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# 2,4-Bis(diphenylphosphanyl)-1,1,2,3,3,4-hexaphenyl-1,3-diphospha-2,4-diboracyclobutane tetrahydrofuran sesquisolvate

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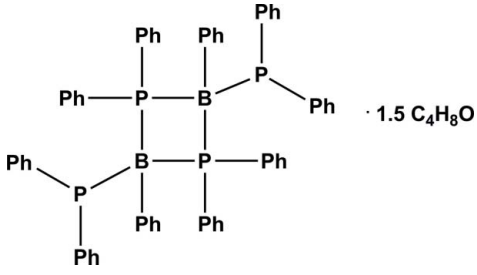
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.003 Å; disorder in solvent or counterion; $R$ factor = 0.041; $wR$ factor = 0.096; data-to-parameter ratio = 19.5.

In the title compound, $C_{60}H_{50}B_2P_4\cdot1.5C_4H_8O$, the diphosphadiborane molecule lies on an inversion centre, whereas the disordered tetrahydrofuran solvent molecule is in a general position with a partial occupancy of 0.75. The diphosphadiborane molecule consists of an ideal planar four-membered $B_2P_2$ ring with an additional phenyl and a $-PPh_2$ group attached to each B atom.

## Related literature

For the structure of a monomeric diphosphaborane molecule, see: Bartlett *et al.* (1988). For assumed monomeric $PhB(PPh_2)_2$, see: Coates & Livingstone (1961). For the structures of other dimeric boron-bridged bisphosphine compounds, see: Herdtweck *et al.* (1997); Kaufmann *et al.* (1997); Nöth (1987).




## Experimental

### Crystal data

$C_{60}H_{50}B_2P_4\cdot1.5C_4H_8O$
$M_r$ = 1024.66
Orthorhombic, *Pbca*
$a$ = 19.2421 (4) Å
$b$ = 11.6938 (2) Å
$c$ = 24.9769 (5) Å
$V$ = 5620.13 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 150 K
0.35 × 0.28 × 0.20 mm

### Data collection

Stoe IPDS II diffractometer
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)
$T_{min}$ = 0.927, $T_{max}$ = 0.986
91233 measured reflections
6705 independent reflections
4392 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.072

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.096
$S$ = 0.87
6705 reflections
343 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); 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: YK2048).

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# supplementary materials

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## 2,4-Bis(diphenylphosphanyl)-1,1,2,3,3,4-hexaphenyl-1,3-diphospha-2,4-diboracyclobutane tetrahydrofuran sesquisolvate

**Normen Peulecke, Bernd H. Müller, Anke Spannenberg and Uwe Rosenthal**

### Comment

We became interested in such a class of compounds, because the boron-bridged bisphosphines could be potential ligands for the chromium catalyzed selective oligomerization of ethene, like PNP. Unfortunately the synthesis of $PhB(PPh_2)_2$, according to the literature (Coates & Livingstone, 1961), failed and always ended up with insoluble polymer. Therefore we changed the procedure using $LiPPh_2$ instead of $HPPh_2$. Examples of structurally characterized borone-bridged bisphosphines are known (Herdtweck *et al.*, 1997; Kaufmann *et al.*, 1997; Nöth, 1987). Only bulky substituents at the boron lead to a monomeric structure (Bartlett *et al.*, 1988). In the present publication, we report on the formation of the dimeric $C_{60}H_{50}B_2P_4$. In the structure of the title compound, the diphosphadiborane molecule occupies the position at an inversion center, whereas the solvent molecule of tetrahydrofuran lies in general position with partial occupancy equal to 0.75. In the tetrahydrofuran molecule the O atom is disordered over two sites with occupancies of 0.341 (9): 0.409 (9). All P—B distances in the four-membered ring are essentially identical [B1—P2 = 2.030 (3) Å and B1—$P2^i$ = 2.036 (2) Å], and also the B1—P1 bond distance of 2.043 (2) Å is not significantly different. In the $B_2P_2$ ring, angles of nearly 90° were observed [P2—B1—$P2^i$ = 87.24 (9)° and B1—P2—$B1^i$ = 92.75°].

