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Bis[(4-bromobenzoylmethyl)triphenylphosphonium] di-μ-bromido-bis[dibromidomercurate(IV)]

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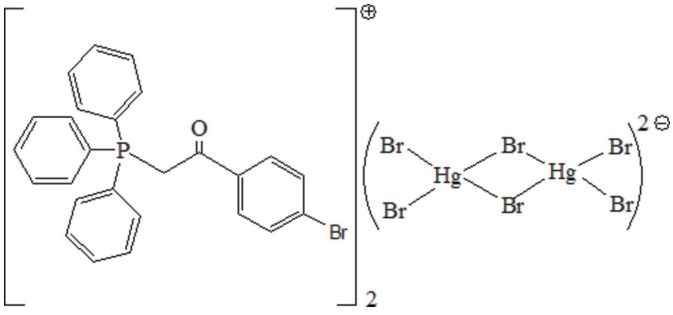
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.076; data-to-parameter ratio = 21.4.

Colourless needle-shaped crystals of the title compound, $(C_{26}H_{21}BrOP)_2[Hg_2Br_6]$, have been prepared by addition of a solution of $HgBr_2$ in methanol to a solution of (4-bromobenzoylmethyl)triphenylphosphorane in dry methanol. The compound features $Hg_2Br_6^{2-}$ dianions, whose site symmetry is $\overline{1}$.

Related literature

For other hexabromodimercurates, see: Bell *et al.* (2002); Fábry & Maximov (1991); Pickardt & Wischlinski (1999). For related literature, see: Hu *et al.* (2003); Nockemann & Meyer (2002); Sabounchei *et al.* (2007); Thiel *et al.* (1994).



Experimental

Crystal data

$(C_{26}H_{21}BrOP)_2[Hg_2Br_6]$
M_r = 1801.18
Monoclinic, $P2_1/n$
a = 9.4146 (6) Å
b = 21.8848 (14) Å
c = 13.2675 (9) Å
β = 100.785 (5)°
V = 2685.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 11.76 mm^{-1}
T = 120 (2) K
0.5 × 0.12 × 0.1 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: numerical [shape of crystal determined optically (*X-SHAPE*; Stoe & Cie, 2005)
T_{min} = 0.200, T_{max} = 0.300
19321 measured reflections
6386 independent reflections
5929 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.076
S = 1.17
6386 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.64 e Å^{-3}
$\Delta\rho_{min}$ = −1.32 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2042).

References

Bell, N. A., Coles, S. J., Constable, C. P., Hursthouse, M. B., Light, M. E., Mansor, R. & Salvin, N. J. (2002). *Polyhedron*, **21**, 1845–1855.
Fábry, J. & Maximov, B.A. (1991). *Acta Cryst.* C**47**, 51–53.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hu, N., Norifusa, T. & Aoki, K. (2003). *Dalton Trans.* pp. 335–341.
Nockemann, P. & Meyer, G. (2002). *Acta Cryst.* E**58**, m529–m530.
Pickardt, J. & Wischlinski, P. (1999). *Z. Anorg. Allg. Chem.* **625**, 1527–1531.
Sabounchei, S. J., Dadras, A., Jafarzadeh, M. & Khavasi, H. R. (2007). *Acta Cryst.* E**63**, o3160.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2005). *X-AREA* and *X-SHAPE*. Stoe & Cie GmbH, Darmstadt, Germany.
Thiel, J., Bu, X. & Coppens, P. (1994). *Acta Cryst.* C**50**, 23–25.

