

Onyango M. Tedmann,<sup>a</sup> Peter Y. Zavalij,<sup>b\*</sup> Stanley K. Madan<sup>a</sup> and Scott R.J. Oliver<sup>c</sup><sup>a</sup>Department of Chemistry, Binghamton University, Vestal Parkway East, Binghamton, NY 13902-6000, USA, <sup>b</sup>Institute for Materials Research and Department of Chemistry, Binghamton University, Vestal Parkway East, Binghamton, NY 13902-6000, USA, and <sup>c</sup>Department of Chemistry and Biochemistry, University of California at Santa Cruz, 1156 High Street, Santa Cruz, CA 95064, USACorrespondence e-mail:  
zavalij@binghamton.edu

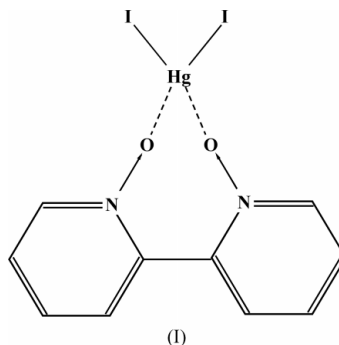
## Key indicators

Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.020$  Å  
 $R$  factor = 0.054  
 $wR$  factor = 0.069  
Data-to-parameter ratio = 15.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.(2,2'-Bipyridine  $N,N'$ -dioxide- $\kappa^2O,O'$ )diiodo-mercury(II)

The title compound,  $[\text{HgI}_2(\text{C}_{10}\text{H}_8\text{N}_2\text{O}_2)]$ , is a further example of a mercury halide complex of the chelating BipyO<sub>2</sub> ligand (BipyO<sub>2</sub> is 2,2'-bipyridine  $N,N'$ -dioxide). As observed for similar compounds, the coordination polyhedron of the Hg atom is a severely distorted tetrahedron, in which Hg is coordinated by two I atoms and two O atoms of the ligand.

## Comment

Recently, we reported the crystal structures of 2,2'-bipyridine  $N,N'$ -dioxide (BipyO<sub>2</sub>) complexes of mercury dichloride,  $[\text{HgCl}_2(\text{BipyO}_2)]$  (Tedmann *et al.*, 2004), and mercury dibromide,  $[\text{HgBr}_2(\text{BipyO}_2)]$  (Tedmann *et al.*, 2005). In a continuing program of study of such mercury halide complexes of this bidentate ligand, we have now synthesized the title iodide complex,  $[\text{HgI}_2(\text{BipyO}_2)]$ , (I), using the same synthetic route. Unlike the other mercury halide complexes of BipyO<sub>2</sub>, this is the first time, to our knowledge, that the iodide complex has been synthesized. We report its crystal structure here.

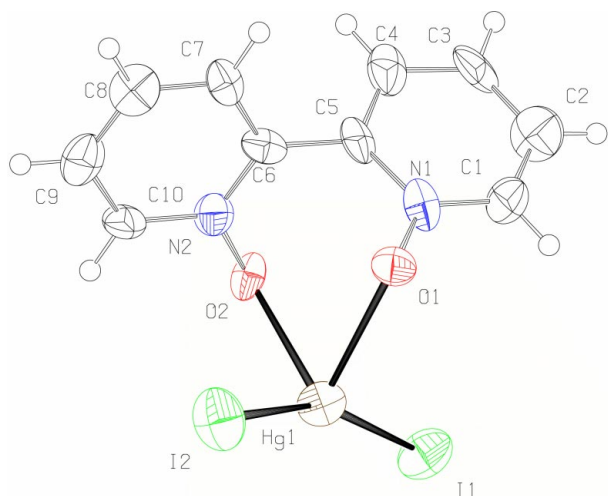


Previous IR characterization of the other mercury halide complexes indicated a pseudo-tetrahedral Hg environment (Ahuja & Singh, 1973). This finding was ascribed to the fact that the frequencies of metal-halogen stretching modes in coordination compounds are halogen-dependent (Coates & Ridley, 1964; Deacon & Green, 1966; Deacon *et al.*, 1968).

In the structure of (I), two I atoms and two O atoms from the chelating BipyO<sub>2</sub> ligand form the coordination polyhedron of each Hg atom, which can be described as a highly distorted tetrahedron (Fig. 1). Similar deformation was found in the mercury dichloride and dibromide complexes (Tedmann *et al.* 2004, 2005). The distortion is illustrated by the angles in the complex (Table 1). The dihedral angle between the two ligand rings is 62.0 (2)°. The intermolecular dative bond distance between the O and N atoms of BipyO<sub>2</sub> is 2.945 (6) Å.

The mean intramolecular Hg—I bond length is 2.598 (1) Å. There is also a weak intermolecular contact, Hg1...I1

Received 10 December 2004  
Accepted 20 December 2004  
Online 8 January 2005



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

4.263 (2) Å, which links  $\text{HgI}_2\text{-BipyO}_2$  molecules into a chain, shown in Fig. 2. Selected bond lengths and angles of (I) are listed in Table 1.

## Experimental

Following the procedure described by Simpson *et al.* (1963), 2,2'-bipyridine was first oxidized to tris-2,2'-bipyridine-1,1'-dioxide. Needle-like colorless crystals of (I) were then obtained using the method of Ahuja & Singh (1973). The crystals were dried at room temperature in air. As a precaution, due to the poisonous nature of the fumes emitted by mercury salts during reactions, this experiment should only be carried out in a fume hood.

