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

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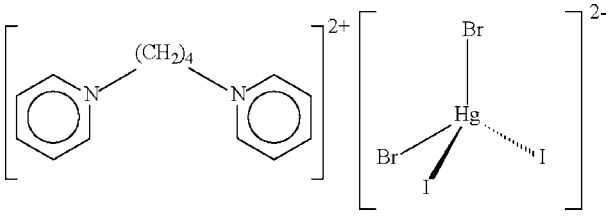
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.009 Å; disorder in main residue; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 18.8.

The Hg atom in the title compound, $(C_{14}H_{18}N_2)[HgBr_2I_2]$, is coordinated by four halogen atoms in a tetrahedral geometry. The four halogen atoms are disordered between I and Br, with the I:Br ratios being 0.824 (2):0.176 (2), 0.614 (2):0.386 (2), 0.325 (2):0.675 (2) and 0.237 (2):0.763 (2). The cation is disordered over two orientations and each was refined with an occupancy of 0.50.

Related literature

For the related butanedipyridinium bromidotrichloridomercurate, see: Niu *et al.* (2007).



Experimental

Crystal data

$(C_{14}H_{18}N_2)[HgBr_2I_2]$
M_r = 828.51
Orthorhombic, *Pbca*
a = 16.0181 (8) Å
b = 15.3290 (7) Å
c = 17.2550 (8) Å
V = 4236.8 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 13.95 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.059, T_{max} = 0.165
(expected range = 0.022–0.061)
31877 measured reflections
3722 independent reflections
2713 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.01
3722 reflections
198 parameters
226 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.03 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected bond lengths (Å).

Hg1—Br1	2.73 (2)	Hg1—I1	2.718 (2)
Hg1—Br2	2.70 (2)	Hg1—I2	2.777 (6)
Hg1—Br3	2.61 (4)	Hg1—I3	2.72 (5)
Hg1—Br4	2.646 (9)	Hg1—I4	2.75 (2)

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2389).

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supplementary materials

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

H.-D. Jia, Z.-J. Li, Y.-Y. Niu, X.-C. Liu and S. W. Ng

Comment

The preceding study reports the structure of 1,2-butanedipyridinium bromotrichloromercurate(II) (Niu *et al.*, 2007). Replacing the mercuric dichloride reactant by mercuric diiodide furnishes a similar tetrahalogenomercurate. The anion of the salt is composed two bromines and two chlorines that are disordered (Fig. 1); the metal atom shows tetrahedral coordination. Selected bond distances are given 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 diiodide (0.091 g, 0.2 mmol) in DMF (10 ml). The mixture was set aside for the formation of colorless crystals in 30% yield after several days.

Refinement

The four halogen atoms lie in general positions. Initial attempts to refine the structure with either four iodines or four bromines gave unacceptably high *R*-indices and large peaks/deep holes. The four halogen atoms were then refined as four (I+Br) mixtures; one attempt had the mixtures to have the same displacement parameters as well as sharing the same sites. A second attempt allowed the components having the same displacement parameters only. The second led to a formulation consisting of approximately two I and two Br atoms. The use of a restraint that fixed the number of I and Br atoms as exactly two I and two Br led to occupancies of 0.824 (2), 0.614 (2), 0.325 (2) and 0.237 (2), respectively, for I1, I2, I3 and I4, and 0.176 (2), 0.386 (2), 0.675 (2) and 0.763 (2), respectively, for Br1, Br2, Br3 and Br4.

The formulation is in fair agreement with CH&N elemental analysis, and furthermore, there were neither large peaks nor deep holes in the difference Fourier map; the final difference Fourier map had a large peak at 0.77 Å from Hg1. 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 pyridyl rings were refined as rigid hexagons (C—C = C—N = 1.39 Å). The C(sp^3)—C(sp^3) 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

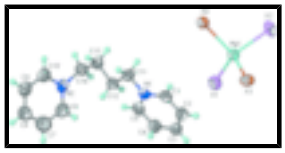

Fig. 1. The molecular structure of $[C_{14}H_{18}N_2][HgBr_2I_2]$. Displacement ellipsoids are drawn at the 50% probability level. The bromine and iodine atoms are disordered; the figure depicts the anion as an $[HgX_4]^{2-}$ species. Hydrogen atoms are drawn as spheres of arbitrary radius. Only one of the components of the disordered cation is shown.