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Bis[(4-bromobenzoylmethyl)triphenylphosphonium] di-μ-bromido-bis-[dibromidomercurate(IV)]

Seyyed Javad Sabounchei, Alireza Dadras, Vida Jodaian, Hassan Nemattalab and Hamid Reza Khavasi

S1. Comment

Colourless, needle-shaped crystals of $C_{26}H_{21}HgBr_3OP$ were obtained from a mixture of methanol, dmso and diethyl ether. The crystal structure consists of discrete $[BrC_6H_4COCH_2PPh_3]^+$ cations and $[Hg_2Br_6]^{2-}$ anions (Fig. 1). The crystals are air-stable and resistant to moisture. All atoms occupy general position in the monoclinic space group, $P2_1/n$. The site symmetry of the anion is -1, with the inversion centre halfway between the two Hg atoms. Comparison of the bond lengths and bond angles within the above crystal show that the phosphonium as a ligand is electrostatically under the influence of an anionic part of an bromomercurate in the unit cells (for instance the bond lengths C6—C7, O1—C7, C8—P1 and P1—C9 and bond angles C8—P1—C9, O1—C7—C8 are 1.489 (5), 1.213 (5), 1.804 (4) and 1.800 (4) A° and 106.7 (2) and 120.4 (4)° for title compound and 1.514 (2), 1.256 (2), 1.719 (2) and 1.805 (2) A° and 105.3 (1) and 123.2 (2)° for the phosphorane molecule (Sabounchei *et al.*, 2007)). The bridging Hg—Br bond lengths in the crystal are 2.6693 (4) A° and 2.7920 (4) A°, the terminal Hg—Br distances are 2.5192 (5) A° and 2.5433 (5) A°. These values are well within the reported bond distances (2.703—-2.787 A° for bridging bromide and 2.479–2.532 A° for terminal bromide) in $[Hg_2Br_6]^{-2}$ anions (Nockemann & Meyer, 2002; Thiel *et al.*, 1994; Hu *et al.*, 2003).

S2. Experimental

Starting materials were purchased from commercial sources and used without further purification.The title compound was prepared by addition of solution of $HgBr_2$ (0.18 g, 0.5 mmol) in methanol (15 ml) to a solution of the 4-bromo-benzoylmethylenetriphenylphosphorane (0.229?g, 0.5?mmol) in dry methanol (15 ml) and stirring for 12 h. A white product formed upon slow evaporation ofthe solvent. It was washed several times with dry diethylether and dried *invacuo*. The product was then washed with benzene and dried *in vacuo*. Yield 83%, m.p=290 K. It was recrystallized from a mixture of methanol, dimethylsulfoxide and diethyl ether (1:1:3).

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, U_{iso}=1.2U_{eq} of the respective carrier atom. The largest difference peak and hole (1.64 and -1.32 e.A^{-3}) are found 1.18Å and 0.05Å respectively from Hg.

