Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,1′-(Butane-1,4-diyl)dipyridinium bromidotrichloridomercurate(II)

Yun-Yin Niu,[a] Xiu-Cun Liu,[a] Hong-Wei Hou,[a] Yao-Ting Fan[a] and Seik Weng Ng[b]*

[a]Department of Chemistry, Zhengzhou University, Zhengzhou 450052, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

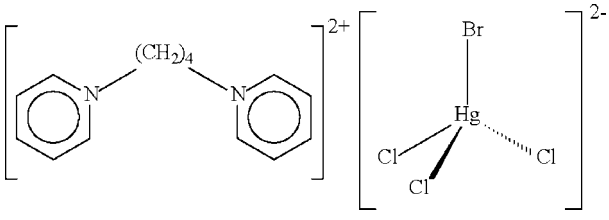
Received 30 May 2007; accepted 5 June 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.008 Å; disorder in main residue; R factor = 0.031; wR factor = 0.081; data-to-parameter ratio = 15.8.

The Hg atom in the title compound, $(C_{14}H_{18}N_2)[HgBrCl_3]$, is coordinated by four halogen atoms in a tetrahedral geometry. The four halogen atoms are each disordered between Br and Cl, with the Br:Cl ratios being 0.218 (2):0.782 (2), 0.136 (2):0.864 (2), 0.090 (2):0.910 (2) and 0.556 (2):0.444 (2). The cation is disordered over two orientations and each was refined with an occupancy of 0.50.

Related literature

For related tetrahalidomercurates, see: Wang *et al.* (2007).



Experimental

Crystal data

$(C_{14}H_{18}N_2)[HgBrCl_3]$
M_r = 601.15
Monoclinic, $P2_1/c$
a = 15.9912 (8) Å
b = 8.7769 (5) Å
c = 14.3189 (9) Å
β = 109.760 (1)°
V = 1891.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 10.67 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.096, T_{max} = 0.415
(expected range = 0.080–0.344)
11857 measured reflections
3316 independent reflections
2809 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.081
S = 1.01
3316 reflections
210 parameters
130 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.84 e Å^{-3}

Table 1
Selected bond lengths (Å).

Hg1—Cl1	2.51 (2)	Hg1—Cl3	2.543 (5)
Hg1—Br1	2.58 (4)	Hg1—Br3	2.46 (2)
Hg1—Cl2	2.529 (15)	Hg1—Cl4	2.545 (18)
Hg1—Br2	2.49 (4)	Hg1—Br4	2.530 (5)

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

The authors thank the National Natural Science Foundation of China (grant No. 20671083), the Henan Province Excellent Young Foundation (grant No. 0612002800), Zhengzhou University and the University of Malaya for supporting this work. We thank Central China Normal University for the diffraction measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2388).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2004). *SAINT* (Version 6.45a) and *SMART* (Version 6.45a). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, Q.-L., Yang, C.-C., Niu, Y.-Y., Liu, X.-C. & Ng, S. W. (2007). *Acta Cryst.* E**63**, m1892.
Westrip, S. P. (2007). *publCIF*. In preparation.

  doi:10.1107/S1600536807027468

supplementary materials

Acta Cryst. (2007). E**63**, m1894 [**doi:10.1107/S1600536807027468**]

1,1'-(Butane-1,4-diyl)dipyridinium bromidotrichloridomercurate(II)

Y.-Y. Niu, X.-C. Liu, H.-W. Hou, Y.-T. Fan and S. W. Ng

Comment

The preceding study reports the structure of the tetrahedral dibromidodichloridomercurate(II), which was isolated as a 1,2-ethanedipyridinium salt (Wang *et al.*, 2007). Replacing the cation by 1,4-butanedipyridinium furnishes a similar tetrahalomercurate. The anion of the salt is composed of one bromine and three chlorine atoms which are disordered (Fig. 1); the metal atom shows tetrahedral coordination. Selected bond distances are listed in Table 1.

Experimental

The salt was synthesized from the reaction of butane-1,4-dipyridinium dibromide (0.026 g, 0.1 mmol) in methanol (5 ml) and mercuric dichloride (0.054 g, 0.2 mmol) in DMF (10 ml). The mixture was set aside for the formation of colourless crystals in 30% yield after several days. CH&N elemental analysis for $C_{14}H_{18}BrCl_3HgN_2$. Calculated: C 27.97, H 3.02, N 4.46%; found C 27.08, H 2.77, N 4.49%.