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

Crystal data

$(C_{14}H_{18}N_2)[HgBr_2I_2]$	$F_{000} = 2976$
$M_r = 828.51$	$D_x = 2.598$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5589 reflections
$a = 16.0181$ (8) Å	$\theta = 2.4$–$22.3°$
$b = 15.3290$ (7) Å	$\mu = 13.95$ mm^{-1}
$c = 17.2550$ (8) Å	$T = 295$ (2) K
$V = 4236.8$ (3) Å^3	Block, colourless
$Z = 8$	0.20 × 0.20 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer	3722 independent reflections
Radiation source: fine-focus sealed tube	2713 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.054$
$T = 298$(2) K	$\theta_{max} = 25.0°$
φ and ω scans	$\theta_{min} = 2.2°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -19 \rightarrow 19$
$T_{min} = 0.059$, $T_{max} = 0.165$	$k = -18 \rightarrow 18$
31877 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 2.7056P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
3722 reflections	$\Delta\rho_{max} = 1.03$ e Å^{-3}
198 parameters	$\Delta\rho_{min} = -0.51$ e Å^{-3}

226 restraints

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Hg1	0.59858 (2)	0.751573 (19)	0.866623 (17)	0.05914 (13)	
I1	0.68911 (13)	0.67185 (13)	0.75380 (15)	0.0712 (4)	0.824 (2)
I2	0.5676 (4)	0.9215 (4)	0.8189 (3)	0.0717 (8)	0.614 (2)
I3	0.677 (4)	0.744 (4)	1.007 (3)	0.0732 (18)	0.325 (2)
I4	0.4457 (13)	0.6720 (11)	0.8836 (11)	0.0691 (8)	0.237 (2)
Br1	0.6735 (11)	0.6560 (12)	0.7524 (12)	0.0712 (4)	0.176 (2)
Br2	0.5830 (10)	0.9228 (10)	0.8330 (7)	0.0717 (8)	0.386 (2)
Br3	0.674 (3)	0.743 (3)	1.000 (2)	0.0732 (18)	0.675 (2)
Br4	0.4489 (6)	0.6863 (4)	0.8958 (5)	0.0691 (8)	0.763 (2)
N1	0.6643 (7)	0.4418 (11)	0.5603 (7)	0.0511 (19)	0.50
C1	0.7070 (9)	0.5169 (11)	0.5387 (7)	0.062 (3)	0.50
H1	0.6879	0.5504	0.4974	0.074*	0.50
C2	0.7784 (8)	0.5420 (10)	0.5788 (10)	0.065 (4)	0.50
H2	0.8070	0.5922	0.5643	0.078*	0.50
C3	0.8070 (8)	0.4919 (12)	0.6405 (9)	0.065 (3)	0.50
H3	0.8547	0.5087	0.6673	0.078*	0.50
C4	0.7643 (12)	0.4168 (12)	0.6621 (9)	0.071 (3)	0.50
H4	0.7835	0.3833	0.7034	0.085*	0.50
C5	0.6930 (11)	0.3918 (10)	0.6220 (9)	0.065 (3)	0.50
H5	0.6644	0.3415	0.6364	0.077*	0.50
N2	0.5665 (12)	0.1988 (7)	0.3523 (6)	0.064 (3)	0.50
C6	0.6475 (11)	0.1667 (10)	0.3470 (13)	0.082 (4)	0.50
H6	0.6907	0.2033	0.3317	0.098*	0.50
C7	0.6638 (9)	0.0798 (11)	0.3645 (15)	0.105 (4)	0.50
H7	0.7179	0.0583	0.3609	0.126*	0.50
C8	0.5991 (11)	0.0251 (7)	0.3874 (11)	0.088 (4)	0.50
H8	0.6100	−0.0330	0.3991	0.105*	0.50
C9	0.5182 (10)	0.0572 (9)	0.3927 (11)	0.084 (4)	0.50
H9	0.4749	0.0205	0.4080	0.101*	0.50
C10	0.5019 (9)	0.1440 (10)	0.3752 (10)	0.075 (3)	0.50
H10	0.4477	0.1655	0.3788	0.090*	0.50
C11	0.5890 (10)	0.4165 (18)	0.5171 (11)	0.059 (3)	0.50
H11A	0.5599	0.4687	0.5005	0.071*	0.50
H11B	0.5521	0.3844	0.5514	0.071*	0.50
C12	0.6080 (10)	0.361 (2)	0.4477 (13)	0.055 (3)	0.50
H12A	0.6348	0.3076	0.4638	0.066*	0.50
H12B	0.6456	0.3923	0.4133	0.066*	0.50
C13	0.5274 (9)	0.3414 (10)	0.4065 (8)	0.063 (4)	0.50
H13A	0.4909	0.3094	0.4412	0.076*	0.50
H13B	0.4999	0.3957	0.3931	0.076*	0.50
C14	0.5405 (11)	0.2897 (8)	0.3354 (7)	0.063 (4)	0.50
H14A	0.5829	0.3176	0.3039	0.075*	0.50

