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[1,2-Bis(diisopropylphosphino)-1,2-dicarba-*closo*-dodecaborane-κ^2P,P']dichloridomercury(II)

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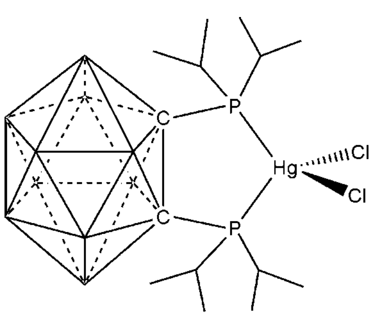
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.038; wR factor = 0.077; data-to-parameter ratio = 17.8.

In the title complex, $[HgCl_2(C_{14}H_{38}B_{10}P_2)]$, the Hg^{II} atom is in a distorted $HgCl_2P_2$ tetrahedral coordination environment. The chelation of the Hg atom by two P atoms and two C atoms from the carborane skeleton results in a nearly planar five-membered ring.

Related literature

For related structures see: Mariyatra *et al.* (2005); Liu *et al.* (2004); Paavola, Kivekäs *et al.* (2002), Paavola, Teixidor *et al.* (2002*a*,*b*). For the synthesis and structure of the ligand, see: Kivekäs *et al.* (1995).



Experimental

Crystal data

$[HgCl_2(C_{14}H_{38}B_{10}P_2)]$
M_r = 647.97
Tetragonal, $I4_1/a$
a = 21.110 (3) Å
c = 24.585 (6) Å
V = 10956 (3) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 5.93 mm^{-1}
T = 298 (2) K
0.53 × 0.49 × 0.47 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.145, T_{max} = 0.167 (expected range = 0.053–0.062)
22446 measured reflections
4815 independent reflections
3491 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.077
S = 1.00
4815 reflections
270 parameters
290 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.37 e Å^{-3}
$\Delta\rho_{min}$ = −1.23 e Å^{-3}

Table 1
Selected bond lengths (Å).

Hg1—Cl1	2.4482 (17)	Hg1—P1	2.5200 (10)
Hg1—Cl2	2.4542 (17)	Hg1—P2	2.5242 (16)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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, 2001); 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: HB2648).

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supplementary materials

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[1,2-Bis(diisopropylphosphino)-1,2-dicarba-*closo*-dodecaborane-κ^2*P*,*P*']dichloridomercury(II)

F. Su, Q. Guo, J. Dou, D. Li and D. Wang

Comment

The synthesis and structure of 1,2-(P^iPr_2)$_2$-1,2-$C_2B_{10}H_{10}$ was reported by Kivekäs *et al.* (1995). Since then, only a few complexes containing this ligand have been described, containing Pt(II) and Pd(II) (Paavola *et al.* (2002,2002*a*,b). We now report the structure of this ligand combined with Hg^{II} and chloride ions as the title compound, (I).

As shown in Fig. 1, The Hg^{II} atom in (I) is in a distorted $HgCl_2P_2$ tetrahedral coordination environment (Table 1). The Hg—P distances in (I) are longer than those of 2.3991Å in [Ph_3PHg*Cl*(µ-*Cl*)$_2$*Cl*$HgPPh_3$] (Mariyatra *et al.*, 2005). The Hg—Cl distances in (I) are also longer than the corresponding distance of 2.4015 (8)Å for in the Mariyatra *et al.* (2005) phase. The Cl—Hg—Cl angle in (I) of 104.81 (6) Å, is slight bigger than that of 101.19 (4)° in [$(HgCl_2)_2((C_6H_{11})_3P)_2$] (Liu *et al.*, 2004).

The chelation of the mercury(II) atom in (I) with phosphorus atoms and carbon atoms form a nearly planar five-membered ring with a maximum deviation of 0.033Å for C2. The torsion angle P1—C1—C2—P2 in (I) is 5.8 (6)°, which is smaller than that of 12.1 (2)° in the free ligand (Kivekas *et al.*, 1995).

