

# Crystal structure of *catena*-poly[[diiodido-mercury(II)]- $\mu$ -2,2'-dithiobis(pyridine *N*-oxide)- $\kappa^2$ O:O']<sup>1</sup>

Rüdiger W. Seidel<sup>a\*</sup> and Iris M. Oppel<sup>b</sup><sup>a</sup>Lehrstuhl für Analytische Chemie, Ruhr-Universität Bochum, Universitätsstrasse 150, 44780 Bochum, Germany, and<sup>b</sup>Institut für Anorganische Chemie, Rheinisch-Westfälische Technische Hochschule Aachen, Landoltweg 1, 52074 Aachen, Germany. \*Correspondence e-mail: Ruediger.Seidel@rub.de

Received 16 February 2018

Accepted 22 February 2018

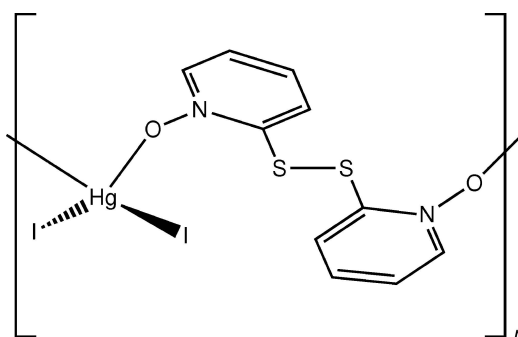
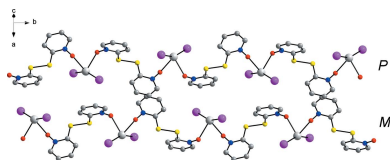
Edited by H. Ishida, Okayama University, Japan

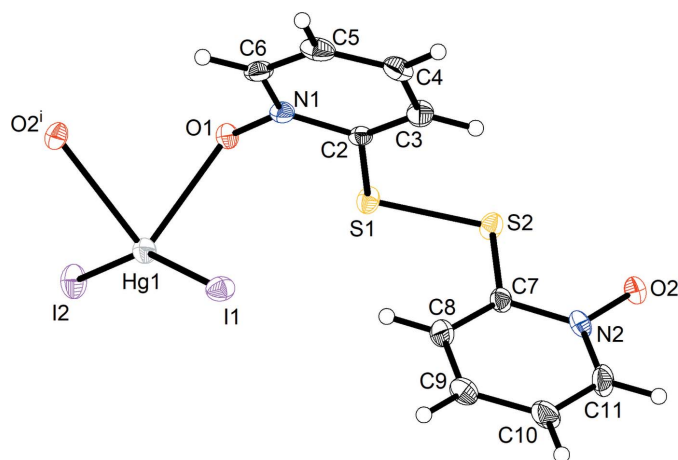
<sup>1</sup> Dedicated to Professor Peter Imming on the occasion of his 60th birthday.**Keywords:** crystal structure; one-dimensional coordination polymer; 2,2'-dithiobis(pyridine *N*-oxide); Hg<sup>II</sup> complex; disulfide compound.**CCDC reference:** 1825194**Supporting information:** this article has supporting information at journals.iucr.org/e

The title compound, [HgI<sub>2</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>)]<sub>n</sub>, a one-dimensional coordination polymer with HgI<sub>2</sub> units and 2,2'-dithiobis(pyridine *N*-oxide) spacer ligands in an alternating fashion, forms helical chains running along the *b* axis in the crystal. Within a single coordination polymer strand, the axially chiral 2,2'-dithiobis(pyridine *N*-oxide) ligands are homochiral, but the enantiomeric conformation is present in adjacent strands. Within a coordination polymer strand, the iodido ligands point towards the centroids of the aromatic rings of the pyridine *N*-oxide moieties in the coordination sphere of Hg<sup>II</sup>. Moreover, intra-strand C—H···O and C—H···I interactions, and inter-strand short S···I and S···O contacts are observed.

## 1. Chemical context

Research into one-dimensional coordination polymers has been an active field of research, not only due to the usually easy and straightforward synthesis, but also due to interesting structural features and introduction of these compounds as new materials such as coordination polymeric gels, fibres and nanostructures (Leong & Vittal, 2011). In the context of our structural studies on coordination polymers and discrete metallocsupramolecular assemblies containing disulfide-based bridging (spacer) ligands (Seidel *et al.*, 2013), 2,2'-dithiobis(pyridine *N*-oxide) has attracted our interest. Recently, we reported one-dimensional coordination polymers from 2,2'-dithiobis(pyridine *N*-oxide), and Zn<sup>II</sup> and Cd<sup>II</sup> halides (Seidel *et al.*, 2017), which represented the first structurally characterised coordination polymers containing 2,2'-dithiobis(pyridine *N*-oxide) as a spacer ligand (*i.e.* involving both pyridine *N*-oxide moieties as coordinating groups). As a continuation of this work, we herein report the crystal structure of a one-dimensional coordination polymer formed from 2,2'-dithiobis(pyridine *N*-oxide) and HgI<sub>2</sub>.