Refinement

The four halogens lie in general positions. Initial attempts to refine the structure with either four bromines or four chlorines gave unacceptably high *R*-indices and large peaks/deep holes. The four halogen atoms were then refined as four (Br+Cl) mixtures; one attempt had the mixtures to have the same displacement parameters as well as sharing the same site. A second attempt had the components having the same displacement parameters only. The second led to a formulation consisting of approximately one Br and three Cl atoms. The use of a restraint that fixed the number of Br and Cl atoms as exactly 1 Br and 3 C l led to occupancies of 0.218 (2), 0.136 (2), 0.090 (2) and 0.556 (2), respectively, Br1, Br2, Br3 and Br4, and 0.782 (2), 0.864 (2), 0.910 (2) and 0.444 (2), respectively, for Cl1, Cl2, Cl3 and Cl4. The formulation is in good agreement with CH&N elemental analysis, and furthermore, there were neither large peaks nor deep holes in the difference Fourier map. Other formulations led to somewhat larger peaks/deep holes.

The cation is disordered over two orientations and each was refined with an occupancy of 0.50. The occupancy could not be refined. The pyridyl rings were refined as rigid hexagons (C—C = C—N = 1.39 Å). The C(sp^3)—C(sp3) and N—C(sp^3) distances were restrained to 1.50 (1) Å, and the 1,3-related distances to 2.45 (1) Å; additionally, the alphatic carbon atom bonded to the nitrogen atom was retrained to lie on the plane of the ring. The displacement parameters of the primed atoms were set to those of the unprimed ones and they were restrained to be nearly isotropic. C-bound H atoms were generated geometrically (C—H 0.93 and 0.97 Å), and were included in the refinement in the riding-model approximation, with *U*(H) set to 1.2U_{eq}(C).

Figures

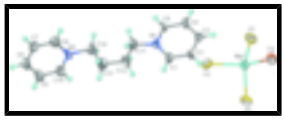


Fig. 1. The molecular structure of $[C_{14}H_{18}N_2][HgBrCl_3]$. Displacement ellipsoids are drawn at the 50% probability level. The bromine and chlorine atoms are disordered; the figure depicts the anion as an $[HgX_4]^{2-}$ species. Hydrogen atoms are drawn as spheres of arbitrary radius.

1,1'-(Butane-1,4-diyl)dipyridinium bromidotrichloridomercurate(II)

Crystal data

$(C_{14}H_{18}N_2)[HgBrCl_3]$	F_{000} = 1128
M_r = 601.15	D_x = 2.111 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4607 reflections
a = 15.9912 (8) Å	θ = 2.7–26.4º
b = 8.7769 (5) Å	μ = 10.67 mm^{-1}
c = 14.3189 (9) Å	T = 295 (2) K
β = 109.760 (1)º	Block, colourless
V = 1891.4 (2) Å^3	0.20 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker APEX area-detector diffractometer	3316 independent reflections
Radiation source: fine-focus sealed tube	2809 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −19→15
T_{min} = 0.096, T_{max} = 0.415	k = −10→10
11857 measured reflections	l = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H-atom parameters constrained
$wR(F^2)$ = 0.081	$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.263P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
3316 reflections	$\Delta\rho_{max}$ = 0.77 e Å^{-3}