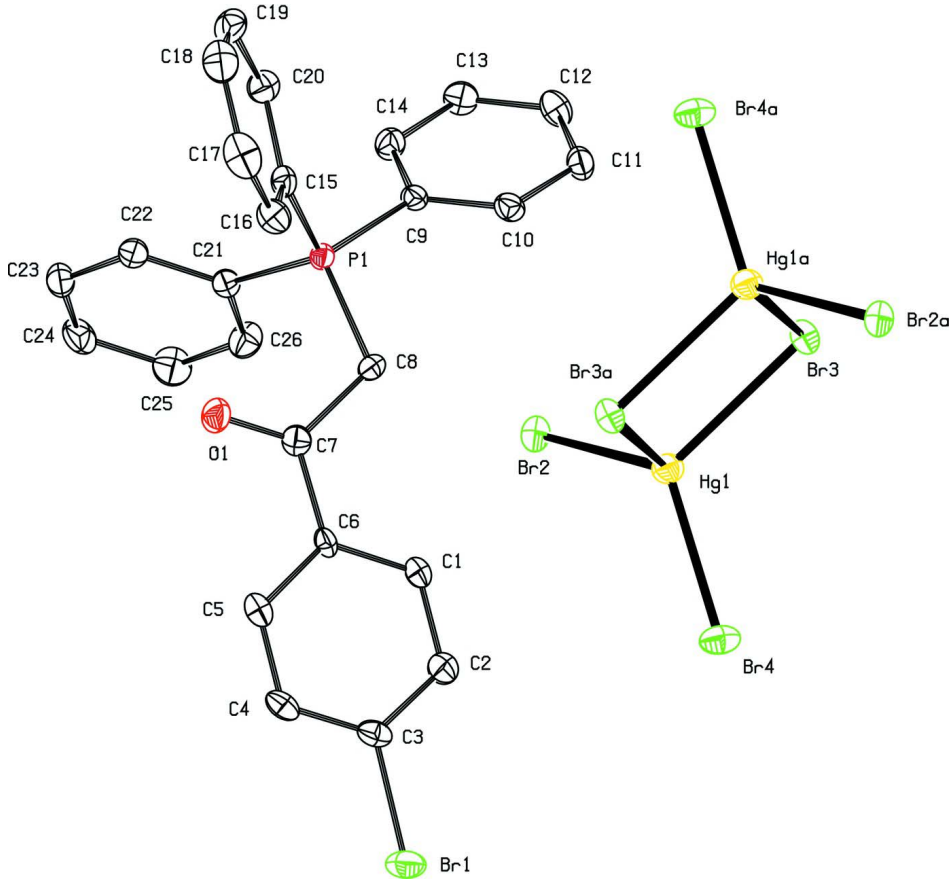

Figure 1

View of (I) (30% probability displacement ellipsoids), symmetry code (i)1 - *x*,-*y*,2 - *z*.

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Crystal data

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Hall symbol: -P 2yn
$a = 9.4146\ (6)$ Å
$b = 21.8848\ (14)$ Å
$c = 13.2675\ (9)$ Å
$\beta = 100.785\ (5)°$
$V = 2685.3\ (3)$ Å^3
$Z = 2$
$F(000) = 1680$
$D_x = 2.228$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2500 reflections
$\theta = 1.8–28.0°$
$\mu = 11.76$ mm^{-1}
$T = 120$ K
Needle, colourless
0.5 × 0.12 × 0.1 mm

Data collection

Stoe IPDSII diffractometer
ω scan
Absorption correction: numerical (shape of crystal determined optically)
$T_{min} = 0.200$, $T_{max} = 0.300$
19321 measured reflections
6386 independent reflections
5929 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 28.0°$, $\theta_{min} = 1.8°$
$h = -12\rightarrow12$
$k = -27\rightarrow28$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.076$
$S = 1.17$
6386 reflections
298 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0312P)^2 + 4.7097P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.018$
$\Delta\rho_{max} = 1.64$ e Å^{-3}
$\Delta\rho_{min} = -1.32$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.459203 (16)	0.045660 (7)	0.872826 (12)	0.02046 (6)
Br1	−0.20000 (5)	0.01733 (2)	0.54508 (3)	0.02701 (10)
Br2	0.41038 (4)	0.160021 (18)	0.86866 (3)	0.02001 (9)
Br3	0.70223 (4)	0.011883 (18)	0.99824 (3)	0.01917 (9)
Br4	0.39811 (5)	−0.00959 (2)	0.70367 (3)	0.02576 (10)
C1	0.0365 (4)	0.0819 (2)	0.8196 (3)	0.0216 (8)
H1	0.1321	0.0808	0.854	0.026*
C2	−0.0011 (4)	0.0538 (2)	0.7241 (3)	0.0230 (8)
H2	0.0686	0.035	0.6936	0.028*
C3	−0.1454 (4)	0.05466 (19)	0.6753 (3)	0.0196 (8)
C4	−0.2511 (4)	0.08368 (19)	0.7184 (3)	0.0196 (8)
H4	−0.3469	0.0839	0.6845	0.024*
C5	−0.2114 (4)	0.11225 (18)	0.8126 (3)	0.0176 (7)
H5	−0.2812	0.1321	0.8417	0.021*
C6	−0.0678 (4)	0.11159 (17)	0.8644 (3)	0.0146 (7)
C7	−0.0321 (4)	0.14202 (18)	0.9665 (3)	0.0176 (7)
C8	0.1241 (4)	0.13891 (19)	1.0237 (3)	0.0175 (7)
H8A	0.1881	0.1431	0.9746	0.021*
H8B	0.1413	0.0991	1.0556	0.021*
C9	0.3623 (4)	0.20382 (18)	1.1473 (3)	0.0150 (7)
C10	0.4485 (4)	0.15232 (18)	1.1426 (3)	0.0183 (7)
H10	0.4062	0.1142	1.1275	0.022*
C11	0.5986 (4)	0.1587 (2)	1.1606 (3)	0.0207 (8)
H11	0.6567	0.1248	1.156	0.025*
C12	0.6615 (4)	0.2155 (2)	1.1854 (3)	0.0234 (8)
H12	0.7617	0.2194	1.1983	0.028*
C13	0.5753 (4)	0.2667 (2)	1.1912 (3)	0.0228 (8)
H13	0.6177	0.3045	1.2087	0.027*
C14	0.4254 (4)	0.26093 (19)	1.1708 (3)	0.0205 (8)
H14	0.3675	0.2951	1.1729	0.025*
C15	0.1055 (4)	0.17780 (19)	1.2365 (3)	0.0172 (7)