**Figure 1**  
Displacement ellipsoid plot (50% probability level) of the title compound, showing the repeat unit of the coordination polymer and the coordination sphere of  $\text{Hg}^{\text{II}}$ . H atoms are represented by small spheres of arbitrary radii. [Symmetry code: (i)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ].

## 2. Structural commentary

The title compound, (I), is a one-dimensional coordination polymer consisting of  $\text{HgI}_2$  units joined by 2,2'-dithiobis(pyridine *N*-oxide) as bridging ligands in a  $\mu\text{-}\kappa^2\text{O}:\text{O}'$  coordination mode. Fig. 1 depicts the repeat unit of the coordination polymer and the coordination sphere of the  $\text{Hg}^{\text{II}}$  ion. The  $\text{Hg}^{\text{II}}$  ion is tetracoordinated by two iodide ligands and two O atoms of the bridging ligands, with a coordination sphere that is best described as a severely distorted tetrahedron or a seesaw form (Yang *et al.*, 2007). The C2–S1–S2–C7 torsion angle is  $77.2(2)^\circ$ , which corresponds to the *P* form of the axially chiral *gauche* conformation of the disulfide-based ligand in the chosen asymmetric unit. The dihedral angle between the planes of the aromatic N1/C2–C6 and N2/C7–C11 rings is  $71.8(2)^\circ$ .

The strand of the coordination polymer propagates along a  $2_1$ -screw axis parallel to the *b* axis (Fig. 2). Within a single strand, 2,2'-dithiobis(pyridine *N*-oxide) exhibits exclusively either the right-handed *P* or the left-handed *M* conformation,

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

<i>D</i> –H $\cdots$ <i>A</i>	<i>D</i> –H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> –H $\cdots$ <i>A</i>
C3–H3 $\cdots$ I2 <sup>i</sup>	0.95	3.00	3.776 (6)	140
C11–H11 $\cdots$ O1 <sup>i</sup>	0.95	2.59	3.268 (7)	129

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

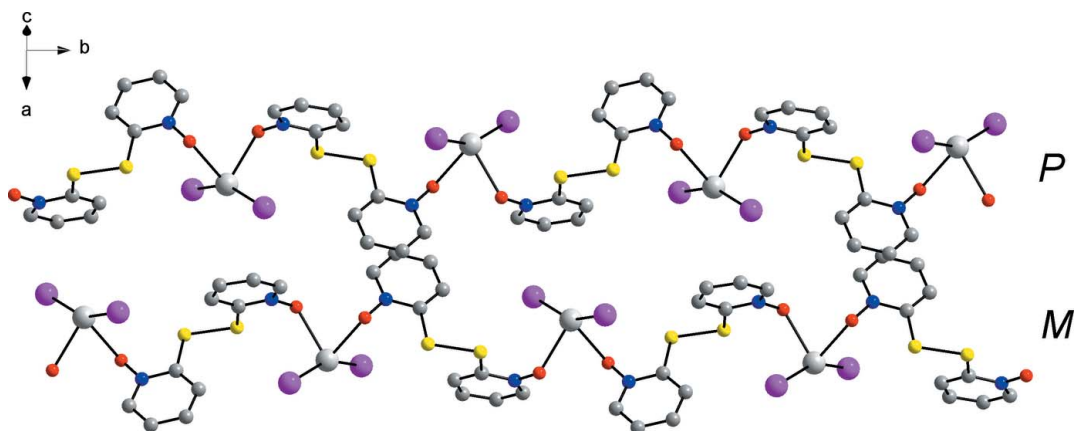
*i.e.* the bridging ligands in each coordination polymer chain are homochiral. The centrosymmetric crystal structure (space group  $P2_1/n$ ) features, however, both enantiomeric conformations in adjacent strands, as shown in Fig. 2.