### Crystal data

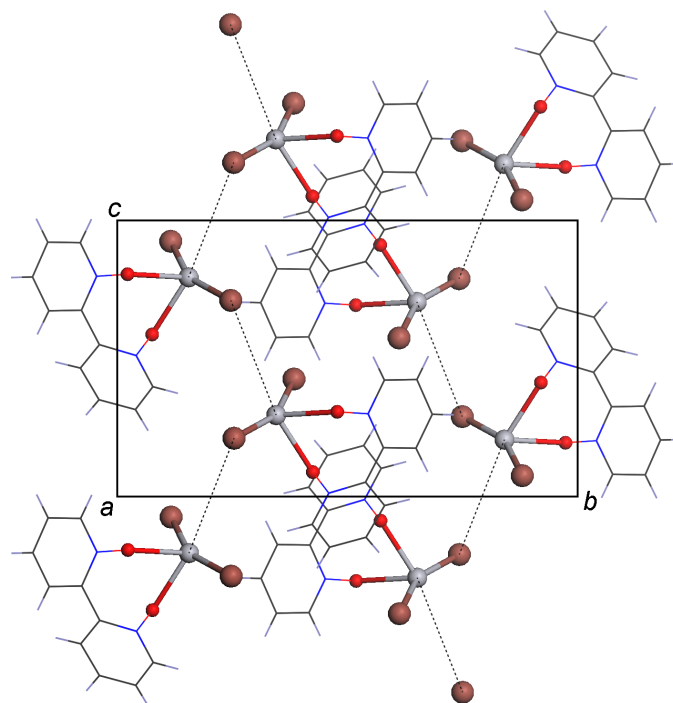
$[\text{HgI}_2(\text{C}_{10}\text{H}_8\text{N}_2\text{O}_2)]$	$D_x = 3.043 \text{ Mg m}^{-3}$
$M_r = 642.57$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2443 reflections
$a = 9.433$ (4) Å	$\theta = 2.3\text{--}22.4^\circ$
$b = 15.690$ (7) Å	$\theta_{\text{max}} = 25.0^\circ$
$c = 10.024$ (5) Å	$\mu = 15.37 \text{ mm}^{-1}$
$\beta = 108.998$ (6)°	$T = 296$ (2) K
$V = 1402.8$ (11) Å <sup>3</sup>	Needle, colorless
$Z = 4$	$0.25 \times 0.04 \times 0.02 \text{ mm}$

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	2413 independent reflections
$\omega$ scans	1448 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.099$
$T_{\text{min}} = 0.334$ , $T_{\text{max}} = 0.794$	$\theta_{\text{max}} = 25.0^\circ$
8603 measured reflections	$h = -11 \rightarrow 11$
	$k = -18 \rightarrow 18$
	$l = -11 \rightarrow 11$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0001P)^2]$
$wR(F^2) = 0.069$	where $P = [\max(F_o^2, 0) + 2F_c^2]/3$
$S = 0.86$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2413 reflections	$\Delta\rho_{\text{max}} = 0.83 \text{ e \AA}^{-3}$
154 parameters	$\Delta\rho_{\text{min}} = -0.94 \text{ e \AA}^{-3}$



**Figure 2**  
A view of the molecular packing of (I). Thin dashed lines show weak  $\text{Hg}\cdots\text{I}$  bonds.

**Table 1**

Selected geometric parameters (Å, °).

Hg1—O1	2.426 (8)	Hg1—I1	2.5992 (14)
Hg1—O2	2.465 (8)	Hg1 $\cdots$ I1 <sup>i</sup>	4.263 (2)
Hg1—I2	2.5963 (15)		
O1—Hg1—O2	74.9 (3)	O1—Hg1—I1	104.8 (2)
O1—Hg1—I2	91.7 (2)	O2—Hg1—I1	94.92 (19)
O2—Hg1—I2	102.66 (19)	I2—Hg1—I1	158.54 (4)
C4—C5—C6—C7	−62 (2)		

Symmetry codes: (i)  $x, -y + \frac{3}{2}, z - \frac{1}{2}$ .

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

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); 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.

This work was supported by an NSF CAREER Award (DMR-0239607).

## References

- Accelrys (2001). *Materials Studio*. Accelrys Inc., San Diego, California, USA.
- Ahuja, I. S. & Singh, R. (1973). *Indian J. Chem.* **11**, 1070–1071.
- Bruker (1999). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Coates, G. E. & Ridley, D. J. (1964). *J. Chem. Soc.* pp. 166–168.
- Deacon, G. B. & Green, J. H. S. (1966). *J. Chem. Soc. Chem. Commun.* pp. 629–631.
- Deacon, G. B., Green, J. H. S. & Harrison, D. J. (1968). *Spectrochim. Acta A*, **24**, 1921–1922.

- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Simpson, P. G., Vinciguerra, A. & Quagliano J. V. (1963). *Inorg. Chem.* **2**, 282–284.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Tedmann, O. M., Zavalij, P. Y., Madan, S. K. & Oliver, S. R. J. (2004). *Acta Cryst.* **E60**, m1706–m1707.
- Tedmann, O. M., Zavalij, P. Y., Madan, S. K. & Oliver, S. R. J. (2005). *Acta Cryst.* **E61**, m212–m213.