15—P2—C7	104.87 (13)	B5—B9—B12	107.0 (3)
C21—P2—C7	103.16 (13)	B4—B9—B12	107.3 (3)
B2—C1—B3	62.72 (18)	B10—B9—B12	59.8 (2)
B2—C1—B4	113.4 (2)	B8—B9—H9	121.7
B3—C1—B4	61.85 (18)	B5—B9—H9	122.2
B2—C1—B6	61.75 (18)	B4—B9—H9	121.9
B3—C1—B6	112.9 (2)	B10—B9—H9	122.0
B4—C1—B6	112.5 (2)	B12—B9—H9	122.3
B2—C1—B5	112.7 (2)	B5—B10—B6	60.6 (2)
B3—C1—B5	112.4 (2)	B5—B10—B12	107.8 (3)
B4—C1—B5	61.70 (19)	B6—B10—B12	107.1 (3)
B6—C1—B5	61.7 (2)	B5—B10—B9	60.1 (2)

B2—C1—P1	125.8 (2)	B6—B10—B9	108.4 (3)
B3—C1—P1	120.49 (19)	B12—B10—B9	60.2 (2)
B4—C1—P1	112.7 (2)	B5—B10—B11	107.7 (3)
B6—C1—P1	121.37 (19)	B6—B10—B11	59.2 (2)
B5—C1—P1	113.4 (2)	B12—B10—B11	59.5 (2)
B3—C7—B2	62.71 (18)	B9—B10—B11	107.8 (3)
B3—C7—B11	113.2 (2)	B5—B10—H10	121.5
B2—C7—B11	61.95 (18)	B6—B10—H10	121.9
B3—C7—B12	112.8 (2)	B12—B10—H10	122.2
B2—C7—B12	112.6 (2)	B9—B10—H10	121.4
B11—C7—B12	61.47 (19)	B11—B10—H10	122.3
B3—C7—B8	62.01 (19)	C7—B11—B6	105.6 (2)
B2—C7—B8	113.3 (2)	C7—B11—B12	59.30 (18)
B11—C7—B8	112.3 (2)	B6—B11—B12	108.4 (3)
B12—C7—B8	61.7 (2)	C7—B11—B2	58.80 (17)
B3—C7—P2	125.42 (19)	B6—B11—B2	60.08 (19)
B2—C7—P2	119.9 (2)	B12—B11—B2	108.3 (2)
B11—C7—P2	113.1 (2)	C7—B11—B10	105.8 (2)
B12—C7—P2	113.8 (2)	B6—B11—B10	60.2 (2)
B8—C7—P2	121.35 (19)	B12—B11—B10	60.2 (2)
C1—B2—C7	102.7 (2)	B2—B11—B10	108.2 (3)
C1—B2—B6	59.77 (18)	C7—B11—H11	124.0
C7—B2—B6	105.4 (2)	B6—B11—H11	122.1
C1—B2—B11	105.5 (2)	B12—B11—H11	121.2
C7—B2—B11	59.24 (18)	B2—B11—H11	121.5
B6—B2—B11	59.45 (19)	B10—B11—H11	122.0
C1—B2—B3	58.81 (17)	C7—B12—B11	59.23 (19)
C7—B2—B3	58.29 (17)	C7—B12—B8	59.23 (18)
B6—B2—B3	108.1 (2)	B11—B12—B8	108.4 (2)
B11—B2—B3	107.4 (2)	C7—B12—B10	105.9 (3)
C1—B2—H2	124.3	B11—B12—B10	60.3 (2)
C7—B2—H2	124.8	B8—B12—B10	107.9 (3)
B6—B2—H2	121.8	C7—B12—B9	105.5 (3)
B11—B2—H2	122.3	B11—B12—B9	108.3 (3)
B3—B2—H2	121.8	B8—B12—B9	59.6 (2)
C7—B3—C1	102.9 (2)	B10—B12—B9	60.0 (2)
C7—B3—B4	105.9 (2)	C7—B12—H12	123.8
C1—B3—B4	59.35 (17)	B11—B12—H12	121.1
C7—B3—B8	59.69 (18)	B8—B12—H12	121.6
C1—B3—B8	105.7 (2)	B10—B12—H12	122.1
B4—B3—B8	59.8 (2)	B9—B12—H12	122.3
C7—B3—B2	58.99 (17)	C8—C2—C3	117.7 (3)
C1—B3—B2	58.47 (17)	C8—C2—P1	126.8 (2)
B4—B3—B2	107.9 (2)	C3—C2—P1	115.3 (2)
B8—B3—B2	108.4 (2)	C4—C3—C2	121.3 (3)
C7—B3—H3	124.2	C4—C3—H3A	119.4
C1—B3—H3	124.6	C2—C3—H3A	119.4
B4—B3—H3	121.9	C5—C4—C3	120.1 (3)
B8—B3—H3	121.7	C5—C4—H4A	119.9