H14B	0.4891	0.2887	0.3057	0.075*	0.50
N1'	0.6530 (7)	0.4378 (11)	0.5467 (7)	0.0511 (19)	0.50
C1'	0.6846 (9)	0.5220 (10)	0.5408 (8)	0.062 (3)	0.50
H1'	0.6626	0.5605	0.5045	0.074*	0.50
C2'	0.7490 (8)	0.5488 (9)	0.5893 (10)	0.065 (4)	0.50
H2'	0.7701	0.6051	0.5854	0.078*	0.50
C3'	0.7818 (8)	0.4913 (12)	0.6437 (9)	0.065 (3)	0.50
H3'	0.8249	0.5092	0.6761	0.078*	0.50
C4'	0.7502 (12)	0.4071 (11)	0.6495 (9)	0.071 (3)	0.50
H4'	0.7722	0.3686	0.6859	0.085*	0.50
C5'	0.6859 (11)	0.3803 (9)	0.6010 (9)	0.065 (3)	0.50
H5'	0.6647	0.3240	0.6049	0.077*	0.50
N2'	0.5766 (12)	0.1750 (6)	0.3511 (6)	0.064 (3)	0.50
C6'	0.6585 (11)	0.1463 (10)	0.3439 (12)	0.082 (4)	0.50
H6'	0.6984	0.1821	0.3212	0.098*	0.50
C7'	0.6807 (9)	0.0640 (11)	0.3706 (15)	0.105 (4)	0.50
H7'	0.7355	0.0447	0.3658	0.126*	0.50
C8'	0.6210 (11)	0.0104 (8)	0.4046 (11)	0.088 (4)	0.50
H8'	0.6359	−0.0447	0.4225	0.105*	0.50
C9'	0.5391 (10)	0.0391 (9)	0.4118 (10)	0.084 (4)	0.50
H9'	0.4992	0.0033	0.4345	0.101*	0.50
C10'	0.5169 (9)	0.1215 (10)	0.3851 (10)	0.075 (3)	0.50
H10'	0.4620	0.1407	0.3899	0.090*	0.50
C11'	0.5849 (10)	0.4077 (18)	0.4962 (11)	0.059 (3)	0.50
H11C	0.5580	0.4580	0.4730	0.071*	0.50
H11D	0.5437	0.3776	0.5275	0.071*	0.50
C12'	0.6136 (11)	0.3480 (19)	0.4332 (13)	0.055 (3)	0.50
H12C	0.6360	0.2948	0.4553	0.066*	0.50
H12D	0.6572	0.3759	0.4031	0.066*	0.50
C13'	0.5401 (10)	0.3271 (9)	0.3818 (9)	0.063 (4)	0.50
H13C	0.4954	0.3030	0.4132	0.076*	0.50
H13D	0.5198	0.3804	0.3582	0.076*	0.50
C14'	0.5622 (11)	0.2640 (8)	0.3201 (7)	0.063 (4)	0.50
H14C	0.6122	0.2838	0.2939	0.075*	0.50
H14D	0.5174	0.2620	0.2823	0.075*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0614 (2)	0.0609 (2)	0.0551 (2)	0.00344 (15)	0.00333 (15)	−0.00355 (15)
I1	0.0754 (10)	0.0702 (10)	0.0680 (4)	−0.0013 (5)	0.0145 (7)	−0.0171 (6)
I2	0.104 (2)	0.0568 (4)	0.0548 (18)	0.0035 (12)	0.0093 (11)	−0.0019 (12)
I3	0.070 (2)	0.0910 (6)	0.058 (5)	0.0138 (12)	−0.011 (3)	−0.002 (3)
I4	0.0619 (9)	0.055 (2)	0.090 (3)	−0.0031 (15)	0.0052 (15)	−0.0088 (13)
Br1	0.0754 (10)	0.0702 (10)	0.0680 (4)	−0.0013 (5)	0.0145 (7)	−0.0171 (6)
Br2	0.104 (2)	0.0568 (4)	0.0548 (18)	0.0035 (12)	0.0093 (11)	−0.0019 (12)
Br3	0.070 (2)	0.0910 (6)	0.058 (5)	0.0138 (12)	−0.011 (3)	−0.002 (3)
Br4	0.0619 (9)	0.055 (2)	0.090 (3)	−0.0031 (15)	0.0052 (15)	−0.0088 (13)