Experimental

The title compound was synthesizd by the reaction of 1 mmol $HgCl_2$ and 1 mmol 1,2-(P^iPr_2)$_2$-1,2-$C_2B_{10}H_{10}$ in 10 ml dichloromethane under the protection of N_2. The mixture was refluxed for 4 h, then a colourless solution formed, and colourless blocks of (I) were obtained from a dichloromethane/n-hexane solution (61.7%, m.p. 405–406 K). FTIR (KBr) \v (cm^{-1}): 2990, 2968, 2932, 2875 (C—H); 2615, 2603, 2586, 2558 (B—H); 1072 (C—P).

Refinement

All H atoms were placed geometrically (B—H = 1.10 Å, C—H = 0.96–0.98 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(B) or 1.5U_{eq}(C).

Figures

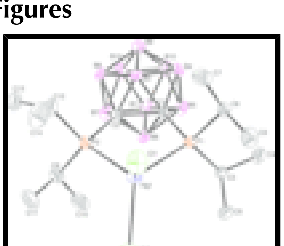


Fig. 1. The molecular structure of (I), with 30% probability displacement ellipsoids (H atoms omitted for clarity).

[1,2-Bis(diisopropylphosphino)-1,2-dicarba-*closo*-dodecaborane-\ κ²*P*,*P*']dichloridomercury(II)

Crystal data

$[HgCl_2(C_{14}H_{38}B_{10}P_2)]$	$Z = 16$
$M_r = 647.97$	$F_{000} = 5056$
Tetragonal, $I4_1/a$	$D_x = 1.571$ Mg m^{-3}
Hall symbol: -I 4ad	Mo *K*α radiation λ = 0.71073 Å
$a = 21.110$ (3) Å	Cell parameters from 5681 reflections
$b = 21.110$ (3) Å	θ = 2.3–25.3°
$c = 24.585$ (6) Å	$\mu = 5.93$ mm^{-1}
α = 90°	$T = 298$ (2) K
β = 90°	Block, colorless
γ = 90°	0.53 × 0.49 × 0.47 mm
$V = 10956$ (3) Å^3	

Data collection

Bruker SMART CCD diffractometer	4815 independent reflections
Radiation source: fine-focus sealed tube	3491 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.081$
$T = 298(2)$ K	$\theta_{max} = 25.0°$
ω scans	$\theta_{min} = 1.9°$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -25 \rightarrow 23$
$T_{min} = 0.145$, $T_{max} = 0.167$	$k = -17 \rightarrow 25$
22446 measured reflections	$l = -29 \rightarrow 27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.031P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.002$
4815 reflections	$\Delta\rho_{max} = 1.37$ e Å^{-3}
270 parameters	$\Delta\rho_{min} = -1.23$ e Å^{-3}
290 restraints	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 $F^2 > \sigma(F^2)$ 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	0.88138 (6)	0.58515 (7)	0.21383 (4)	0.0258 (3)
Hg1	0.906748 (11)	0.554286 (12)	0.117243 (8)	0.03997 (11)
P2	1.02256 (7)	0.53987 (8)	0.13960 (5)	0.0344 (4)
Cl1	0.87446 (8)	0.63978 (9)	0.05593 (7)	0.0653 (5)
Cl2	0.85996 (8)	0.45816 (8)	0.07802 (7)	0.0598 (5)
B3	1.0185 (3)	0.6349 (3)	0.2328 (2)	0.0303 (16)
H3	1.0115	0.6728	0.2028	0.036*
B4	0.9818 (3)	0.6364 (4)	0.2987 (2)	0.0391 (19)
H4	0.9519	0.6761	0.3122	0.047*
B5	0.9646 (3)	0.5571 (3)	0.3155 (2)	0.0401 (19)
H5	0.9232	0.5447	0.3406	0.048*
B6	0.9896 (3)	0.5093 (3)	0.2589 (2)	0.0319 (16)
H6	0.9638	0.4667	0.2457	0.038*
B7	1.0743 (3)	0.5145 (4)	0.2565 (3)	0.0413 (19)
H7	1.1044	0.4750	0.2430	0.050*
B8	1.0922 (3)	0.5945 (3)	0.2405 (3)	0.0379 (18)
H8	1.1341	0.6074	0.2164	0.046*
B9	1.0649 (3)	0.6428 (4)	0.2937 (3)	0.046 (2)
H9	1.0894	0.6872	0.3041	0.056*
B10	1.0309 (3)	0.5941 (4)	0.3432 (3)	0.050 (2)
H10	1.0334	0.6065	0.3866	0.060*
B11	1.0350 (3)	0.5142 (4)	0.3206 (3)	0.047 (2)
H11	1.0393	0.4738	0.3486	0.057*
B12	1.0978 (3)	0.5680 (4)	0.3086 (3)	0.050 (2)
H12	1.1436	0.5629	0.3294	0.060*
C1	0.9610 (2)	0.5824 (3)	0.24933 (18)	0.0280 (12)
C2	1.0262 (2)	0.5577 (3)	0.21524 (19)	0.0301 (12)
C3	0.8303 (3)	0.5299 (3)	0.2536 (2)	0.0326 (13)
H3A	0.8588	0.4975	0.2683	0.039*
C4	0.7960 (3)	0.5584 (3)	0.3027 (2)	0.0508 (17)
H4A	0.7646	0.5880	0.2903	0.076*
H4B	0.8260	0.5799	0.3255	0.076*
H4C	0.7758	0.5252	0.3230	0.076*