## 3. Supramolecular features

In a single strand, the iodide ligands point towards the centroids of the aromatic rings of the pyridine *N*-oxide moieties in the coordination sphere of  $\text{Hg}^{\text{II}}$ , but  $\text{I}\cdots\pi$  interactions are not observed. The  $\text{I}\cdots\text{Cg}$  distances are long [ $\text{I1}\cdots\text{Cg1} = 3.940(2) \text{\AA}$  and  $\text{I2}\cdots\text{Cg2}^{\text{ii}} = 4.205(2) \text{\AA}$ ] and the  $\text{Hg}\text{--}\text{I}\cdots\text{Cg}$  angles are acute [ $\text{Hg1}\text{--}\text{I1}\cdots\text{Cg1} = 77.94(3)^\circ$  and  $\text{Hg1}\text{--}\text{I2}\cdots\text{Cg2}^{\text{ii}} = 68.79(3)^\circ$ ] [ $\text{Cg1}$  and  $\text{Cg2}$  are the centroids of the N1/C2–C6 and N2/C7–C11 rings, respectively; symmetry code: (ii)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ]. In the chain, potentially structure-influencing C–H $\cdots$ O and C–H $\cdots$ I interactions can be identified (Table 1). The disulfide moiety is involved in two inter-strand contacts that are shorter than the sum of the van der Waals radii (Bondi, 1964); the short contacts [ $\text{S1}\cdots\text{I1}^{\text{iii}} = 3.5983(13) \text{\AA}$  and  $\text{S2}\cdots\text{O2}^{\text{iv}} = 3.263(4) \text{\AA}$ ; symmetry codes: (iii)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (iv)  $-x + 2, -y + 1, -z + 2$ ], connect adjacent chains into a layer structure parallel to  $(\bar{1}01)$ .

## 4. Database survey

A search for structures containing 2,2'-dithiobis(pyridine *N*-oxide) in the Cambridge Structural Database (CSD; Groom *et al.*, 2016) via the WebCSD interface (Thomas *et al.*, 2010) in February 2018 revealed the aforementioned one-dimensional coordination polymers containing  $\text{Zn}^{\text{II}}$  and  $\text{Cd}^{\text{II}}$  halide units (Seidel *et al.*, 2017). In addition, there is an  $\text{Na}^{\text{I}}$  coordination



**Figure 2**  
Two adjacent coordination polymer strands of the title compound, viewed along the  $[101]$  direction. *P* and *M* denote the handedness of the 2,2'-dithiobis(pyridine *N*-oxide) ligand in the chains. H atoms have been omitted for clarity.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	[HgI <sub>2</sub> (C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub> )] <sub>n</sub>
<i>M<sub>r</sub></i>	706.69
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	108
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.4207 (3), 18.7599 (7), 11.6463 (4)
β (°)	100.887 (4)
<i>V</i> (Å <sup>3</sup> )	1592.13 (10)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	13.81
Crystal size (mm)	0.16 × 0.10 × 0.04
Data collection	
Diffractometer	Oxford Diffraction Xcalibur2
Absorption correction	empirical (using intensity measurements) ( <i>ShxAbs</i> ; Spek, 2009)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.614, 0.885
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	21770, 6430, 4209
<i>R</i> <sub>int</sub>	0.069
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.842
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.047, 0.059, 1.02
No. of reflections	6430
No. of parameters	172
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	1.64, -1.39

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *DIAMOND* (Brandenburg, 2016) and *enCIFer* (Allen *et al.*, 2004).

polymer, wherein the Na<sup>I</sup> ions are bridged *via* only one pyridine *N*-oxide moiety of the ligand in a μ-κ<sup>2</sup>*O*:*O* coordination mode (Ravindran Durai Nayagam, 2010). The crystal structures of the free, unsolvated 2,2'-dithiobis(pyridine *N*-oxide) (CSD refcode RIRPEN; Bodige *et al.*, 1997) and some cocrystals (Bodige *et al.*, 1997; Bond & Jones, 2000a,b) have also been reported.

The isomorphous series of one-dimensional Zn<sup>II</sup> coordination polymers, [ZnX<sub>2</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>)<sub>n</sub>] [*X* = Cl, Br, I; C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub> is 2,2'-dithiobis(pyridine *N*-oxide)] (Seidel *et al.*, 2017) and (I) are topologically related but not isostructural. The Hg—I and Hg—O bond lengths in (I) are longer by *ca* 0.09 and 0.48 Å, respectively, than the corresponding Zn—I and Zn—O bond lengths in [ZnI<sub>2</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>)<sub>n</sub>] (CSD refcode XAMNUX; Seidel *et al.*, 2017). The deviations of the I—Hg—I and O—Hg—O angles from the ideal tetrahedral angle of 109.5° are considerably larger in (I) than those of the corresponding I—Zn—I and O—Zn—O angles in XAMNUX. In (2,2'-bipyridine *N,N'*-dioxide)diiodidomercury(II) (CSD refcode FAYKEW; Tedmann *et al.*, 2005), so far the only Hg<sup>II</sup> complex with two pyridine *N*-oxide and two iodide ligands in the CSD, the I—Hg—I angle is 158.54 (4)°, which is similar to that of 155.113 (16)° observed in (I). The C2—S1—S2—C7 torsion angle in (I) [77.2 (2)°] is markedly smaller than that in RIRPEN, which is very close to the preferred value of 90° [89.89 (9)°], indicating some torsional strain in (I).