210 parameters	$\Delta\rho_{min} = -0.84$ e Å^{-3}
130 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Hg1	0.254133 (15)	0.47282 (3)	0.529270 (15)	0.05327 (11)	
Br1	0.180 (3)	0.253 (4)	0.411 (2)	0.0635 (18)	0.218 (2)
Br2	0.415 (3)	0.435 (4)	0.623 (3)	0.0563 (12)	0.136 (2)
Br3	0.2771 (14)	0.660 (2)	0.4126 (18)	0.0577 (7)	0.090 (2)
Br4	0.1650 (4)	0.5446 (5)	0.6389 (4)	0.0643 (7)	0.556 (2)
Cl1	0.1756 (17)	0.251 (3)	0.4255 (15)	0.0635 (18)	0.782 (2)
Cl2	0.4166 (11)	0.4121 (14)	0.6159 (11)	0.0563 (12)	0.864 (2)
Cl3	0.2607 (3)	0.6920 (5)	0.4159 (4)	0.0577 (7)	0.910 (2)
Cl4	0.1718 (14)	0.5153 (17)	0.6513 (14)	0.0643 (7)	0.444 (2)
N1	0.5444 (6)	0.0632 (18)	0.3892 (8)	0.0415 (18)	0.50
C1	0.5126 (7)	0.2014 (16)	0.4108 (11)	0.049 (2)	0.50
H1	0.5517	0.2820	0.4356	0.059*	0.50
C2	0.4226 (8)	0.2193 (12)	0.3955 (13)	0.047 (3)	0.50
H2	0.4014	0.3118	0.4100	0.057*	0.50
C3	0.3643 (6)	0.0990 (12)	0.3585 (9)	0.045 (3)	0.50
H3	0.3041	0.1109	0.3482	0.054*	0.50
C4	0.3960 (8)	−0.0393 (12)	0.3368 (10)	0.047 (3)	0.50
H4	0.3570	−0.1198	0.3121	0.056*	0.50
C5	0.4861 (8)	−0.0572 (14)	0.3522 (10)	0.045 (2)	0.50
H5	0.5073	−0.1497	0.3377	0.054*	0.50
N2	0.8831 (4)	−0.0935 (9)	0.3268 (6)	0.051 (2)	0.50
C6	0.9378 (8)	−0.1770 (12)	0.4066 (7)	0.071 (2)	0.50
H6	0.9134	−0.2292	0.4479	0.085*	0.50
C7	1.0288 (7)	−0.1824 (17)	0.4249 (8)	0.056 (2)	0.50
H7	1.0654	−0.2382	0.4783	0.067*	0.50
C8	1.0651 (4)	−0.1044 (18)	0.3632 (10)	0.058 (3)	0.50
H8	1.1260	−0.1080	0.3754	0.070*	0.50
C9	1.0104 (7)	−0.0209 (15)	0.2834 (9)	0.074 (2)	0.50
H9	1.0348	0.0313	0.2421	0.089*	0.50
C10	0.9194 (7)	−0.0155 (10)	0.2651 (6)	0.058 (3)	0.50
H10	0.8828	0.0403	0.2117	0.070*	0.50
C11	0.6368 (10)	0.020 (4)	0.4005 (15)	0.055 (3)	0.50
H11A	0.6758	0.0525	0.4654	0.066*	0.50
H11B	0.6407	−0.0897	0.3971	0.066*	0.50
C12	0.6673 (6)	0.0893 (13)	0.3235 (9)	0.060 (3)	0.50
H12A	0.6549	0.1977	0.3197	0.072*	0.50
H12B	0.6347	0.0447	0.2595	0.072*	0.50
C13	0.7646 (6)	0.0649 (11)	0.3455 (9)	0.065 (2)	0.50
H13A	0.7945	0.0679	0.4167	0.078*	0.50
H13B	0.7879	0.1473	0.3164	0.078*	0.50