C5	0.7850 (3)	0.4955 (3)	0.2166 (2)	0.0515 (18)
H5A	0.7646	0.4620	0.2364	0.077*
H5B	0.8079	0.4778	0.1864	0.077*
H5C	0.7537	0.5246	0.2034	0.077*
C6	0.8465 (3)	0.6652 (3)	0.2224 (2)	0.0380 (14)
H6A	0.8417	0.6741	0.2613	0.046*
C7	0.8844 (3)	0.7185 (3)	0.1962 (3)	0.0577 (18)
H7A	0.8959	0.7066	0.1598	0.087*
H7B	0.9220	0.7263	0.2171	0.087*
H7C	0.8590	0.7563	0.1951	0.087*
C8	0.7808 (3)	0.6633 (3)	0.1959 (3)	0.0584 (18)
H8A	0.7606	0.7037	0.2001	0.088*
H8B	0.7556	0.6312	0.2131	0.088*
H8C	0.7851	0.6537	0.1579	0.088*
C9	1.0537 (3)	0.4602 (3)	0.1261 (3)	0.0523 (16)
H9A	1.0981	0.4580	0.1375	0.063*
C10	1.0167 (4)	0.4082 (3)	0.1536 (3)	0.078 (2)
H10A	0.9722	0.4173	0.1511	0.116*
H10B	1.0288	0.4057	0.1912	0.116*
H10C	1.0255	0.3686	0.1360	0.116*
C11	1.0495 (4)	0.4506 (4)	0.0638 (3)	0.085 (2)
H11A	1.0616	0.4080	0.0549	0.128*
H11B	1.0774	0.4798	0.0459	0.128*
H11C	1.0068	0.4580	0.0519	0.128*
C12	1.0783 (3)	0.5968 (3)	0.1081 (2)	0.0502 (16)
H12A	1.0793	0.6333	0.1326	0.060*
C13	1.1470 (3)	0.5732 (4)	0.1045 (3)	0.069 (2)
H13A	1.1509	0.5437	0.0750	0.104*
H13B	1.1584	0.5527	0.1380	0.104*
H13C	1.1748	0.6086	0.0983	0.104*
C14	1.0553 (4)	0.6221 (4)	0.0543 (3)	0.093 (3)
H14A	1.0866	0.6501	0.0393	0.140*
H14B	1.0164	0.6448	0.0596	0.140*
H14C	1.0483	0.5875	0.0297	0.140*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0229 (8)	0.0301 (9)	0.0245 (7)	−0.0001 (7)	−0.0025 (6)	−0.0018 (6)
Hg1	0.03668 (17)	0.05346 (19)	0.02979 (13)	0.00074 (13)	−0.00920 (11)	−0.00648 (11)
P2	0.0269 (9)	0.0513 (10)	0.0249 (7)	0.0046 (8)	−0.0005 (7)	−0.0113 (7)
Cl1	0.0625 (12)	0.0856 (14)	0.0479 (9)	0.0170 (11)	−0.0108 (9)	0.0162 (10)
Cl2	0.0628 (12)	0.0618 (12)	0.0547 (10)	−0.0097 (10)	−0.0096 (9)	−0.0179 (9)
B3	0.030 (4)	0.032 (4)	0.030 (3)	−0.008 (3)	−0.001 (3)	−0.006 (3)
B4	0.037 (4)	0.052 (5)	0.029 (3)	0.002 (4)	0.000 (3)	−0.018 (3)
B5	0.035 (4)	0.062 (5)	0.023 (3)	−0.005 (4)	0.002 (3)	0.009 (3)
B6	0.026 (4)	0.033 (4)	0.036 (3)	0.001 (3)	0.002 (3)	0.011 (3)
B7	0.029 (4)	0.056 (5)	0.038 (4)	0.006 (4)	−0.007 (3)	0.009 (4)