### Experimental

$PhBCl_2$ (0.817 ml, 6.3 mmol) was added to a solution of 25 mL $Ph_2PLi$ (0.5*M* in thf) in 20 ml of thf at -40°C and the resulting solution was stirred at room temperature for 48 h. Subsequently, the formed light brown solution was filtered, reduced to the half, over-layered with *n*-hexane and stored at 0°C. Crystals of the title compound appeared, which were suitable for crystal structure analysis. The white compound was fully characterized by standard analytical methods *e.g.* $^{31}$P-NMR: ($C_6D_6$): -10.7(br), -42.2(tr) p.p.m..

### Refinement

H atoms were placed in idealized positions with d(C—H) = 0.95 Å (CH), 0.99 Å ($CH_2$) and refined using a riding model with $U_{iso}$(H) fixed at 1.2 $U_{eq}$(C).

### Computing details

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA* (Stoe & Cie, 2005); data reduction: *X-AREA* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

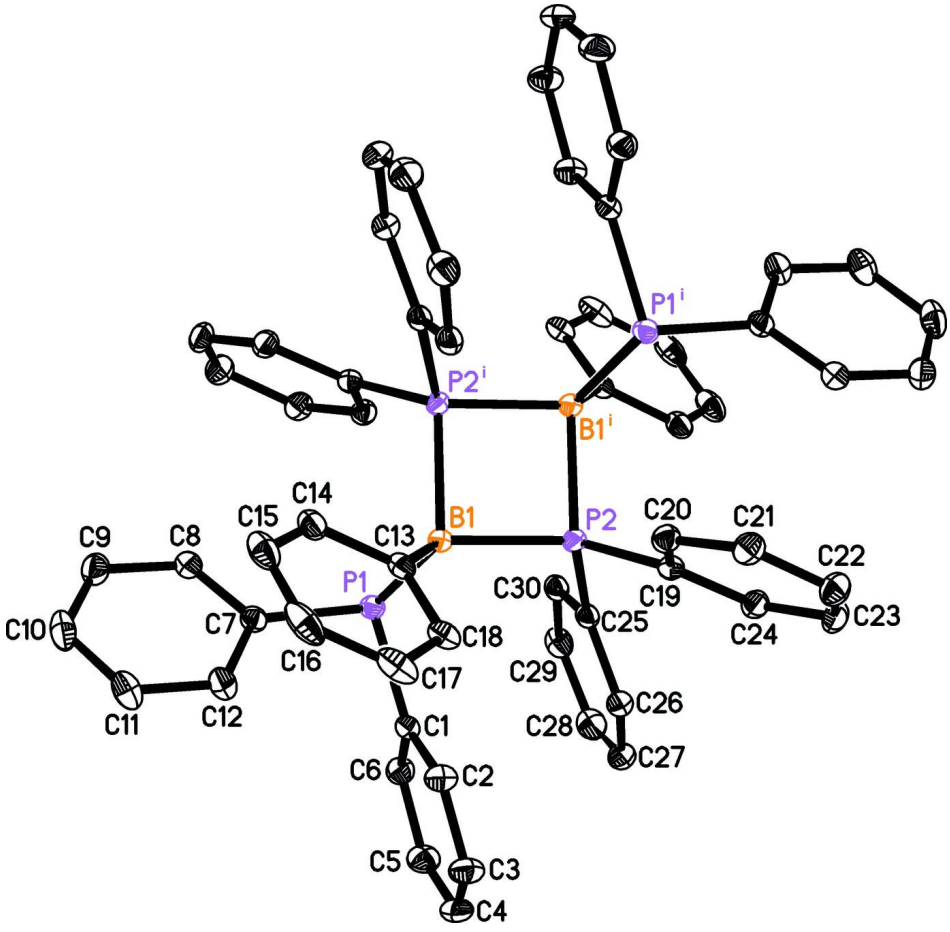


**Figure 1**

The structure of the diphosphadiborane molecule showing the atom-labelling scheme. Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level.

