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# 1,2-Bis(diphenylphosphino)-1,2-dicarba-*closo*-dodecaborane

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The title compound, $C_{26}H_{30}B_{10}P_2$, was synthesized by the reaction of 1,2-dilithiocarborane with diphenylchorophosphine in diethyl ether. The molecular symmetry of the molecule deviates from $C_{2v}$ because of the different mutual orientations of the phenyl groups. The two P atoms of the –$PPh_2$ groups and two cage C atoms are almost coplanar, with a P—C—C—P torsion angle of 10.6 (3)°.

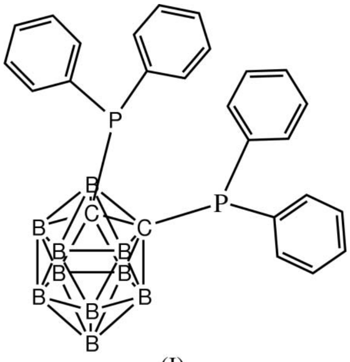
**Key indicators**

Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.006 Å
$R$ factor = 0.049
$wR$ factor = 0.145
Data-to-parameter ratio = 19.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

## Comment

Carboranes, despite their high cost, are uniquely suitable for several applications (Pleasek, 1992). Owing to their interesting chemical and physical properties, organic or organo-element derivatives of dicarba-*closo*-dodecaboranes have received much attention during the past few decades. These types of compounds can be used as catalysts (Hart & Owen, 1985; Longato & Bresadola, 1982), as precursors for ceramic materials (Hsu *et al.*, 1991) and in medical areas (Hawthorne, 1993; Gielen *et al.*, 1995). 1,2-Dicarba-*closo*-dodecaborane is an icosahedral cluster with two C atoms in adjacent positions. The first diphosphine derivative was reported by Alexander & Schroeder (1963). Since then, these types of compounds have been widely used as ligands in the area of transition metal chemistry (Al-Baker *et al.*, 1987; Crespo *et al.*,1992; Bembenek *et al.*, 1994).



(I)

The molecular structure of the title compound is shown in Fig. 1. The molecule is composed of an icosahedral carborane skeleton with –$PPh_2$ groups bonded to the two adjacent cage C (Cc) atoms. The relative orientations of the phenyl groups are quite different, and, as a result, the molecular symmetry of the molecule deviates from $C_{2v}$. The two phosphorus and two cage C atoms are almost coplanar, the P1—C1—C2—P2 torsion angle being 10.6 (3)°. The two P—Cc—Cc angles in the title compound are 116.6 (2) and 111.07 (19)° for C2—C1—P1 and C1—C2—P2, respectively. The corresponding angles in 1,2-

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$(PClPh)_2$-1,2-$C_2B_{10}H_{10}$ (Balema *et al.*, 1998) are 112.89 (13) and 112.19 (13)°, and in 1,2-$(P^iPr_2)_2$-1,2-$C_2B_{10}H_{10}$ (Kivekäs *et al.*, 1995) they are 112.9 (2) and 112.3 (1)°. The Cc—P, Cc—B, B—B and Cc—Cc distances in the title compound (Table 1) are in agreement with these two literature structures.

## Experimental

The title compound was prepared according to the literature method (Alexander & Schroeder, 1963). The product was recrystallized from petroleum ether (b.p. 333–383 K) and dried in a vacuum (65%) (m.p. 490–493 K). The white solid was dissolved in dichloromethane, and crystals suitable for X-ray diffraction were obtained after partial evaporation of the solvent.

### *Crystal data*

$C_{26}H_{30}B_{10}P_2$
$M_r = 512.54$
Monoclinic, $P2_1/n$
$a = 16.315$ (6) Å
$b = 10.387$ (4) Å
$c = 17.768$ (6) Å
$\beta = 111.845$ (5)°
$V = 2795.0$ (17) Å$^3$
$Z = 4$
$D_x = 1.218$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 4735 reflections
$\theta = 2.3$–26.3°
$\mu = 0.17$ mm$^{-1}$
$T = 298$ (2) K
Block, white
0.43 × 0.41 × 0.40 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.930$, $T_{\max} = 0.934$
17791 measured reflections
6721 independent reflections
4367 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.046$
$\theta_{\max} = 28.4°$
$h = -21 \rightarrow 21$
$k = -12 \rightarrow 13$
$l = -11 \rightarrow 23$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.145$
$S = 1.02$
6721 reflections
343 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 1.0346P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.58$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.33$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| P1—C1 | 1.889 (3) | B3—C1 | 1.717 (5) |
| P2—C2 | 1.880 (3) | B3—B9 | 1.778 (5) |
| B6—C2 | 1.708 (5) | B3—B4 | 1.792 (6) |
| B6—C1 | 1.732 (5) | B4—C1 | 1.711 (5) |
| B6—B11 | 1.763 (5) | B4—B9 | 1.774 (6) |
| B6—B7 | 1.779 (5) | B4—B10 | 1.775 (6) |
| B6—B5 | 1.783 (5) | B4—B5 | 1.778 (6) |
| B7—C2 | 1.714 (5) | B5—C1 | 1.714 (5) |
| B7—B11 | 1.764 (6) | B5—B10 | 1.778 (6) |
| B7—B12 | 1.767 (6) | B5—B11 | 1.782 (6) |
| B7—B8 | 1.772 (6) | B11—B12 | 1.789 (6) |
| B8—C2 | 1.716 (5) | B11—B10 | 1.799 (6) |
| B8—B12 | 1.768 (6) | B12—B10 | 1.767 (6) |
| B8—B9 | 1.775 (6) | B12—B9 | 1.776 (6) |
| B8—B3 | 1.779 (5) | B9—B10 | 1.779 (6) |
| B3—C2 | 1.714 (5) | C2—C1 | 1.697 (4) |
| | | | |
| C1—C2—P2 | 111.07 (19) | C2—C1—P1 | 116.6 (2) |

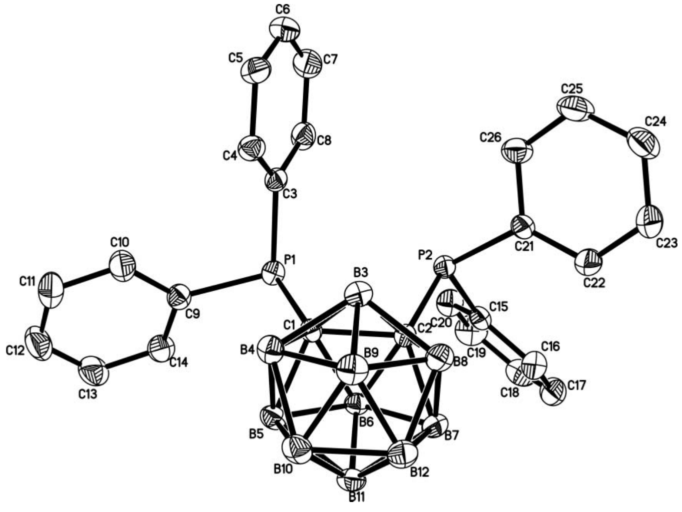

**Figure 1**
The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

All H were placed in calculated postions with C—H = 0.93 Å and B—H = 1.10 Å. They were included in the refinement with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(C,B).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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