B8	0.022 (4)	0.060 (5)	0.032 (3)	−0.008 (4)	−0.001 (3)	−0.005 (4)
B9	0.033 (4)	0.061 (6)	0.045 (4)	−0.005 (4)	−0.008 (4)	−0.020 (4)
B10	0.036 (5)	0.093 (7)	0.020 (3)	0.003 (5)	−0.011 (3)	−0.012 (4)
B11	0.033 (4)	0.075 (6)	0.034 (4)	0.006 (4)	−0.004 (3)	0.028 (4)
B12	0.031 (4)	0.089 (7)	0.031 (4)	0.003 (5)	−0.008 (3)	−0.008 (4)
C1	0.023 (3)	0.038 (3)	0.023 (2)	−0.001 (2)	0.001 (2)	−0.002 (2)
C2	0.026 (3)	0.037 (3)	0.027 (2)	0.004 (2)	0.002 (2)	−0.003 (2)
C3	0.027 (3)	0.040 (3)	0.030 (3)	−0.008 (3)	0.001 (2)	−0.002 (2)
C4	0.038 (4)	0.068 (4)	0.046 (3)	−0.004 (3)	0.009 (3)	−0.001 (3)
C5	0.041 (4)	0.066 (4)	0.047 (3)	−0.018 (4)	0.003 (3)	−0.005 (3)
C6	0.033 (3)	0.045 (3)	0.037 (3)	0.005 (3)	−0.003 (3)	−0.004 (3)
C7	0.063 (4)	0.039 (4)	0.071 (4)	0.007 (4)	−0.009 (4)	−0.002 (3)
C8	0.047 (4)	0.064 (4)	0.064 (4)	0.017 (4)	−0.011 (3)	0.002 (4)
C9	0.042 (3)	0.060 (4)	0.055 (3)	0.010 (3)	−0.004 (3)	−0.021 (3)
C10	0.083 (5)	0.054 (5)	0.096 (5)	0.018 (4)	−0.004 (5)	−0.028 (4)
C11	0.073 (5)	0.109 (5)	0.075 (4)	0.014 (4)	0.001 (4)	−0.052 (4)
C12	0.038 (3)	0.073 (4)	0.039 (3)	−0.003 (3)	0.006 (3)	0.000 (3)
C13	0.041 (4)	0.105 (5)	0.062 (4)	−0.007 (4)	0.016 (3)	−0.015 (4)
C14	0.081 (5)	0.142 (7)	0.057 (4)	−0.012 (5)	0.005 (4)	0.029 (5)

Geometric parameters (Å, °)