## 2,4-Bis(diphenylphosphanyl)-1,1,2,3,3,4-hexaphenyl- 1,3-diphospha-2,4-diboracyclobutane tetrahydrofuran sesquisolvate

*Crystal data*

$C_{60}H_{50}B_2P_4 \cdot 1.5C_4H_8O$
$M_r = 1024.66$
Orthorhombic, *Pbca*
$a = 19.2421$ (4) Å
$b = 11.6938$ (2) Å
$c = 24.9769$ (5) Å
$V = 5620.13$ (19) Å$^3$
$Z = 4$
$F(000) = 2160$
$D_x = 1.211$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6569 reflections
$\theta = 1.6$–$28.0°$
$\mu = 0.18$ mm$^{-1}$
$T = 150$ K
Prism, colourless
0.35 × 0.28 × 0.20 mm

*Data collection*

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)
$T_{min} = 0.927$, $T_{max} = 0.986$

91233 measured reflections
6705 independent reflections
4392 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.2°$
$h = -25 \rightarrow 25$
$k = -15 \rightarrow 15$
$l = -32 \rightarrow 32$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.096$
$S = 0.87$
6705 reflections
343 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.0P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.64$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > \sigma(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1A | 0.1872 (2) | 0.6123 (6) | 0.2276 (2) | 0.061 (2)* | 0.341 (9) |
| O1B | 0.1940 (2) | 0.5614 (5) | 0.24577 (17) | 0.0613 (19)* | 0.409 (9) |
| C31 | 0.2198 (2) | 0.5279 (4) | 0.1944 (2) | 0.0981 (17) | 0.75 |
| H31A | 0.1909 | 0.5086 | 0.1629 | 0.118* | 0.341 (9) |
| H31B | 0.2305 | 0.4572 | 0.2147 | 0.118* | 0.341 (9) |
| H31C | 0.1834 | 0.5419 | 0.1672 | 0.118* | 0.409 (9) |
| H31D | 0.2297 | 0.4448 | 0.1948 | 0.118* | 0.409 (9) |
| C32 | 0.2832 (2) | 0.5897 (4) | 0.17909 (16) | 0.0913 (16) | 0.75 |
| H32A | 0.2749 | 0.6378 | 0.1471 | 0.110* | 0.75 |
| H32B | 0.3214 | 0.5356 | 0.1711 | 0.110* | 0.75 |
| C33 | 0.3004 (2) | 0.6610 (4) | 0.22580 (13) | 0.0766 (13) | 0.75 |
| H33A | 0.3059 | 0.7420 | 0.2151 | 0.092* | 0.75 |
| H33B | 0.3441 | 0.6346 | 0.2427 | 0.092* | 0.75 |
| C34 | 0.24158 (17) | 0.6479 (4) | 0.26295 (13) | 0.0627 (10) | 0.75 |
| H34A | 0.2513 | 0.5891 | 0.2905 | 0.075* | 0.341 (9) |
| H34B | 0.2301 | 0.7211 | 0.2808 | 0.075* | 0.341 (9) |
| H34C | 0.2595 | 0.6279 | 0.2989 | 0.075* | 0.409 (9) |
| H34D | 0.2167 | 0.7217 | 0.2659 | 0.075* | 0.409 (9) |
| C1 | 1.06155 (9) | −0.01162 (16) | 0.34268 (7) | 0.0246 (4) | |
| C2 | 1.00019 (10) | 0.02724 (18) | 0.31988 (7) | 0.0307 (4) | |
| H2 | 0.9719 | 0.0795 | 0.3392 | 0.037* | |
| C3 | 0.97947 (11) | −0.00883 (19) | 0.26950 (8) | 0.0364 (5) | |