C16	0.0059 (4)	0.1308 (2)	1.2391 (3)	0.0233 (8)
H16	−0.0286	0.1079	1.1805	0.028*
C17	−0.0408 (5)	0.1186 (2)	1.3301 (4)	0.0300 (10)
H17	−0.1067	0.0873	1.3326	0.036*
C18	0.0096 (5)	0.1526 (2)	1.4175 (4)	0.0303 (10)
H18	−0.0234	0.1442	1.4778	0.036*
C19	0.1093 (5)	0.1993 (2)	1.4156 (3)	0.0266 (9)
H19	0.1429	0.2221	1.4743	0.032*
C20	0.1586 (5)	0.21153 (19)	1.3246 (3)	0.0213 (8)
H20	0.2267	0.2421	1.3229	0.026*
C21	0.0937 (4)	0.26785 (17)	1.0688 (3)	0.0153 (7)
C22	−0.0084 (4)	0.29971 (18)	1.1122 (3)	0.0175 (7)
H22	−0.0356	0.2855	1.1718	0.021*
C23	−0.0689 (4)	0.3527 (2)	1.0657 (3)	0.0223 (8)
H23	−0.1374	0.3739	1.0942	0.027*
C24	−0.0282 (5)	0.3743 (2)	0.9772 (4)	0.0261 (9)
H24	−0.0693	0.41	0.9467	0.031*
C25	0.0741 (5)	0.3429 (2)	0.9334 (4)	0.0285 (9)
H25	0.1011	0.3575	0.874	0.034*
C26	0.1351 (5)	0.2896 (2)	0.9792 (3)	0.0241 (8)
H26	0.2033	0.2684	0.9505	0.029*
P1	0.16840 (10)	0.19701 (4)	1.12096 (7)	0.01362 (18)
O1	−0.1233 (3)	0.16804 (15)	1.0042 (2)	0.0243 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.02434 (9)	0.01809 (8)	0.01816 (9)	0.00154 (5)	0.00193 (6)	0.00013 (5)
Br1	0.0272 (2)	0.0325 (2)	0.0190 (2)	−0.00427 (17)	−0.00171 (15)	−0.00519 (16)
Br2	0.02090 (18)	0.01773 (18)	0.0232 (2)	0.00194 (14)	0.00861 (14)	0.00331 (14)
Br3	0.01555 (16)	0.01933 (19)	0.02263 (19)	0.00089 (13)	0.00359 (14)	0.00510 (14)
Br4	0.0335 (2)	0.0234 (2)	0.01901 (19)	−0.00529 (16)	0.00126 (16)	−0.00361 (15)
C1	0.0133 (16)	0.027 (2)	0.023 (2)	0.0043 (15)	−0.0005 (14)	−0.0037 (16)
C2	0.0169 (17)	0.026 (2)	0.025 (2)	0.0005 (15)	0.0016 (15)	−0.0049 (17)
C3	0.0219 (18)	0.0197 (19)	0.0151 (18)	−0.0015 (15)	−0.0020 (14)	0.0027 (14)
C4	0.0138 (16)	0.0213 (19)	0.0213 (19)	−0.0041 (14)	−0.0027 (14)	0.0033 (15)
C5	0.0136 (15)	0.0174 (18)	0.0217 (19)	0.0001 (14)	0.0031 (14)	0.0062 (15)
C6	0.0091 (14)	0.0137 (17)	0.0203 (19)	0.0008 (12)	0.0008 (13)	0.0006 (14)
C7	0.0155 (16)	0.0161 (17)	0.0212 (19)	−0.0022 (13)	0.0035 (14)	−0.0011 (14)
C8	0.0168 (17)	0.0197 (18)	0.0160 (17)	0.0009 (14)	0.0030 (13)	−0.0059 (15)
C9	0.0123 (15)	0.0192 (18)	0.0135 (17)	−0.0002 (13)	0.0019 (12)	−0.0010 (14)
C10	0.0176 (17)	0.0163 (18)	0.0195 (19)	−0.0009 (14)	−0.0007 (14)	−0.0006 (14)
C11	0.0154 (17)	0.021 (2)	0.025 (2)	0.0031 (14)	0.0026 (15)	−0.0004 (16)
C12	0.0136 (16)	0.027 (2)	0.029 (2)	−0.0018 (15)	0.0026 (15)	0.0024 (17)
C13	0.0189 (18)	0.020 (2)	0.028 (2)	−0.0063 (15)	0.0030 (15)	−0.0041 (16)
C14	0.0195 (18)	0.0180 (19)	0.024 (2)	0.0000 (15)	0.0036 (15)	−0.0033 (15)
C15	0.0137 (16)	0.0192 (18)	0.0195 (18)	0.0022 (14)	0.0055 (13)	0.0012 (14)
C16	0.0206 (18)	0.024 (2)	0.025 (2)	−0.0014 (15)	0.0035 (16)	0.0023 (16)