P1—C6	1.856 (6)	B10—B12	1.739 (10)
P1—C3	1.865 (5)	B10—B11	1.778 (11)
P1—C1	1.896 (5)	B10—H10	1.1000
Hg1—Cl1	2.4482 (17)	B11—B12	1.769 (10)
Hg1—Cl2	2.4542 (17)	B11—H11	1.1000
Hg1—P1	2.5200 (10)	B12—H12	1.1000
Hg1—P2	2.5242 (16)	C1—C2	1.694 (6)
P2—C9	1.836 (7)	C3—C5	1.507 (7)
P2—C12	1.851 (6)	C3—C4	1.531 (7)
P2—C2	1.899 (5)	C3—H3A	0.9800
B3—C1	1.691 (8)	C4—H4A	0.9600
B3—C2	1.693 (8)	C4—H4B	0.9600
B3—B8	1.783 (9)	C4—H4C	0.9600
B3—B4	1.795 (8)	C5—H5A	0.9600
B3—B9	1.798 (9)	C5—H5B	0.9600
B3—H3	1.1000	C5—H5C	0.9600
B4—C1	1.722 (8)	C6—C7	1.523 (8)
B4—B10	1.752 (10)	C6—C8	1.532 (7)
B4—B5	1.763 (10)	C6—H6A	0.9800
B4—B9	1.764 (10)	C7—H7A	0.9600
B4—H4	1.1000	C7—H7B	0.9600
B5—C1	1.713 (7)	C7—H7C	0.9600
B5—B10	1.743 (10)	C8—H8A	0.9600
B5—B11	1.745 (10)	C8—H8B	0.9600
B5—B6	1.797 (9)	C8—H8C	0.9600
B5—H5	1.1000	C9—C10	1.507 (9)
B6—C2	1.673 (8)	C9—C11	1.548 (9)

B6—C1	1.674 (8)	C9—H9A	0.9800
B6—B7	1.793 (9)	C10—H10A	0.9600
B6—B11	1.797 (9)	C10—H10B	0.9600
B6—H6	1.1000	C10—H10C	0.9600
B7—C2	1.701 (8)	C11—H11A	0.9600
B7—B8	1.775 (10)	C11—H11B	0.9600
B7—B12	1.778 (10)	C11—H11C	0.9600
B7—B11	1.781 (9)	C12—C14	1.507 (8)
B7—H7	1.1000	C12—C13	1.537 (8)
B8—C2	1.711 (8)	C12—H12A	0.9800
B8—B9	1.756 (9)	C13—H13A	0.9600
B8—B12	1.770 (9)	C13—H13B	0.9600
B8—H8	1.1000	C13—H13C	0.9600
B9—B10	1.748 (11)	C14—H14A	0.9600
B9—B12	1.765 (11)	C14—H14B	0.9600
B9—H9	1.1000	C14—H14C	0.9600