| | | | | |
|---|---|---|---|---|
| H3 | 0.9371 | 0.0185 | 0.2547 | 0.044* |
| C4 | 1.01996 (11) | −0.0841 (2) | 0.24080 (8) | 0.0369 (5) |
| H4 | 1.0057 | −0.1089 | 0.2063 | 0.044* |
| C5 | 1.08146 (11) | −0.12344 (19) | 0.26268 (8) | 0.0369 (5) |
| H5 | 1.1099 | −0.1749 | 0.2430 | 0.044* |
| C6 | 1.10164 (10) | −0.08786 (17) | 0.31321 (7) | 0.0308 (4) |
| H6 | 1.1437 | −0.1161 | 0.3280 | 0.037* |
| C7 | 1.13848 (10) | 0.16430 (16) | 0.39173 (7) | 0.0257 (4) |
| C8 | 1.20183 (10) | 0.18941 (18) | 0.41622 (7) | 0.0299 (4) |
| H8 | 1.2214 | 0.1365 | 0.4408 | 0.036* |
| C9 | 1.23674 (11) | 0.29054 (19) | 0.40521 (9) | 0.0376 (5) |
| H9 | 1.2794 | 0.3070 | 0.4228 | 0.045* |
| C10 | 1.20972 (12) | 0.36709 (19) | 0.36884 (9) | 0.0414 (5) |
| H10 | 1.2332 | 0.4369 | 0.3617 | 0.050* |
| C11 | 1.14820 (11) | 0.34169 (18) | 0.34279 (9) | 0.0383 (5) |
| H11 | 1.1302 | 0.3933 | 0.3169 | 0.046* |
| C12 | 1.11277 (10) | 0.24195 (18) | 0.35416 (8) | 0.0319 (4) |
| H12 | 1.0704 | 0.2259 | 0.3362 | 0.038* |
| C13 | 0.98211 (9) | 0.19751 (16) | 0.43708 (7) | 0.0240 (4) |
| C14 | 1.01833 (11) | 0.29722 (16) | 0.45140 (7) | 0.0304 (4) |
| H14 | 1.0579 | 0.2909 | 0.4740 | 0.036* |
| C15 | 0.99832 (12) | 0.40388 (18) | 0.43376 (9) | 0.0390 (5) |
| H15 | 1.0236 | 0.4696 | 0.4448 | 0.047* |
| C16 | 0.94210 (12) | 0.41587 (19) | 0.40029 (9) | 0.0427 (6) |
| H16 | 0.9291 | 0.4892 | 0.3874 | 0.051* |
| C17 | 0.90491 (12) | 0.32050 (19) | 0.38570 (8) | 0.0382 (5) |
| H17 | 0.8659 | 0.3282 | 0.3627 | 0.046* |
| C18 | 0.92386 (10) | 0.21293 (17) | 0.40430 (7) | 0.0280 (4) |
| H18 | 0.8967 | 0.1484 | 0.3946 | 0.034* |
| C19 | 0.86269 (9) | −0.06475 (16) | 0.46070 (6) | 0.0237 (4) |
| C20 | 0.82663 (9) | 0.03413 (16) | 0.47541 (7) | 0.0263 (4) |
| H20 | 0.8517 | 0.1014 | 0.4844 | 0.032* |
| C21 | 0.75461 (10) | 0.03493 (18) | 0.47697 (8) | 0.0314 (4) |
| H21 | 0.7306 | 0.1022 | 0.4876 | 0.038* |
| C22 | 0.71758 (10) | −0.06199 (19) | 0.46314 (8) | 0.0344 (4) |
| H22 | 0.6682 | −0.0612 | 0.4639 | 0.041* |
| C23 | 0.75253 (10) | −0.15974 (18) | 0.44826 (8) | 0.0328 (4) |
| H23 | 0.7271 | −0.2259 | 0.4381 | 0.039* |
| C24 | 0.82462 (10) | −0.16246 (17) | 0.44795 (7) | 0.0280 (4) |
| H24 | 0.8482 | −0.2313 | 0.4390 | 0.034* |
| C25 | 0.98791 (10) | −0.18291 (16) | 0.42454 (7) | 0.0243 (4) |
| C26 | 0.95519 (11) | −0.21012 (17) | 0.37607 (7) | 0.0295 (4) |
| H26 | 0.9138 | −0.1714 | 0.3660 | 0.035* |
| C27 | 0.98292 (11) | −0.29323 (18) | 0.34282 (8) | 0.0359 (5) |
| H27 | 0.9600 | −0.3124 | 0.3104 | 0.043* |
| C28 | 1.04372 (12) | −0.34830 (17) | 0.35668 (8) | 0.0385 (5) |
| H28 | 1.0624 | −0.4054 | 0.3338 | 0.046* |
| C29 | 1.07740 (11) | −0.32094 (17) | 0.40355 (8) | 0.0337 (5) |
| H29 | 1.1197 | −0.3581 | 0.4126 | 0.040* |