C17	0.024 (2)	0.029 (2)	0.039 (3)	−0.0019 (17)	0.0095 (18)	0.013 (2)
C18	0.032 (2)	0.036 (3)	0.026 (2)	0.0083 (19)	0.0124 (18)	0.0119 (19)
C19	0.033 (2)	0.030 (2)	0.018 (2)	0.0100 (18)	0.0087 (17)	0.0020 (17)
C20	0.0246 (19)	0.0178 (18)	0.021 (2)	0.0005 (15)	0.0045 (15)	0.0012 (15)
C21	0.0146 (15)	0.0132 (16)	0.0176 (18)	−0.0013 (13)	0.0022 (13)	−0.0003 (14)
C22	0.0163 (16)	0.0171 (18)	0.0190 (18)	−0.0015 (14)	0.0031 (14)	−0.0011 (14)
C23	0.0180 (17)	0.021 (2)	0.027 (2)	0.0036 (15)	0.0021 (15)	−0.0024 (17)
C24	0.026 (2)	0.022 (2)	0.027 (2)	0.0052 (16)	−0.0022 (17)	0.0054 (17)
C25	0.035 (2)	0.028 (2)	0.024 (2)	0.0027 (19)	0.0077 (18)	0.0090 (18)
C26	0.030 (2)	0.021 (2)	0.023 (2)	0.0024 (17)	0.0095 (17)	0.0018 (16)
P1	0.0123 (4)	0.0141 (4)	0.0147 (4)	0.0004 (3)	0.0032 (3)	−0.0015 (3)
O1	0.0159 (13)	0.0271 (16)	0.0300 (16)	0.0008 (11)	0.0050 (11)	−0.0085 (13)

Geometric parameters (Å, º)