B2—B3—H3	121.5	C3—C4—H4A	119.9
C1—B4—B8	105.6 (2)	C4—C5—C6	120.3 (3)
C1—B4—B3	58.80 (17)	C4—C5—H5A	119.9
B8—B4—B3	60.16 (19)	C6—C5—H5A	119.9
C1—B4—B9	106.1 (2)	C5—C6—C8	119.7 (3)
B8—B4—B9	60.0 (2)	C5—C6—H6A	120.1
B3—B4—B9	108.4 (3)	C8—C6—H6A	120.1
C1—B4—B5	59.49 (18)	C6—C8—C2	120.9 (3)
B8—B4—B5	107.8 (3)	C6—C8—H8A	119.6
B3—B4—B5	108.1 (2)	C2—C8—H8A	119.6
B9—B4—B5	59.9 (2)	C10—C9—C14	117.6 (3)
C1—B4—H4	123.8	C10—C9—P1	114.5 (2)
B8—B4—H4	122.3	C14—C9—P1	127.9 (2)
B3—B4—H4	121.4	C9—C10—C11	120.7 (3)
B9—B4—H4	121.9	C9—C10—H10A	119.6
B5—B4—H4	121.5	C11—C10—H10A	119.6
C1—B5—B10	105.8 (3)	C12—C11—C10	120.7 (4)
C1—B5—B9	105.6 (2)	C12—C11—H11A	119.7
B10—B5—B9	60.6 (2)	C10—C11—H11A	119.7
C1—B5—B4	58.81 (18)	C11—C12—C13	119.9 (3)
B10—B5—B4	108.4 (3)	C11—C12—H12A	120.0
B9—B5—B4	59.9 (2)	C13—C12—H12A	120.0
C1—B5—B6	59.00 (18)	C14—C13—C12	119.7 (3)
B10—B5—B6	60.1 (2)	C14—C13—H13	120.2
B9—B5—B6	108.4 (3)	C12—C13—H13	120.2
B4—B5—B6	107.9 (2)	C13—C14—C9	121.3 (3)
C1—B5—H5	124.1	C13—C14—H14	119.4
B10—B5—H5	121.7	C9—C14—H14	119.4
B9—B5—H5	121.9	C16—C15—C20	118.3 (3)
B4—B5—H5	121.6	C16—C15—P2	114.1 (2)
B6—B5—H5	121.5	C20—C15—P2	127.5 (2)
C1—B6—B11	105.3 (2)	C17—C16—C15	120.4 (3)
C1—B6—B2	58.48 (17)	C17—C16—H16	119.8
B11—B6—B2	60.48 (19)	C15—C16—H16	119.8
C1—B6—B10	105.4 (2)	C18—C17—C16	120.4 (3)
B11—B6—B10	60.7 (2)	C18—C17—H17	119.8
B2—B6—B10	108.9 (2)	C16—C17—H17	119.8
C1—B6—B5	59.27 (18)	C17—C18—C19	120.2 (3)
B11—B6—B5	107.8 (3)	C17—C18—H18	119.9
B2—B6—B5	108.0 (2)	C19—C18—H18	119.9
B10—B6—B5	59.3 (2)	C18—C19—C20	120.1 (3)
C1—B6—H6	124.3	C18—C19—H19	119.9
B11—B6—H6	122.0	C20—C19—H19	119.9
B2—B6—H6	121.2	C19—C20—C15	120.6 (3)
B10—B6—H6	121.9	C19—C20—H20	119.7
B5—B6—H6	121.8	C15—C20—H20	119.7
C7—B8—B4	105.0 (2)	C26—C21—C22	117.1 (3)
C7—B8—B9	106.1 (2)	C26—C21—P2	126.6 (2)
B4—B8—B9	60.2 (2)	C22—C21—P2	116.0 (2)