| | | | | |
|---|---|---|---|---|
| C30 | 1.04967 (10) | −0.23923 (16) | 0.43754 (7) | 0.0268 (4) |
| H30 | 1.0729 | −0.2213 | 0.4700 | 0.032* |
| B1 | 1.01311 (10) | 0.07717 (18) | 0.45461 (7) | 0.0212 (4) |
| P1 | 1.09614 (2) | 0.02764 (4) | 0.409099 (17) | 0.02250 (11) |
| P2 | 0.95699 (2) | −0.06707 (4) | 0.467327 (17) | 0.02053 (10) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C31 | 0.079 (3) | 0.089 (4) | 0.126 (4) | −0.017 (3) | −0.022 (3) | −0.053 (3) |
| C32 | 0.098 (4) | 0.128 (4) | 0.048 (2) | −0.003 (3) | 0.015 (2) | −0.035 (3) |
| C33 | 0.081 (3) | 0.080 (3) | 0.069 (3) | −0.027 (2) | 0.015 (2) | −0.019 (2) |
| C34 | 0.048 (2) | 0.089 (3) | 0.0510 (19) | −0.013 (2) | 0.0032 (16) | −0.0253 (19) |
| C1 | 0.0280 (9) | 0.0259 (10) | 0.0200 (8) | −0.0036 (8) | 0.0021 (7) | 0.0005 (7) |
| C2 | 0.0311 (10) | 0.0355 (11) | 0.0256 (9) | 0.0051 (9) | −0.0015 (8) | −0.0013 (8) |
| C3 | 0.0369 (11) | 0.0464 (13) | 0.0260 (9) | 0.0042 (10) | −0.0062 (8) | 0.0006 (9) |
| C4 | 0.0420 (12) | 0.0480 (13) | 0.0207 (9) | −0.0042 (10) | −0.0003 (8) | −0.0058 (9) |
| C5 | 0.0399 (12) | 0.0422 (13) | 0.0285 (10) | 0.0029 (10) | 0.0061 (8) | −0.0082 (9) |
| C6 | 0.0287 (10) | 0.0343 (11) | 0.0294 (9) | 0.0007 (9) | 0.0010 (8) | −0.0022 (8) |
| C7 | 0.0261 (9) | 0.0268 (10) | 0.0243 (9) | −0.0006 (8) | 0.0043 (7) | −0.0015 (7) |
| C8 | 0.0293 (10) | 0.0337 (11) | 0.0267 (9) | −0.0032 (8) | 0.0019 (8) | 0.0003 (8) |
| C9 | 0.0321 (11) | 0.0420 (12) | 0.0387 (11) | −0.0092 (9) | 0.0044 (9) | −0.0064 (10) |
| C10 | 0.0395 (12) | 0.0311 (12) | 0.0535 (13) | −0.0086 (10) | 0.0155 (10) | 0.0006 (10) |
| C11 | 0.0370 (12) | 0.0322 (12) | 0.0458 (12) | 0.0028 (9) | 0.0100 (10) | 0.0113 (9) |
| C12 | 0.0271 (10) | 0.0330 (11) | 0.0355 (10) | −0.0004 (8) | 0.0028 (8) | 0.0068 (9) |
| C13 | 0.0284 (9) | 0.0237 (9) | 0.0199 (8) | 0.0006 (8) | 0.0053 (7) | 0.0009 (7) |
| C14 | 0.0389 (11) | 0.0246 (10) | 0.0276 (9) | −0.0031 (9) | 0.0080 (8) | 0.0011 (8) |
| C15 | 0.0532 (13) | 0.0237 (11) | 0.0401 (11) | −0.0005 (10) | 0.0192 (10) | 0.0018 (9) |
| C16 | 0.0525 (13) | 0.0302 (12) | 0.0455 (12) | 0.0149 (10) | 0.0232 (10) | 0.0159 (10) |
| C17 | 0.0359 (11) | 0.0462 (13) | 0.0324 (10) | 0.0167 (10) | 0.0111 (9) | 0.0150 (9) |
| C18 | 0.0290 (10) | 0.0321 (10) | 0.0229 (8) | 0.0056 (8) | 0.0054 (7) | 0.0043 (8) |
| C19 | 0.0248 (8) | 0.0265 (9) | 0.0198 (8) | −0.0023 (8) | −0.0019 (7) | 0.0022 (7) |
| C20 | 0.0278 (9) | 0.0252 (10) | 0.0257 (8) | −0.0013 (8) | −0.0036 (7) | 0.0019 (7) |
| C21 | 0.0294 (10) | 0.0317 (11) | 0.0331 (10) | 0.0033 (8) | −0.0045 (8) | 0.0013 (8) |
| C22 | 0.0230 (9) | 0.0424 (12) | 0.0379 (10) | −0.0015 (9) | −0.0057 (8) | 0.0018 (9) |
| C23 | 0.0290 (10) | 0.0330 (11) | 0.0363 (10) | −0.0093 (9) | −0.0073 (8) | 0.0008 (9) |
| C24 | 0.0289 (10) | 0.0267 (10) | 0.0285 (9) | −0.0021 (8) | −0.0035 (8) | 0.0012 (8) |