C14	0.7849 (5)	−0.0846 (11)	0.3060 (8)	0.058 (2)	0.50
H14A	0.7659	−0.1685	0.3381	0.069*	0.50
H14B	0.7535	−0.0911	0.2352	0.069*	0.50
N1'	0.5395 (6)	0.0366 (18)	0.3852 (8)	0.0415 (18)	0.50
C1'	0.5296 (7)	0.1906 (17)	0.4015 (11)	0.049 (2)	0.50
H1'	0.5785	0.2553	0.4171	0.059*	0.50
C2'	0.4467 (8)	0.2480 (12)	0.3944 (13)	0.047 (3)	0.50
H2'	0.4401	0.3511	0.4053	0.057*	0.50
C3'	0.3737 (6)	0.1514 (12)	0.3711 (10)	0.045 (3)	0.50
H3'	0.3182	0.1898	0.3664	0.054*	0.50
C4'	0.3835 (7)	−0.0027 (12)	0.3549 (10)	0.047 (3)	0.50
H4'	0.3346	−0.0673	0.3393	0.056*	0.50
C5'	0.4664 (8)	−0.0601 (13)	0.3619 (10)	0.045 (2)	0.50
H5'	0.4730	−0.1632	0.3510	0.054*	0.50
N2'	0.8955 (4)	−0.0307 (10)	0.3618 (6)	0.051 (2)	0.50
C6'	0.9442 (8)	−0.1532 (12)	0.4144 (7)	0.071 (2)	0.50
H6'	0.9242	−0.2062	0.4590	0.085*	0.50
C7'	1.0227 (8)	−0.1965 (15)	0.4003 (9)	0.056 (2)	0.50
H7'	1.0552	−0.2785	0.4355	0.067*	0.50
C8'	1.0525 (5)	−0.1173 (17)	0.3336 (10)	0.058 (3)	0.50
H8'	1.1051	−0.1463	0.3242	0.070*	0.50
C9'	1.0039 (8)	0.0051 (14)	0.2810 (9)	0.074 (2)	0.50
H9'	1.0239	0.0581	0.2363	0.089*	0.50
C10'	0.9254 (7)	0.0485 (10)	0.2951 (7)	0.058 (3)	0.50
H10'	0.8929	0.1304	0.2598	0.070*	0.50
C11'	0.6329 (11)	−0.004 (4)	0.3962 (13)	0.055 (3)	0.50
H11C	0.6735	0.0614	0.4456	0.066*	0.50
H11D	0.6447	−0.1086	0.4186	0.066*	0.50
C12'	0.6475 (5)	0.0143 (14)	0.2997 (8)	0.060 (3)	0.50
H12C	0.6470	0.1219	0.2840	0.072*	0.50
H12D	0.5991	−0.0341	0.2479	0.072*	0.50
C13'	0.7332 (5)	−0.0535 (14)	0.3013 (8)	0.065 (2)	0.50
H13C	0.7332	−0.1614	0.3161	0.078*	0.50
H13D	0.7383	−0.0435	0.2359	0.078*	0.50
C14'	0.8112 (5)	0.0193 (12)	0.3753 (8)	0.058 (2)	0.50
H14C	0.8126	−0.0073	0.4416	0.069*	0.50
H14D	0.8058	0.1291	0.3684	0.069*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.05137 (18)	0.04907 (17)	0.06456 (16)	−0.00278 (9)	0.02638 (13)	−0.00031 (10)
Br1	0.068 (3)	0.0608 (8)	0.076 (5)	−0.0161 (14)	0.043 (3)	−0.018 (3)
Br2	0.0542 (9)	0.047 (4)	0.061 (2)	0.011 (3)	0.0108 (12)	−0.007 (2)
Br3	0.047 (2)	0.055 (2)	0.0626 (8)	−0.0058 (11)	0.0074 (12)	0.0138 (13)
Br4	0.0685 (12)	0.0632 (19)	0.0745 (16)	0.0078 (13)	0.0418 (12)	0.0016 (11)
Cl1	0.068 (3)	0.0608 (8)	0.076 (5)	−0.0161 (14)	0.043 (3)	−0.018 (3)
Cl2	0.0542 (9)	0.047 (4)	0.061 (2)	0.011 (3)	0.0108 (12)	−0.007 (2)

