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(2,2′-Bipyridine *N*,*N*′-dioxide-κ^2O,O')dibromomercury(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.018 Å
R factor = 0.042
wR factor = 0.113
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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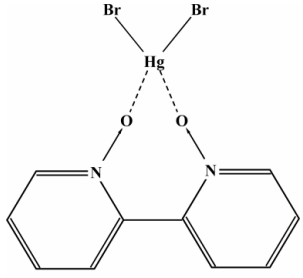
The title compound, $[HgBr_2(C_{10}H_8N_2O_2)]$, has an Hg atom surrounded by two Br atoms and two O atoms from a chelating $BipyO_2$ ligand ($BipyO_2$ is 2,2′-bipyridine *N*,*N*′-dioxide), forming a severely distorted tetrahedron. In addition, two weak Hg···Br bonds link these complexes into a chain.

Comment

The bidentate ligand 2,2′-bipyridine *N*,*N*′-dioxide ($BipyO_2$) is known to form coordination compounds with mercury halide salts (Ahuja & Singh 1973). In that study, structural information was derived exclusively from IR spectroscopy. UV spectra were not studied, due to a lack of *d*–*d* transitions in Hg^{II}. The structure contains seven-membered rings, since both O atoms of $BipyO_2$ are coordinated to the same metal ion (Vinciguerra *et al.*, 1963; Madan & Bull, 1964). We present here the single-crystal X-ray structure determination of the title mercury(II) bromide $BipyO_2$ complex, $[HgBr_2(BipyO_2)]$, (I).



(I)

The Hg atom in (I) is four-coordinated, by two Br atoms and two O atoms from the chelating $BipyO_2$ ligand (Fig. 1). The geometry around the Hg center is distorted from tetrahedral (Table 1), while the average Hg—Br bond length is 2.443 (1) Å and Hg—O is 2.451 (7) Å.

There are also weak intermolecular bonds, Hg···Br2 3.523 (1) and Hg···Br1 3.587 (2) Å, which link the complexes into a chain along the *b* axis (Fig. 2). The chains pack into layers parallel to the $(\bar{1}01)$ plane. The Hg···Hg distance along the chain is 4.498 (2) Å. Our results are consistent with the previous IR characterization (Ahuja & Singh 1973).

Experimental

To obtain the title compound, (I), 2,2′-bipyridyl was oxidized to $BipyO_2$ following the procedure described by Simpson *et al.* (1963). The method described by Ahuja & Singh (1973) was then followed to yield the corresponding colorless plate-like crystals. These were dried

in air at room temperature. As a precaution, since mercury salts are known to sublime as poisonous fumes, these experiments need to be performed in a chemical fume hood.

Crystal data

$[HgBr_2(C_{10}H_8N_2O_2)]$	D_x = 2.816 Mg m^{-3}
M_r = 548.59	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2815 reflections
a = 9.826 (3) Å	θ = 2.3–23.1°
b = 8.235 (2) Å	μ = 18.06 mm^{-1}
c = 16.073 (5) Å	T = 295 (2) K
β = 95.857 (5)°	Plate, colorless
V = 1293.8 (7) Å^3	0.22 × 0.10 × 0.04 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2292 independent reflections
	1618 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.068
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
	$h = -11 \rightarrow 11$
T_{min} = 0.138, T_{max} = 0.531	$k = -9 \rightarrow 9$
10 469 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.042	$w = 1/[\sigma^2(F_o^2) + (0.001P)^2 + 2.15P]$ where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$wR(F^2)$ = 0.113	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.72 e Å^{-3}
2292 reflections	$\Delta\rho_{min}$ = −0.93 e Å^{-3}
154 parameters	

Table 1
Selected geometric parameters (Å, °).

Hg1—O2	2.442 (7)	Hg1—O1	2.460 (7)
Hg1—Br2	2.4432 (14)	Hg1···Br2^{i}	3.5226 (14)
Hg1—Br1	2.4433 (13)	Hg1···Br1^{ii}	3.5871 (15)
O2—Hg1—Br2	97.17 (17)	O2—Hg1—O1	72.0 (2)
O2—Hg1—Br1	101.08 (17)	Br2—Hg1—O1	105.28 (17)
Br2—Hg1—Br1	157.72 (5)	Br1—Hg1—O1	92.52 (16)
N1—C5—C6—N2	−63.9 (11)		

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x, -y+1, -z$.

H atoms were treated as riding, with C—H distances of 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C)..

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Materials Studio* (Accelrys, 2001) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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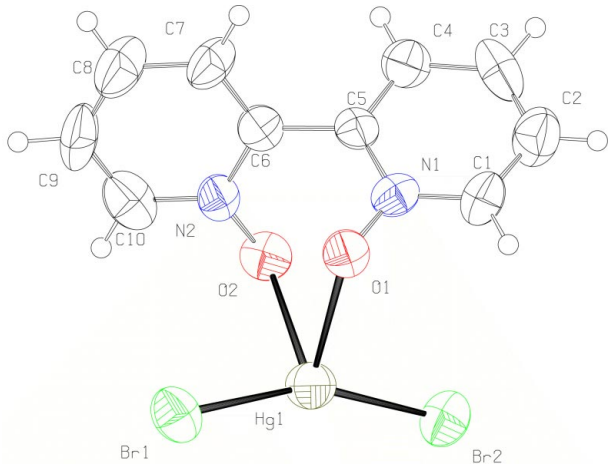

Figure 1
A view of (I), showing the numbering scheme employed. Displacement ellipsoids are drawn at the 50% probability level. H atoms are displayed with arbitrarily small radii.

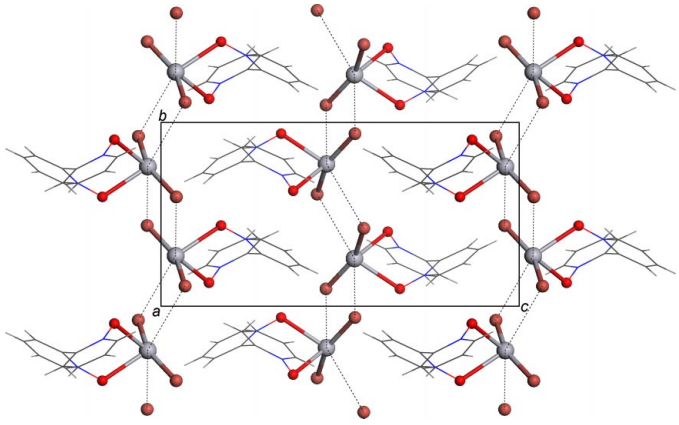

Figure 2
A view of the molecular packing of (I). Thin dashed lines show weak Hg···Br bonds.

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