| C25 | 0.0300 (10) | 0.0207 (9) | 0.0221 (8) | −0.0051 (8) | 0.0038 (7) | −0.0002 (7) |
| C26 | 0.0335 (10) | 0.0294 (10) | 0.0255 (9) | −0.0058 (9) | 0.0008 (8) | −0.0008 (7) |
| C27 | 0.0471 (13) | 0.0333 (11) | 0.0271 (9) | −0.0123 (10) | 0.0023 (9) | −0.0075 (8) |
| C28 | 0.0524 (13) | 0.0265 (11) | 0.0367 (11) | −0.0033 (10) | 0.0130 (10) | −0.0102 (9) |
| C29 | 0.0394 (11) | 0.0244 (10) | 0.0375 (11) | 0.0005 (8) | 0.0080 (9) | 0.0003 (8) |
| C30 | 0.0306 (10) | 0.0236 (10) | 0.0263 (9) | −0.0034 (8) | 0.0037 (8) | 0.0015 (7) |
| B1 | 0.0235 (9) | 0.0220 (10) | 0.0182 (9) | −0.0021 (8) | −0.0006 (7) | 0.0005 (7) |
| P1 | 0.0239 (2) | 0.0231 (2) | 0.0206 (2) | 0.0002 (2) | −0.00034 (18) | 0.00079 (18) |
| P2 | 0.0229 (2) | 0.0195 (2) | 0.01925 (19) | −0.00212 (19) | −0.00134 (18) | −0.00060 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1A—C34 | 1.431 (3) | C12—H12 | 0.9500 |
| O1A—C31 | 1.433 (4) | C13—C18 | 1.400 (3) |
| O1B—C34 | 1.429 (3) | C13—C14 | 1.405 (3) |
| O1B—C31 | 1.430 (4) | C13—B1 | 1.590 (3) |
| C31—C32 | 1.470 (3) | C14—C15 | 1.378 (3) |
| C31—H31A | 0.9900 | C14—H14 | 0.9500 |
| C31—H31B | 0.9900 | C15—C16 | 1.374 (3) |
| C31—H31C | 0.9900 | C15—H15 | 0.9500 |
| C31—H31D | 0.9900 | C16—C17 | 1.374 (3) |
| C32—C33 | 1.471 (3) | C16—H16 | 0.9500 |
| C32—H32A | 0.9900 | C17—C18 | 1.390 (3) |
| C32—H32B | 0.9900 | C17—H17 | 0.9500 |
| C33—C34 | 1.472 (3) | C18—H18 | 0.9500 |
| C33—H33A | 0.9900 | C19—C24 | 1.394 (3) |
| C33—H33B | 0.9900 | C19—C20 | 1.398 (3) |
| C34—H34A | 0.9900 | C19—P2 | 1.8222 (18) |
| C34—H34B | 0.9900 | C20—C21 | 1.386 (3) |
| C34—H34C | 0.9900 | C20—H20 | 0.9500 |
| C34—H34D | 0.9900 | C21—C22 | 1.383 (3) |
| C1—C2 | 1.387 (3) | C21—H21 | 0.9500 |
| C1—C6 | 1.390 (3) | C22—C23 | 1.377 (3) |
| C1—P1 | 1.8455 (18) | C22—H22 | 0.9500 |
| C2—C3 | 1.386 (3) | C23—C24 | 1.388 (3) |
| C2—H2 | 0.9500 | C23—H23 | 0.9500 |
| C3—C4 | 1.377 (3) | C24—H24 | 0.9500 |
| C3—H3 | 0.9500 | C25—C30 | 1.397 (3) |
| C4—C5 | 1.382 (3) | C25—C26 | 1.401 (2) |
| C4—H4 | 0.9500 | C25—P2 | 1.8251 (19) |
| C5—C6 | 1.385 (3) | C26—C27 | 1.385 (3) |
| C5—H5 | 0.9500 | C26—H26 | 0.9500 |
| C6—H6 | 0.9500 | C27—C28 | 1.380 (3) |
| C7—C8 | 1.395 (3) | C27—H27 | 0.9500 |
| C7—C12 | 1.396 (3) | C28—C29 | 1.376 (3) |
| C7—P1 | 1.8454 (19) | C28—H28 | 0.9500 |
| C8—C9 | 1.388 (3) | C29—C30 | 1.385 (3) |
| C8—H8 | 0.9500 | C29—H29 | 0.9500 |
| C9—C10 | 1.377 (3) | C30—H30 | 0.9500 |
| C9—H9 | 0.9500 | B1—P2 | 2.028 (2) |
| C10—C11 | 1.383 (3) | B1—P2$^{i}$ | 2.0361 (18) |
| C10—H10 | 0.9500 | B1—P1 | 2.045 (2) |
| C11—C12 | 1.381 (3) | P2—B1$^{i}$ | 2.0363 (18) |
| C11—H11 | 0.9500 | | |
| | | | |
| C34—O1A—C31 | 103.7 (3) | C9—C10—H10 | 120.2 |
| C34—O1B—C31 | 104.0 (3) | C11—C10—H10 | 120.2 |
| O1B—C31—C32 | 112.7 (3) | C12—C11—C10 | 120.5 (2) |
| O1A—C31—C32 | 100.1 (4) | C12—C11—H11 | 119.8 |
| O1B—C31—H31A | 125.6 | C10—C11—H11 | 119.8 |