N1	0.053 (4)	0.054 (3)	0.047 (4)	0.008 (3)	0.003 (3)	0.001 (3)
C1	0.059 (6)	0.055 (4)	0.072 (5)	0.007 (5)	0.004 (5)	0.004 (4)
C2	0.066 (7)	0.066 (5)	0.063 (5)	−0.005 (5)	0.015 (6)	−0.007 (4)
C3	0.059 (6)	0.071 (5)	0.064 (5)	0.003 (5)	0.002 (5)	−0.013 (4)
C4	0.080 (6)	0.070 (5)	0.063 (5)	0.004 (5)	−0.011 (5)	−0.001 (4)
C5	0.079 (5)	0.056 (5)	0.059 (7)	0.004 (4)	0.006 (5)	−0.002 (5)
N2	0.069 (5)	0.069 (6)	0.054 (4)	−0.015 (5)	−0.008 (4)	−0.004 (4)
C6	0.078 (6)	0.087 (7)	0.081 (5)	−0.013 (5)	0.011 (5)	−0.005 (5)
C7	0.103 (7)	0.106 (7)	0.106 (6)	0.008 (5)	0.007 (5)	−0.010 (5)
C8	0.097 (7)	0.078 (6)	0.088 (7)	0.002 (5)	−0.016 (6)	0.000 (5)
C9	0.087 (7)	0.080 (6)	0.086 (7)	−0.013 (5)	−0.010 (5)	0.004 (5)
C10	0.068 (6)	0.074 (6)	0.082 (6)	−0.005 (5)	−0.002 (5)	−0.001 (5)
C11	0.052 (4)	0.067 (5)	0.058 (7)	0.001 (4)	0.002 (4)	−0.003 (5)
C12	0.054 (4)	0.055 (6)	0.055 (6)	0.001 (4)	0.003 (4)	0.001 (4)
C13	0.064 (5)	0.062 (5)	0.064 (7)	−0.002 (4)	−0.001 (5)	−0.003 (5)
C14	0.064 (6)	0.065 (6)	0.058 (5)	0.009 (5)	−0.011 (5)	0.001 (5)
N1'	0.053 (4)	0.054 (3)	0.047 (4)	0.008 (3)	0.003 (3)	0.001 (3)
C1'	0.059 (6)	0.055 (4)	0.072 (5)	0.007 (5)	0.004 (5)	0.004 (4)
C2'	0.066 (7)	0.066 (5)	0.063 (5)	−0.005 (5)	0.015 (6)	−0.007 (4)
C3'	0.059 (6)	0.071 (5)	0.064 (5)	0.003 (5)	0.002 (5)	−0.013 (4)
C4'	0.080 (6)	0.070 (5)	0.063 (5)	0.004 (5)	−0.011 (5)	−0.001 (4)
C5'	0.079 (5)	0.056 (5)	0.059 (7)	0.004 (4)	0.006 (5)	−0.002 (5)
N2'	0.069 (5)	0.069 (6)	0.054 (4)	−0.015 (5)	−0.008 (4)	−0.004 (4)
C6'	0.078 (6)	0.087 (7)	0.081 (5)	−0.013 (5)	0.011 (5)	−0.005 (5)
C7'	0.103 (7)	0.106 (7)	0.106 (6)	0.008 (5)	0.007 (5)	−0.010 (5)
C8'	0.097 (7)	0.078 (6)	0.088 (7)	0.002 (5)	−0.016 (6)	0.000 (5)
C9'	0.087 (7)	0.080 (6)	0.086 (7)	−0.013 (5)	−0.010 (5)	0.004 (5)
C10'	0.068 (6)	0.074 (6)	0.082 (6)	−0.005 (5)	−0.002 (5)	−0.001 (5)
C11'	0.052 (4)	0.067 (5)	0.058 (7)	0.001 (4)	0.002 (4)	−0.003 (5)
C12'	0.054 (4)	0.055 (6)	0.055 (6)	0.001 (4)	0.003 (4)	0.001 (4)
C13'	0.064 (5)	0.062 (5)	0.064 (7)	−0.002 (4)	−0.001 (5)	−0.003 (5)
C14'	0.064 (6)	0.065 (6)	0.058 (5)	0.009 (5)	−0.011 (5)	0.001 (5)