Hg1—Br4	2.5192 (5)	C12—C13	1.394 (6)
Hg1—Br2	2.5433 (5)	C12—H12	0.93
Hg1—Br3	2.6693 (4)	C13—C14	1.391 (5)
Hg1—Br3^{i}	2.7919 (4)	C13—H13	0.93
Br1—C3	1.893 (4)	C14—H14	0.93
Br3—Hg1^{i}	2.7919 (4)	C15—C20	1.394 (6)
C1—C2	1.392 (6)	C15—C16	1.396 (6)
C1—C6	1.400 (5)	C15—P1	1.794 (4)
C1—H1	0.93	C16—C17	1.386 (6)
C2—C3	1.391 (6)	C16—H16	0.93
C2—H2	0.93	C17—C18	1.384 (8)
C3—C4	1.391 (6)	C17—H17	0.93
C4—C5	1.385 (6)	C18—C19	1.389 (7)
C4—H4	0.93	C18—H18	0.93
C5—C6	1.398 (5)	C19—C20	1.397 (6)
C5—H5	0.93	C19—H19	0.93
C6—C7	1.489 (5)	C20—H20	0.93
C7—O1	1.213 (5)	C21—C22	1.395 (5)
C7—C8	1.526 (5)	C21—C26	1.403 (6)
C8—P1	1.804 (4)	C21—P1	1.787 (4)
C8—H8A	0.97	C22—C23	1.384 (6)
C8—H8B	0.97	C22—H22	0.93
C9—C14	1.394 (6)	C23—C24	1.386 (6)
C9—C10	1.397 (5)	C23—H23	0.93
C9—P1	1.800 (4)	C24—C25	1.395 (7)
C10—C11	1.396 (5)	C24—H24	0.93
C10—H10	0.93	C25—C26	1.388 (6)
C11—C12	1.391 (6)	C25—H25	0.93
C11—H11	0.93	C26—H26	0.93
Br4—Hg1—Br2	116.277 (15)	C14—C13—H13	120.1
Br4—Hg1—Br3	116.655 (15)	C12—C13—H13	120.1
Br2—Hg1—Br3	114.607 (14)	C13—C14—C9	119.9 (4)

Br4—Hg1—Br3^{i}	105.642 (15)	C13—C14—H14	120
Br2—Hg1—Br3^{i}	109.895 (13)	C9—C14—H14	120
Br3—Hg1—Br3^{i}	89.686 (12)	C20—C15—C16	120.4 (4)
Hg1—Br3—Hg1^{i}	90.314 (12)	C20—C15—P1	117.9 (3)
C2—C1—C6	120.8 (4)	C16—C15—P1	121.6 (3)
C2—C1—H1	119.6	C17—C16—C15	119.1 (4)
C6—C1—H1	119.6	C17—C16—H16	120.4
C3—C2—C1	118.5 (4)	C15—C16—H16	120.4
C3—C2—H2	120.7	C18—C17—C16	120.8 (4)
C1—C2—H2	120.7	C18—C17—H17	119.6
C4—C3—C2	121.7 (4)	C16—C17—H17	119.6
C4—C3—Br1	118.6 (3)	C17—C18—C19	120.4 (4)
C2—C3—Br1	119.6 (3)	C17—C18—H18	119.8
C5—C4—C3	119.0 (3)	C19—C18—H18	119.8
C5—C4—H4	120.5	C18—C19—C20	119.4 (4)
C3—C4—H4	120.5	C18—C19—H19	120.3
C4—C5—C6	120.8 (4)	C20—C19—H19	120.3
C4—C5—H5	119.6	C15—C20—C19	119.8 (4)
C6—C5—H5	119.6	C15—C20—H20	120.1
C5—C6—C1	119.1 (4)	C19—C20—H20	120.1
C5—C6—C7	118.4 (3)	C22—C21—C26	120.1 (4)
C1—C6—C7	122.5 (3)	C22—C21—P1	121.7 (3)
O1—C7—C6	121.9 (3)	C26—C21—P1	118.1 (3)
O1—C7—C8	120.4 (4)	C23—C22—C21	119.5 (4)
C6—C7—C8	117.7 (3)	C23—C22—H22	120.2
C7—C8—P1	113.4 (3)	C21—C22—H22	120.2
C7—C8—H8A	108.9	C22—C23—C24	120.5 (4)
P1—C8—H8A	108.9	C22—C23—H23	119.8
C7—C8—H8B	108.9	C24—C23—H23	119.8
P1—C8—H8B	108.9	C23—C24—C25	120.5 (4)
H8A—C8—H8B	107.7	C23—C24—H24	119.8
C14—C9—C10	120.4 (3)	C25—C24—H24	119.8
C14—C9—P1	119.5 (3)	C26—C25—C24	119.5 (4)
C10—C9—P1	120.1 (3)	C26—C25—H25	120.2
C11—C10—C9	119.4 (4)	C24—C25—H25	120.2
C11—C10—H10	120.3	C25—C26—C21	119.9 (4)
C9—C10—H10	120.3	C25—C26—H26	120
C12—C11—C10	120.1 (4)	C21—C26—H26	120
C12—C11—H11	119.9	C21—P1—C15	111.40 (18)
C10—C11—H11	119.9	C21—P1—C9	108.34 (18)
C11—C12—C13	120.4 (4)	C15—P1—C9	109.79 (17)
C11—C12—H12	119.8	C21—P1—C8	108.25 (18)
C13—C12—H12	119.8	C15—P1—C8	112.16 (19)
C14—C13—C12	119.8 (4)	C9—P1—C8	106.72 (17)