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|---|---|---|---|
| O1A—C31—H31A | 111.8 | C11—C12—C7 | 120.84 (19) |
| C32—C31—H31A | 111.8 | C11—C12—H12 | 119.6 |
| O1B—C31—H31B | 81.0 | C7—C12—H12 | 119.6 |
| O1A—C31—H31B | 111.8 | C18—C13—C14 | 116.06 (17) |
| C32—C31—H31B | 111.8 | C18—C13—B1 | 125.14 (17) |
| H31A—C31—H31B | 109.5 | C14—C13—B1 | 118.58 (16) |
| O1B—C31—H31C | 109.0 | C15—C14—C13 | 122.1 (2) |
| O1A—C31—H31C | 88.5 | C15—C14—H14 | 119.0 |
| C32—C31—H31C | 109.0 | C13—C14—H14 | 119.0 |
| H31B—C31—H31C | 129.5 | C16—C15—C14 | 120.5 (2) |
| O1B—C31—H31D | 109.0 | C16—C15—H15 | 119.8 |
| O1A—C31—H31D | 138.9 | C14—C15—H15 | 119.8 |
| C32—C31—H31D | 109.0 | C15—C16—C17 | 119.23 (19) |
| H31A—C31—H31D | 83.9 | C15—C16—H16 | 120.4 |
| H31C—C31—H31D | 107.8 | C17—C16—H16 | 120.4 |
| C31—C32—C33 | 105.0 (3) | C16—C17—C18 | 120.6 (2) |
| C31—C32—H32A | 110.8 | C16—C17—H17 | 119.7 |
| C33—C32—H32A | 110.8 | C18—C17—H17 | 119.7 |
| C31—C32—H32B | 110.8 | C17—C18—C13 | 121.5 (2) |
| C33—C32—H32B | 110.8 | C17—C18—H18 | 119.3 |
| H32A—C32—H32B | 108.8 | C13—C18—H18 | 119.3 |
| C32—C33—C34 | 105.6 (3) | C24—C19—C20 | 118.51 (16) |
| C32—C33—H33A | 110.6 | C24—C19—P2 | 122.12 (14) |
| C34—C33—H33A | 110.6 | C20—C19—P2 | 118.87 (14) |
| C32—C33—H33B | 110.6 | C21—C20—C19 | 120.61 (18) |
| C34—C33—H33B | 110.6 | C21—C20—H20 | 119.7 |
| H33A—C33—H33B | 108.8 | C19—C20—H20 | 119.7 |
| O1B—C34—C33 | 112.1 (3) | C22—C21—C20 | 120.17 (19) |
| O1A—C34—C33 | 101.7 (3) | C22—C21—H21 | 119.9 |
| O1B—C34—H34A | 80.7 | C20—C21—H21 | 119.9 |
| O1A—C34—H34A | 111.4 | C23—C22—C21 | 119.75 (18) |
| C33—C34—H34A | 111.4 | C23—C22—H22 | 120.1 |
| O1B—C34—H34B | 127.1 | C21—C22—H22 | 120.1 |
| O1A—C34—H34B | 111.4 | C22—C23—C24 | 120.57 (18) |
| C33—C34—H34B | 111.4 | C22—C23—H23 | 119.7 |
| H34A—C34—H34B | 109.3 | C24—C23—H23 | 119.7 |
| O1B—C34—H34C | 109.2 | C23—C24—C19 | 120.35 (18) |
| O1A—C34—H34C | 138.2 | C23—C24—H24 | 119.8 |
| C33—C34—H34C | 109.2 | C19—C24—H24 | 119.8 |
| H34B—C34—H34C | 82.8 | C30—C25—C26 | 118.43 (17) |
| O1B—C34—H34D | 109.2 | C30—C25—P2 | 119.41 (13) |
| O1A—C34—H34D | 86.8 | C26—C25—P2 | 121.88 (15) |
| C33—C34—H34D | 109.2 | C27—C26—C25 | 120.28 (19) |
| H34A—C34—H34D | 130.1 | C27—C26—H26 | 119.9 |
| H34C—C34—H34D | 107.9 | C25—C26—H26 | 119.9 |
| C2—C1—C6 | 117.71 (17) | C28—C27—C26 | 120.24 (19) |
| C2—C1—P1 | 126.48 (14) | C28—C27—H27 | 119.9 |
| C6—C1—P1 | 115.81 (14) | C26—C27—H27 | 119.9 |
| C3—C2—C1 | 121.20 (19) | C29—C28—C27 | 120.29 (19) |