Geometric parameters (Å, °)

Hg1—Br1	2.73 (2)	C13—H13A	0.97
Hg1—Br2	2.70 (2)	C13—H13B	0.97
Hg1—Br3	2.61 (4)	C14—H14A	0.97
Hg1—Br4	2.646 (9)	C14—H14B	0.97
Hg1—I1	2.718 (2)	N1'—C1'	1.39
Hg1—I2	2.777 (6)	N1'—C5'	1.39
Hg1—I3	2.72 (5)	N1'—C11'	1.470 (8)
Hg1—I4	2.75 (2)	C1'—C2'	1.39
N1—C1	1.39	C1'—H1'	0.93
N1—C5	1.39	C2'—C3'	1.39
N1—C11	1.470 (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'	1.483 (9)
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	1.484 (9)	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'	1.493 (9)
C9—C10	1.39	C11'—H11C	0.97
C9—H9	0.93	C11'—H11D	0.97
C10—H10	0.93	C12'—C13'	1.509 (9)
C11—C12	1.496 (9)	C12'—H12C	0.97
C11—H11A	0.97	C12'—H12D	0.97
C11—H11B	0.97	C13'—C14'	1.481 (8)
C12—C13	1.506 (9)	C13'—H13C	0.97
C12—H12A	0.97	C13'—H13D	0.97
C12—H12B	0.97	C14'—H14C	0.97
C13—C14	1.475 (8)	C14'—H14D	0.97
Br3—Hg1—I3	0(2)	C13—C12—H12B	110.0
Br3—Hg1—Br4	103.6 (10)	H12A—C12—H12B	108.3
I3—Hg1—Br4	103.4 (13)	C14—C13—C12	112.4 (8)
Br3—Hg1—I4	107.4 (11)	C14—C13—H13A	109.1
I3—Hg1—I4	107.2 (14)	C12—C13—H13A	109.1
Br4—Hg1—I4	6.2 (4)	C14—C13—H13B	109.1
Br3—Hg1—I1	111.3 (10)	C12—C13—H13B	109.1
I3—Hg1—I1	111.6 (13)	H13A—C13—H13B	107.9
Br4—Hg1—I1	116.73 (12)	C13—C14—N2	112.4 (8)
I4—Hg1—I1	110.6 (3)	C13—C14—H14A	109.1
Br3—Hg1—Br1	114.1 (11)	N2—C14—H14A	109.1
I3—Hg1—Br1	114.4 (13)	C13—C14—H14B	109.1
Br4—Hg1—Br1	109.4 (3)	N2—C14—H14B	109.1
I4—Hg1—Br1	103.3 (4)	H14A—C14—H14B	107.9
I1—Hg1—Br1	7.4 (3)	C1'—N1'—C5'	120.0
Br3—Hg1—I2	112.9 (9)	C1'—N1'—C11'	121.2 (15)
I3—Hg1—I2	112.8 (12)	C5'—N1'—C11'	118.8 (15)
Br4—Hg1—I2	104.5 (2)	N1'—C1'—C2'	120.0
I4—Hg1—I2	106.8 (4)	N1'—C1'—H1'	120.0
I1—Hg1—I2	107.74 (13)	C2'—C1'—H1'	120.0
Br1—Hg1—I2	111.6 (4)	C3'—C2'—C1'	120.0
Br3—Hg1—Br2	106.2 (10)	C3'—C2'—H2'	120.0
I3—Hg1—Br2	106.1 (12)	C1'—C2'—H2'	120.0
Br4—Hg1—Br2	108.9 (4)	C4'—C3'—C2'	120.0