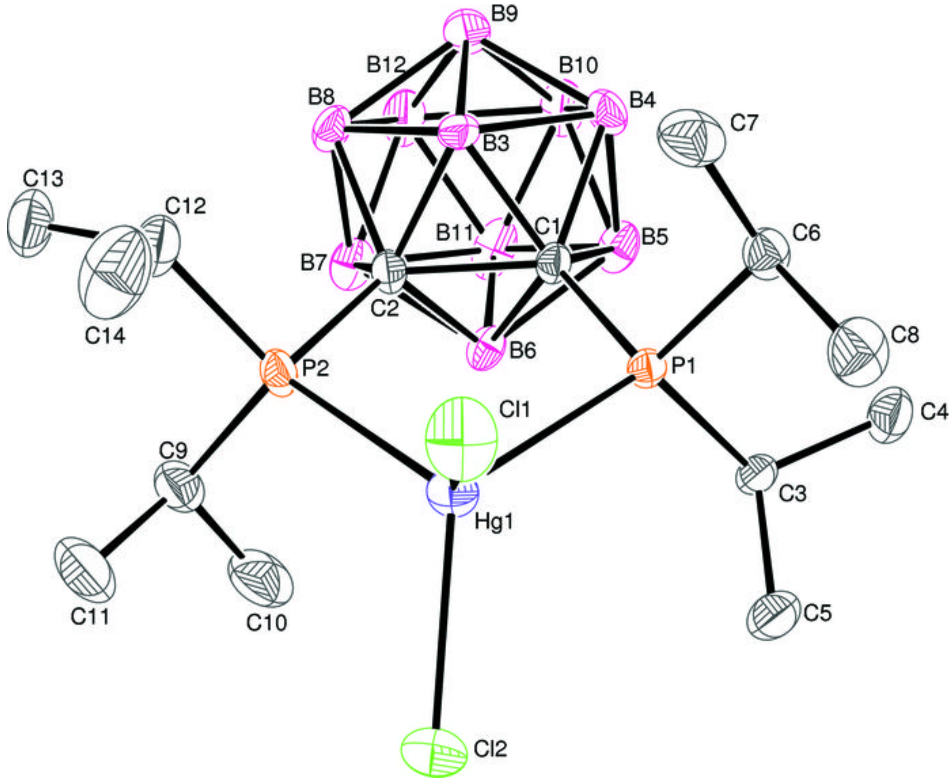
C6—P1—C3	106.3 (3)	B9—B10—H10	121.1
C6—P1—C1	109.1 (2)	B4—B10—H10	120.9
C3—P1—C1	104.6 (2)	B11—B10—H10	121.8
C6—P1—Hg1	115.26 (18)	B5—B11—B12	107.1 (5)
C3—P1—Hg1	117.07 (17)	B5—B11—B10	59.3 (4)
C1—P1—Hg1	103.73 (13)	B12—B11—B10	58.7 (4)
Cl1—Hg1—Cl2	104.81 (6)	B5—B11—B7	109.3 (5)
Cl1—Hg1—P1	109.29 (6)	B12—B11—B7	60.1 (4)
Cl2—Hg1—P1	119.90 (5)	B10—B11—B7	107.3 (5)
Cl1—Hg1—P2	119.51 (6)	B5—B11—B6	60.9 (4)
Cl2—Hg1—P2	112.06 (6)	B12—B11—B6	107.3 (4)
P1—Hg1—P2	91.82 (4)	B10—B11—B6	107.0 (5)
C9—P2—C12	107.0 (3)	B7—B11—B6	60.1 (4)
C9—P2—C2	110.2 (3)	B5—B11—H11	121.2
C12—P2—C2	104.8 (3)	B12—B11—H11	122.6
C9—P2—Hg1	114.7 (2)	B10—B11—H11	123.0
C12—P2—Hg1	116.5 (2)	B7—B11—H11	121.1
C2—P2—Hg1	103.19 (15)	B6—B11—H11	121.8
C1—B3—C2	60.0 (3)	B10—B12—B9	59.8 (4)
C1—B3—B8	106.7 (5)	B10—B12—B11	60.9 (4)
C2—B3—B8	58.9 (4)	B9—B12—B11	108.3 (5)
C1—B3—B4	59.1 (3)	B10—B12—B8	107.9 (5)
C2—B3—B4	106.8 (5)	B9—B12—B8	59.6 (4)
B8—B3—B4	106.8 (5)	B11—B12—B8	108.1 (5)
C1—B3—B9	104.6 (5)	B10—B12—B7	109.1 (5)
C2—B3—B9	104.5 (5)	B9—B12—B7	108.0 (5)
B8—B3—B9	58.7 (4)	B11—B12—B7	60.3 (4)
B4—B3—B9	58.8 (4)	B8—B12—B7	60.0 (4)
C1—B3—H3	122.8	B10—B12—H12	121.2
C2—B3—H3	122.9	B9—B12—H12	122.0
B8—B3—H3	122.5	B11—B12—H12	121.3
B4—B3—H3	122.3	B8—B12—H12	122.0
B9—B3—H3	124.4	B7—B12—H12	121.3