Cl3	0.047 (2)	0.055 (2)	0.0626 (8)	−0.0058 (11)	0.0074 (12)	0.0138 (13)
Cl4	0.0685 (12)	0.0632 (19)	0.0745 (16)	0.0078 (13)	0.0418 (12)	0.0016 (11)
N1	0.034 (3)	0.041 (5)	0.047 (2)	−0.001 (2)	0.011 (2)	−0.004 (2)
C1	0.039 (5)	0.057 (4)	0.058 (4)	0.012 (4)	0.024 (3)	−0.008 (3)
C2	0.032 (6)	0.052 (5)	0.064 (3)	0.006 (4)	0.023 (5)	0.005 (4)
C3	0.040 (4)	0.047 (8)	0.050 (4)	0.006 (4)	0.019 (3)	−0.003 (5)
C4	0.035 (4)	0.062 (6)	0.058 (5)	0.005 (4)	0.036 (4)	−0.001 (4)
C5	0.027 (5)	0.057 (4)	0.061 (4)	0.003 (3)	0.028 (4)	0.012 (3)
N2	0.023 (3)	0.063 (7)	0.058 (6)	−0.016 (4)	0.003 (4)	−0.006 (4)
C6	0.056 (4)	0.074 (5)	0.079 (4)	0.006 (4)	0.019 (3)	0.020 (4)
C7	0.045 (4)	0.052 (4)	0.057 (6)	0.003 (3)	−0.002 (4)	−0.014 (4)
C8	0.037 (4)	0.076 (5)	0.057 (8)	−0.005 (4)	0.011 (4)	−0.018 (5)
C9	0.052 (4)	0.088 (6)	0.089 (4)	−0.001 (4)	0.033 (4)	0.020 (4)
C10	0.046 (4)	0.070 (7)	0.060 (6)	0.003 (5)	0.021 (4)	0.008 (5)
C11	0.039 (3)	0.059 (7)	0.063 (3)	0.004 (3)	0.011 (3)	−0.004 (4)
C12	0.043 (5)	0.070 (7)	0.066 (5)	−0.003 (5)	0.018 (4)	0.003 (5)
C13	0.057 (5)	0.072 (5)	0.069 (5)	0.002 (4)	0.025 (5)	−0.008 (4)
C14	0.044 (5)	0.064 (5)	0.064 (4)	−0.003 (4)	0.017 (4)	0.000 (4)
N1'	0.034 (3)	0.041 (5)	0.047 (2)	−0.001 (2)	0.011 (2)	−0.004 (2)
C1'	0.039 (5)	0.057 (4)	0.058 (4)	0.012 (4)	0.024 (3)	−0.008 (3)
C2'	0.032 (6)	0.052 (5)	0.064 (3)	0.006 (4)	0.023 (5)	0.005 (4)
C3'	0.040 (4)	0.047 (8)	0.050 (4)	0.006 (4)	0.019 (3)	−0.003 (5)
C4'	0.035 (4)	0.062 (6)	0.058 (5)	0.005 (4)	0.036 (4)	−0.001 (4)
C5'	0.027 (5)	0.057 (4)	0.061 (4)	0.003 (3)	0.028 (4)	0.012 (3)
N2'	0.023 (3)	0.063 (7)	0.058 (6)	−0.016 (4)	0.003 (4)	−0.006 (4)
C6'	0.056 (4)	0.074 (5)	0.079 (4)	0.006 (4)	0.019 (3)	0.020 (4)
C7'	0.045 (4)	0.052 (4)	0.057 (6)	0.003 (3)	−0.002 (4)	−0.014 (4)
C8'	0.037 (4)	0.076 (5)	0.057 (8)	−0.005 (4)	0.011 (4)	−0.018 (5)
C9'	0.052 (4)	0.088 (6)	0.089 (4)	−0.001 (4)	0.033 (4)	0.020 (4)
C10'	0.046 (4)	0.070 (7)	0.060 (6)	0.003 (5)	0.021 (4)	0.008 (5)
C11'	0.039 (3)	0.059 (7)	0.063 (3)	0.004 (3)	0.011 (3)	−0.004 (4)
C12'	0.043 (5)	0.070 (7)	0.066 (5)	−0.003 (5)	0.018 (4)	0.003 (5)
C13'	0.057 (5)	0.072 (5)	0.069 (5)	0.002 (4)	0.025 (5)	−0.008 (4)
C14'	0.044 (5)	0.064 (5)	0.064 (4)	−0.003 (4)	0.017 (4)	0.000 (4)

Geometric parameters (Å, °)

Hg1—Cl1	2.51 (2)	C13—H13A	0.97
Hg1—Br1	2.58 (4)	C13—H13B	0.97
Hg1—Cl2	2.529 (15)	C14—H14A	0.97
Hg1—Br2	2.49 (4)	C14—H14B	0.97
Hg1—Cl3	2.543 (5)	N1'—C1'	1.39
Hg1—Br3	2.46 (2)	N1'—C5'	1.39
Hg1—Cl4	2.545 (18)	N1'—C11'	1.491 (8)
Hg1—Br4	2.530 (5)	C1'—C2'	1.39
N1—C1	1.39	C1'—H1'	0.93
N1—C5	1.39	C2'—C3'	1.39
N1—C11	1.479 (8)	C2'—H2'	0.93
C1—C2	1.39	C3'—C4'	1.39