C7—B8—B3	58.30 (17)	C23—C22—C21	121.6 (3)
B4—B8—B3	60.02 (19)	C23—C22—H22	119.2
B9—B8—B3	108.4 (2)	C21—C22—H22	119.2
C7—B8—B12	59.05 (19)	C24—C23—C22	120.4 (3)
B4—B8—B12	108.0 (2)	C24—C23—H23	119.8
B9—B8—B12	60.5 (2)	C22—C23—H23	119.8
B3—B8—B12	107.6 (2)	C23—C24—C25	119.1 (4)
C7—B8—H8	124.3	C23—C24—H24	120.4
B4—B8—H8	122.3	C25—C24—H24	120.4
B9—B8—H8	121.6	C24—C25—C26	120.8 (4)
B3—B8—H8	121.8	C24—C25—H25	119.6
B12—B8—H8	121.5	C26—C25—H25	119.6
B8—B9—B5	107.8 (3)	C21—C26—C25	121.0 (3)
B8—B9—B4	59.8 (2)	C21—C26—H26	119.5
B5—B9—B4	60.2 (2)	C25—C26—H26	119.5

Fig. 1

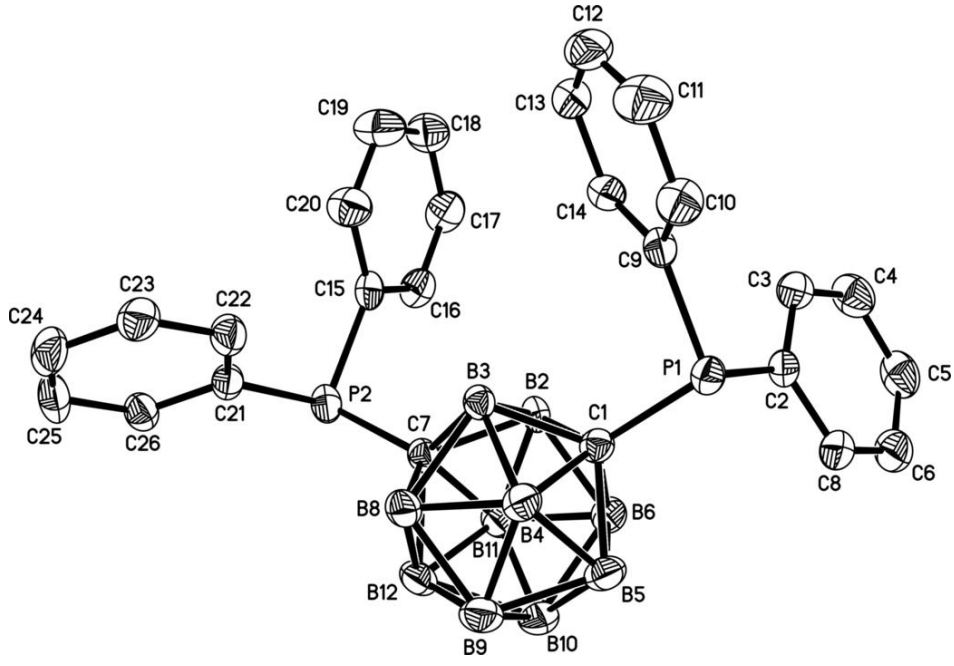

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Fig. 2