I4—Hg1—Br2	111.8 (5)	C4'—C3'—H3'	120.0
I1—Hg1—Br2	109.4 (3)	C2'—C3'—H3'	120.0
Br1—Hg1—Br2	114.0 (5)	C3'—C4'—C5'	120.0
I2—Hg1—Br2	7.1 (3)	C3'—C4'—H4'	120.0
C1—N1—C5	120.0	C5'—C4'—H4'	120.0
C1—N1—C11	119.1 (16)	C4'—C5'—N1'	120.0
C5—N1—C11	120.9 (16)	C4'—C5'—H5'	120.0
N1—C1—C2	120.0	N1'—C5'—H5'	120.0
N1—C1—H1	120.0	C6'—N2'—C10'	120.0
C2—C1—H1	120.0	C6'—N2'—C14'	114.0 (13)
C3—C2—C1	120.0	C10'—N2'—C14'	126.0 (13)
C3—C2—H2	120.0	N2'—C6'—C7'	120.0
C1—C2—H2	120.0	N2'—C6'—H6'	120.0
C2—C3—C4	120.0	C7'—C6'—H6'	120.0
C2—C3—H3	120.0	C8'—C7'—C6'	120.0
C4—C3—H3	120.0	C8'—C7'—H7'	120.0
C3—C4—C5	120.0	C6'—C7'—H7'	120.0
C3—C4—H4	120.0	C7'—C8'—C9'	120.0
C5—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	125.6 (14)	C9'—C10'—N2'	120.0
C10—N2—C14	114.4 (14)	C9'—C10'—H10'	120.0
N2—C6—C7	120.0	N2'—C10'—H10'	120.0
N2—C6—H6	120.0	N1'—C11'—C12'	113.3 (8)
C7—C6—H6	120.0	N1'—C11'—H11C	108.9
C6—C7—C8	120.0	C12'—C11'—H11C	108.9
C6—C7—H7	120.0	N1'—C11'—H11D	108.9
C8—C7—H7	120.0	C12'—C11'—H11D	108.9
C9—C8—C7	120.0	H11C—C11'—H11D	107.7
C9—C8—H8	120.0	C11'—C12'—C13'	108.6 (8)
C7—C8—H8	120.0	C11'—C12'—H12C	110.0
C8—C9—C10	120.0	C13'—C12'—H12C	110.0
C8—C9—H9	120.0	C11'—C12'—H12D	110.0
C10—C9—H9	120.0	C13'—C12'—H12D	110.0
C9—C10—N2	120.0	H12C—C12'—H12D	108.4
C9—C10—H10	120.0	C14'—C13'—C12'	112.0 (8)
N2—C10—H10	120.0	C14'—C13'—H13C	109.2
N1—C11—C12	112.8 (7)	C12'—C13'—H13C	109.2
N1—C11—H11A	109.0	C14'—C13'—H13D	109.2
C12—C11—H11A	109.0	C12'—C13'—H13D	109.2
N1—C11—H11B	109.0	H13C—C13'—H13D	107.9
C12—C11—H11B	109.0	C13'—C14'—N2'	112.3 (8)
H11A—C11—H11B	107.8	C13'—C14'—H14C	109.2
C11—C12—C13	108.6 (8)	N2'—C14'—H14C	109.2
C11—C12—H12A	110.0	C13'—C14'—H14D	109.2
C13—C12—H12A	110.0	N2'—C14'—H14D	109.2

C11—C12—H12B	110.0	H14C—C14'—H14D	107.9
C11—N1—C1—C2	180.0 (3)	C11'—N1'—C1'—C2'	180.0 (3)
C11—N1—C5—C4	180.0 (3)	C11'—N1'—C5'—C4'	−180.0 (3)
C14—N2—C6—C7	180.0 (3)	C14'—N2'—C6'—C7'	180.0 (2)
C14—N2—C10—C9	−180.0 (2)	C14'—N2'—C10'—C9'	−180.0 (3)
C1—N1—C11—C12	87 (2)	C1'—N1'—C11'—C12'	105 (2)
C5—N1—C11—C12	−93 (2)	C5'—N1'—C11'—C12'	−75 (2)
N1—C11—C12—C13	−178 (2)	N1'—C11'—C12'—C13'	−176 (2)
C11—C12—C13—C14	178 (2)	C11'—C12'—C13'—C14'	−177 (2)
C12—C13—C14—N2	70 (2)	C12'—C13'—C14'—N2'	71 (2)
C6—N2—C14—C13	−102.0 (14)	C6'—N2'—C14'—C13'	−113.9 (13)
C10—N2—C14—C13	78.0 (14)	C10'—N2'—C14'—C13'	66.0 (13)

Fig. 1