C1—H1	0.93	C3'—H3'	0.93
C2—C3	1.39	C4'—C5'	1.39
C2—H2	0.93	C4'—H4'	0.93
C3—C4	1.39	C5'—H5'	0.93
C3—H3	0.93	N2'—C6'	1.39
C4—C5	1.39	N2'—C10'	1.39
C4—H4	0.93	N2'—C14'	1.492 (8)
C5—H5	0.93	C6'—C7'	1.39
N2—C6	1.39	C6'—H6'	0.93
N2—C10	1.39	C7'—C8'	1.39
N2—C14	1.498 (8)	C7'—H7'	0.93
C6—C7	1.39	C8'—C9'	1.39
C6—H6	0.93	C8'—H8'	0.93
C7—C8	1.39	C9'—C10'	1.39
C7—H7	0.93	C9'—H9'	0.93
C8—C9	1.39	C10'—H10'	0.93
C8—H8	0.93	C11'—C12'	1.486 (9)
C9—C10	1.39	C11'—H11C	0.97
C9—H9	0.93	C11'—H11D	0.97
C10—H10	0.93	C12'—C13'	1.487 (8)
C11—C12	1.478 (9)	C12'—H12C	0.97
C11—H11A	0.97	C12'—H12D	0.97
C11—H11B	0.97	C13'—C14'	1.481 (8)
C12—C13	1.494 (8)	C13'—H13C	0.97
C12—H12A	0.97	C13'—H13D	0.97
C12—H12B	0.97	C14'—H14C	0.97
C13—C14	1.506 (8)	C14'—H14D	0.97
Cl2—Hg1—Br2	5.1 (9)	C13—C12—H12B	109.3
Cl2—Hg1—Cl3	102.4 (4)	H12A—C12—H12B	108.0
Br2—Hg1—Cl3	100.6 (11)	C12—C13—C14	112.8 (7)
Cl2—Hg1—Br3	96.3 (6)	C12—C13—H13A	109.0
Br2—Hg1—Br3	95.1 (12)	C14—C13—H13A	109.0
Cl3—Hg1—Br3	8.9 (4)	C12—C13—H13B	109.0
Cl2—Hg1—Cl4	112.2 (6)	C14—C13—H13B	109.0
Br2—Hg1—Cl4	109.4 (10)	H13A—C13—H13B	107.8
Cl3—Hg1—Cl4	118.0 (3)	N2—C14—C13	108.4 (6)
Br3—Hg1—Cl4	126.8 (5)	N2—C14—H14A	110.0
Cl2—Hg1—Br4	116.7 (3)	C13—C14—H14A	110.0
Br2—Hg1—Br4	113.4 (9)	N2—C14—H14B	110.0
Cl3—Hg1—Br4	111.18 (10)	C13—C14—H14B	110.0
Br3—Hg1—Br4	120.0 (4)	H14A—C14—H14B	108.4
Cl4—Hg1—Br4	7.0 (4)	C1'—N1'—C5'	120.0
Cl2—Hg1—Cl1	110.7 (7)	C1'—N1'—C11'	112.4 (16)
Br2—Hg1—Cl1	115.8 (9)	C5'—N1'—C11'	127.6 (16)
Cl3—Hg1—Cl1	109.2 (5)	C2'—C1'—N1'	120.0
Br3—Hg1—Cl1	106.0 (7)	C2'—C1'—H1'	120.0
Cl4—Hg1—Cl1	104.4 (6)	N1'—C1'—H1'	120.0
Br4—Hg1—Cl1	106.6 (5)	C1'—C2'—C3'	120.0
Cl2—Hg1—Br1	109.3 (9)	C1'—C2'—H2'	120.0