C1—B4—B10	104.7 (5)	B6—C1—B3	112.3 (4)
C1—B4—B5	58.9 (3)	B6—C1—C2	59.6 (3)
B10—B4—B5	59.4 (4)	B3—C1—C2	60.0 (3)
C1—B4—B9	104.8 (4)	B6—C1—B5	64.1 (4)
B10—B4—B9	59.6 (4)	B3—C1—B5	113.7 (4)
B5—B4—B9	107.1 (5)	C2—C1—B5	109.8 (4)
C1—B4—B3	57.5 (3)	B6—C1—B4	114.8 (4)
B10—B4—B3	107.4 (5)	B3—C1—B4	63.5 (4)
B5—B4—B3	106.4 (5)	C2—C1—B4	110.2 (4)
B9—B4—B3	60.7 (4)	B5—C1—B4	61.8 (4)
C1—B4—H4	124.8	B6—C1—P1	114.3 (4)
B10—B4—H4	122.6	B3—C1—P1	120.3 (4)
B5—B4—H4	122.3	C2—C1—P1	120.1 (3)
B9—B4—H4	122.2	B5—C1—P1	119.0 (3)
B3—B4—H4	122.2	B4—C1—P1	122.0 (3)
C1—B5—B10	105.4 (5)	B6—C2—C1	59.6 (3)
C1—B5—B11	105.5 (4)	B6—C2—B3	112.3 (4)
B10—B5—B11	61.3 (4)	C1—C2—B3	60.0 (3)
C1—B5—B4	59.4 (3)	B6—C2—B7	64.2 (4)
B10—B5—B4	60.0 (4)	C1—C2—B7	110.8 (4)
B11—B5—B4	109.5 (5)	B3—C2—B7	114.9 (5)
C1—B5—B6	56.9 (3)	B6—C2—B8	114.9 (4)
B10—B5—B6	108.6 (5)	C1—C2—B8	110.0 (4)
B11—B5—B6	61.0 (4)	B3—C2—B8	63.2 (4)
B4—B5—B6	107.0 (4)	B7—C2—B8	62.7 (4)
C1—B5—H5	124.9	B6—C2—P2	119.3 (4)
B10—B5—H5	121.6	C1—C2—P2	120.9 (3)
B11—B5—H5	120.9	B3—C2—P2	115.9 (4)
B4—B5—H5	121.4	B7—C2—P2	120.1 (3)
B6—B5—H5	122.3	B8—C2—P2	118.6 (3)
C2—B6—C1	60.8 (3)	C5—C3—C4	111.4 (5)
C2—B6—B7	58.7 (3)	C5—C3—P1	110.6 (4)
C1—B6—B7	107.3 (5)	C4—C3—P1	116.1 (4)
C2—B6—B5	106.8 (5)	C5—C3—H3A	106.0
C1—B6—B5	59.0 (3)	C4—C3—H3A	106.0
B7—B6—B5	106.5 (5)	P1—C3—H3A	106.0
C2—B6—B11	105.0 (5)	C3—C4—H4A	109.5
C1—B6—B11	104.9 (5)	C3—C4—H4B	109.5
B7—B6—B11	59.5 (4)	H4A—C4—H4B	109.5
B5—B6—B11	58.1 (4)	C3—C4—H4C	109.5
C2—B6—H6	122.6	H4A—C4—H4C	109.5
C1—B6—H6	122.3	H4B—C4—H4C	109.5
B7—B6—H6	122.3	C3—C5—H5A	109.5
B5—B6—H6	122.8	C3—C5—H5B	109.5
B11—B6—H6	124.1	H5A—C5—H5B	109.5
C2—B7—B8	58.9 (4)	C3—C5—H5C	109.5
C2—B7—B12	104.8 (5)	H5A—C5—H5C	109.5
B8—B7—B12	59.8 (4)	H5B—C5—H5C	109.5
C2—B7—B11	104.6 (5)	C7—C6—C8	108.3 (5)