Br4—Hg1—Br3—Hg1^{i}	−107.394 (16)	C16—C15—C20—C19	−1.6 (6)
Br2—Hg1—Br3—Hg1^{i}	111.825 (14)	P1—C15—C20—C19	178.2 (3)
Br3^{i}—Hg1—Br3—Hg1^{i}	0	C18—C19—C20—C15	1.2 (6)

C6—C1—C2—C3	−1.6 (7)	C26—C21—C22—C23	0.3 (6)
C1—C2—C3—C4	1.4 (7)	P1—C21—C22—C23	−176.5 (3)
C1—C2—C3—Br1	179.7 (3)	C21—C22—C23—C24	−0.4 (6)
C2—C3—C4—C5	−0.3 (6)	C22—C23—C24—C25	0.2 (7)
Br1—C3—C4—C5	−178.6 (3)	C23—C24—C25—C26	0.0 (7)
C3—C4—C5—C6	−0.6 (6)	C24—C25—C26—C21	0.0 (7)
C4—C5—C6—C1	0.4 (6)	C22—C21—C26—C25	−0.2 (6)
C4—C5—C6—C7	−178.8 (4)	P1—C21—C26—C25	176.8 (4)
C2—C1—C6—C5	0.7 (6)	C22—C21—P1—C15	−4.3 (4)
C2—C1—C6—C7	179.9 (4)	C26—C21—P1—C15	178.8 (3)
C5—C6—C7—O1	−1.4 (6)	C22—C21—P1—C9	−125.2 (3)
C1—C6—C7—O1	179.4 (4)	C26—C21—P1—C9	57.9 (4)
C5—C6—C7—C8	177.9 (4)	C22—C21—P1—C8	119.5 (3)
C1—C6—C7—C8	−1.3 (6)	C26—C21—P1—C8	−57.4 (4)
O1—C7—C8—P1	−20.7 (5)	C20—C15—P1—C21	−72.1 (3)
C6—C7—C8—P1	160.0 (3)	C16—C15—P1—C21	107.6 (3)
C14—C9—C10—C11	−0.6 (6)	C20—C15—P1—C9	47.9 (4)
P1—C9—C10—C11	178.3 (3)	C16—C15—P1—C9	−132.4 (3)
C9—C10—C11—C12	1.5 (6)	C20—C15—P1—C8	166.4 (3)
C10—C11—C12—C13	−0.8 (7)	C16—C15—P1—C8	−13.9 (4)
C11—C12—C13—C14	−0.8 (7)	C14—C9—P1—C21	28.6 (4)
C12—C13—C14—C9	1.7 (7)	C10—C9—P1—C21	−150.4 (3)
C10—C9—C14—C13	−1.0 (6)	C14—C9—P1—C15	−93.3 (3)
P1—C9—C14—C13	−179.9 (3)	C10—C9—P1—C15	87.7 (4)
C20—C15—C16—C17	0.8 (6)	C14—C9—P1—C8	144.9 (3)
P1—C15—C16—C17	−178.9 (3)	C10—C9—P1—C8	−34.1 (4)
C15—C16—C17—C18	0.3 (7)	C7—C8—P1—C21	−43.9 (3)
C16—C17—C18—C19	−0.7 (7)	C7—C8—P1—C15	79.4 (3)
C17—C18—C19—C20	−0.1 (7)	C7—C8—P1—C9	−160.3 (3)

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