Br2—Hg1—Br1	114.4 (11)	C3'—C2'—H2'	120.0
Cl3—Hg1—Br1	104.8 (8)	C4'—C3'—C2'	120.0
Br3—Hg1—Br1	101.2 (9)	C4'—C3'—H3'	120.0
Cl4—Hg1—Br1	109.5 (8)	C2'—C3'—H3'	120.0
Br4—Hg1—Br1	111.5 (7)	C3'—C4'—C5'	120.0
Cl1—Hg1—Br1	5.4 (10)	C3'—C4'—H4'	120.0
C1—N1—C5	120.0	C5'—C4'—H4'	120.0
C1—N1—C11	128.6 (16)	C4'—C5'—N1'	120.0
C5—N1—C11	111.4 (16)	C4'—C5'—H5'	120.0
C2—C1—N1	120.0	N1'—C5'—H5'	120.0
C2—C1—H1	120.0	C6'—N2'—C10'	120.0
N1—C1—H1	120.0	C6'—N2'—C14'	121.5 (8)
C1—C2—C3	120.0	C10'—N2'—C14'	118.5 (8)
C1—C2—H2	120.0	N2'—C6'—C7'	120.0
C3—C2—H2	120.0	N2'—C6'—H6'	120.0
C4—C3—C2	120.0	C7'—C6'—H6'	120.0
C4—C3—H3	120.0	C8'—C7'—C6'	120.0
C2—C3—H3	120.0	C8'—C7'—H7'	120.0
C5—C4—C3	120.0	C6'—C7'—H7'	120.0
C5—C4—H4	120.0	C7'—C8'—C9'	120.0
C3—C4—H4	120.0	C7'—C8'—H8'	120.0
C4—C5—N1	120.0	C9'—C8'—H8'	120.0
C4—C5—H5	120.0	C10'—C9'—C8'	120.0
N1—C5—H5	120.0	C10'—C9'—H9'	120.0
C6—N2—C10	120.0	C8'—C9'—H9'	120.0
C6—N2—C14	121.1 (8)	C9'—C10'—N2'	120.0
C10—N2—C14	118.9 (8)	C9'—C10'—H10'	120.0
N2—C6—C7	120.0	N2'—C10'—H10'	120.0
N2—C6—H6	120.0	C12'—C11'—N1'	110.0 (7)
C7—C6—H6	120.0	C12'—C11'—H11C	109.7
C8—C7—C6	120.0	N1'—C11'—H11C	109.7
C8—C7—H7	120.0	C12'—C11'—H11D	109.7
C6—C7—H7	120.0	N1'—C11'—H11D	109.7
C9—C8—C7	120.0	H11C—C11'—H11D	108.2
C9—C8—H8	120.0	C11'—C12'—C13'	112.1 (8)
C7—C8—H8	120.0	C11'—C12'—H12C	109.2
C8—C9—C10	120.0	C13'—C12'—H12C	109.2
C8—C9—H9	120.0	C11'—C12'—H12D	109.2
C10—C9—H9	120.0	C13'—C12'—H12D	109.2
C9—C10—N2	120.0	H12C—C12'—H12D	107.9
C9—C10—H10	120.0	C14'—C13'—C12'	112.8 (7)
N2—C10—H10	120.0	C14'—C13'—H13C	109.0
C12—C11—N1	112.6 (8)	C12'—C13'—H13C	109.0
C12—C11—H11A	109.1	C14'—C13'—H13D	109.0
N1—C11—H11A	109.1	C12'—C13'—H13D	109.0
C12—C11—H11B	109.1	H13C—C13'—H13D	107.8
N1—C11—H11B	109.1	C13'—C14'—N2'	111.1 (6)
H11A—C11—H11B	107.8	C13'—C14'—H14C	109.4
C11—C12—C13	111.5 (8)	N2'—C14'—H14C	109.4

C11—C12—H12A	109.3	C13'—C14'—H14D	109.4
C13—C12—H12A	109.3	N2'—C14'—H14D	109.4
C11—C12—H12B	109.3	H14C—C14'—H14D	108.0
C11—N1—C1—C2	−179.6 (3)	C11'—N1'—C1'—C2'	−179.8 (2)
C11—N1—C5—C4	179.7 (2)	C11'—N1'—C5'—C4'	179.8 (3)
C14—N2—C6—C7	−179.4 (3)	C14'—N2'—C6'—C7'	−179.8 (3)
C14—N2—C10—C9	179.4 (3)	C14'—N2'—C10'—C9'	179.8 (3)
C1—N1—C11—C12	−74 (2)	C1'—N1'—C11'—C12'	−89 (2)
C5—N1—C11—C12	106 (2)	C5'—N1'—C11'—C12'	91 (2)
N1—C11—C12—C13	171.0 (16)	N1'—C11'—C12'—C13'	−168.6 (16)
C11—C12—C13—C14	86.6 (17)	C11'—C12'—C13'—C14'	−61.7 (19)
C6—N2—C14—C13	100.1 (10)	C12'—C13'—C14'—N2'	−169.3 (9)
C10—N2—C14—C13	−79.3 (10)	C6'—N2'—C14'—C13'	−93.4 (11)
C12—C13—C14—N2	176.8 (9)	C10'—N2'—C14'—C13'	86.8 (11)

Fig. 1