B8—B7—B11	107.3 (5)	C7—C6—P1	114.6 (4)
B12—B7—B11	59.6 (4)	C8—C6—P1	106.7 (4)
C2—B7—B6	57.1 (3)	C7—C6—H6A	109.0
B8—B7—B6	106.1 (5)	C8—C6—H6A	109.0
B12—B7—B6	107.1 (5)	P1—C6—H6A	109.0
B11—B7—B6	60.4 (4)	C6—C7—H7A	109.5
C2—B7—H7	124.8	C6—C7—H7B	109.5
B8—B7—H7	122.1	H7A—C7—H7B	109.5
B12—B7—H7	122.5	C6—C7—H7C	109.5
B11—B7—H7	122.3	H7A—C7—H7C	109.5
B6—B7—H7	122.7	H7B—C7—H7C	109.5
C2—B8—B9	105.5 (5)	C6—C8—H8A	109.5
C2—B8—B12	104.7 (5)	C6—C8—H8B	109.5
B9—B8—B12	60.1 (4)	H8A—C8—H8B	109.5
C2—B8—B7	58.4 (3)	C6—C8—H8C	109.5
B9—B8—B7	108.5 (5)	H8A—C8—H8C	109.5
B12—B8—B7	60.2 (4)	H8B—C8—H8C	109.5
C2—B8—B3	57.9 (3)	C10—C9—C11	108.6 (6)
B9—B8—B3	61.1 (4)	C10—C9—P2	113.6 (5)
B12—B8—B3	108.1 (5)	C11—C9—P2	106.2 (5)
B7—B8—B3	107.0 (5)	C10—C9—H9A	109.4
C2—B8—H8	124.9	C11—C9—H9A	109.4
B9—B8—H8	121.4	P2—C9—H9A	109.4
B12—B8—H8	122.3	C9—C10—H10A	109.5
B7—B8—H8	121.7	C9—C10—H10B	109.5
B3—B8—H8	121.8	H10A—C10—H10B	109.5
B10—B9—B8	108.2 (6)	C9—C10—H10C	109.5
B10—B9—B4	59.9 (4)	H10A—C10—H10C	109.5
B8—B9—B4	109.4 (5)	H10B—C10—H10C	109.5
B10—B9—B12	59.4 (4)	C9—C11—H11A	109.5
B8—B9—B12	60.4 (4)	C9—C11—H11B	109.5
B4—B9—B12	108.0 (6)	H11A—C11—H11B	109.5
B10—B9—B3	107.5 (5)	C9—C11—H11C	109.5
B8—B9—B3	60.2 (4)	H11A—C11—H11C	109.5
B4—B9—B3	60.5 (3)	H11B—C11—H11C	109.5
B12—B9—B3	107.7 (5)	C14—C12—C13	111.6 (5)
B10—B9—H9	122.2	C14—C12—P2	113.2 (5)
B8—B9—H9	120.9	C13—C12—P2	114.5 (5)
B4—B9—H9	121.1	C14—C12—H12A	105.6
B12—B9—H9	122.1	C13—C12—H12A	105.6
B3—B9—H9	121.9	P2—C12—H12A	105.6
B12—B10—B5	108.6 (5)	C12—C13—H13A	109.5
B12—B10—B9	60.8 (4)	C12—C13—H13B	109.5
B5—B10—B9	108.7 (5)	H13A—C13—H13B	109.5
B12—B10—B4	109.6 (5)	C12—C13—H13C	109.5
B5—B10—B4	60.6 (4)	H13A—C13—H13C	109.5
B9—B10—B4	60.5 (4)	H13B—C13—H13C	109.5
B12—B10—B11	60.4 (4)	C12—C14—H14A	109.5
B5—B10—B11	59.4 (4)	C12—C14—H14B	109.5

B9—B10—B11	108.7 (5)	H14A—C14—H14B	109.5
B4—B10—B11	108.5 (5)	C12—C14—H14C	109.5
B12—B10—H10	120.8	H14A—C14—H14C	109.5
B5—B10—H10	121.6	H14B—C14—H14C	109.5

Fig. 1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