| | | | |
|---|---|---|---|
| C3—C2—H2 | 119.4 | C29—C28—H28 | 119.9 |
| C1—C2—H2 | 119.4 | C27—C28—H28 | 119.9 |
| C4—C3—C2 | 120.30 (19) | C28—C29—C30 | 120.0 (2) |
| C4—C3—H3 | 119.9 | C28—C29—H29 | 120.0 |
| C2—C3—H3 | 119.9 | C30—C29—H29 | 120.0 |
| C3—C4—C5 | 119.42 (18) | C29—C30—C25 | 120.69 (18) |
| C3—C4—H4 | 120.3 | C29—C30—H30 | 119.7 |
| C5—C4—H4 | 120.3 | C25—C30—H30 | 119.7 |
| C4—C5—C6 | 120.05 (19) | C13—B1—P2 | 125.41 (13) |
| C4—C5—H5 | 120.0 | C13—B1—P2$^{i}$ | 114.90 (12) |
| C6—C5—H5 | 120.0 | P2—B1—P2$^{i}$ | 87.27 (8) |
| C5—C6—C1 | 121.32 (19) | C13—B1—P1 | 113.00 (12) |
| C5—C6—H6 | 119.3 | P2—B1—P1 | 105.52 (9) |
| C1—C6—H6 | 119.3 | P2$^{i}$—B1—P1 | 107.17 (9) |
| C8—C7—C12 | 117.86 (18) | C7—P1—C1 | 99.40 (8) |
| C8—C7—P1 | 117.71 (14) | C7—P1—B1 | 103.32 (8) |
| C12—C7—P1 | 124.38 (15) | C1—P1—B1 | 106.76 (8) |
| C9—C8—C7 | 121.03 (19) | C19—P2—C25 | 106.41 (9) |
| C9—C8—H8 | 119.5 | C19—P2—B1 | 120.25 (8) |
| C7—C8—H8 | 119.5 | C25—P2—B1 | 110.61 (8) |
| C10—C9—C8 | 120.13 (19) | C19—P2—B1$^{i}$ | 111.67 (8) |
| C10—C9—H9 | 119.9 | C25—P2—B1$^{i}$ | 115.19 (8) |
| C8—C9—H9 | 119.9 | B1—P2—B1$^{i}$ | 92.73 (8) |
| C9—C10—C11 | 119.6 (2) | | |

Symmetry code: (i) $-x+2, -y, -z+1$.