## 5. Synthesis and crystallization

A solution of 20 mg (0.044 mmol) HgI<sub>2</sub> in 2 ml of methanol was mixed with a solution of 12 mg (0.048 mmol) 2,2'-dithiobis(pyridine *N*-oxide) (Acros Organics) in 8 ml of methanol. The reaction mixture was left at room temperature and the solvent was allowed to evaporate slowly. Colourless crystals of (I) suitable for single-crystal X-ray analysis were obtained after *ca* four weeks.

After prolonged standing, colourless crystals of a second product appeared in the crystallization vessel, which were identified as [Hg<sub>2</sub>I<sub>2</sub>(C<sub>5</sub>H<sub>4</sub>NOS)<sub>2</sub>] (C<sub>5</sub>H<sub>4</sub>NOS<sup>-</sup> is pyrithionate) in a preliminary X-ray analysis.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H-atom positions were calculated geometrically and refined using a riding model, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). The C—H bond lengths were set at 0.95 Å.

## Acknowledgements

RWS would like to thank Dr Richard Goddard for helpful discussions. Financial support from Bayer MaterialScience (now Covestro) and the Deutsche Forschungsgemeinschaft (DFG) is gratefully acknowledged.

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## supporting information

*Acta Cryst.* (2018). E74, 433–435 [https://doi.org/10.1107/S2056989018003055]

## Crystal structure of *catena*-poly[[diiodidomercury(II)]- $\mu$ -2,2'-dithiobis(pyridine *N*-oxide)- $\kappa^2$ O:O']

Rüdiger W. Seidel and Iris M. Oppel

### Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SHELXT2014* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/1* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg, 2016); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

### *catena*-Poly[[diiodidomercury(II)]- $\mu$ -2,2'-dithiobis(pyridine *N*-oxide)- $\kappa^2$ O:O']

#### Crystal data

[HgI<sub>2</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>)]

$M_r = 706.69$

Monoclinic,  $P2_1/n$

$a = 7.4207$  (3) Å

$b = 18.7599$  (7) Å

$c = 11.6463$  (4) Å

$\beta = 100.887$  (4)°

$V = 1592.13$  (10) Å<sup>3</sup>

$Z = 4$

$F(000) = 1264$

$D_x = 2.948$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 4297 reflections

$\theta = 3.6$ – $32.1$ °

$\mu = 13.81$  mm<sup>-1</sup>

$T = 108$  K

Plate, colourless

$0.16 \times 0.10 \times 0.04$  mm

#### Data collection

Oxford Diffraction Xcalibur2  
diffractometer

Radiation source: fine-focus sealed X-ray tube,  
Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 8.4171 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: empirical (using  
intensity measurements)  
(*ShxAbs*; Spek, 2009)

$T_{\min} = 0.614$ ,  $T_{\max} = 0.885$

21770 measured reflections

6430 independent reflections

4209 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.069$

$\theta_{\max} = 36.8$ °,  $\theta_{\min} = 3.6$ °

$h = -11 \rightarrow 10$

$k = -26 \rightarrow 31$

$l = -15 \rightarrow 18$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.059$

$S = 1.02$

6430 reflections

172 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0045P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 1.64 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.39 \text{ e } \text{\AA}^{-3}$$

### Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.64620 (3)	0.14596 (2)	0.76452 (2)	0.01829 (5)
I1	0.38759 (5)	0.22283 (2)	0.63732 (3)	0.01977 (9)
I2	0.80134 (6)	0.07571 (2)	0.95050 (3)	0.02410 (9)
S1	0.9109 (2)	0.33156 (8)	0.84420 (11)	0.0169 (3)
S2	0.89904 (19)	0.43914 (8)	0.87677 (12)	0.0182 (3)
O1	0.9177 (5)	0.2100 (2)	0.7332 (3)	0.0175 (8)
O2	0.7700 (5)	0.5690 (2)	0.8952 (3)	0.0183 (8)
N1	0.8795 (6)	0.2607 (3)	0.6515 (4)	0.0162 (10)
N2	0.6271 (6)	0.5263 (2)	0.8586 (4)	0.0178 (10)
C2	0.8761 (7)	0.3286 (3)	0.6896 (4)	0.0135 (11)
C3	0.8382 (8)	0.3838 (3)	0.6102 (4)	0.0199 (13)
H3	0.839772	0.431876	0.636054	0.024*
C4	0.7978 (7)	0.3676 (3)	0.4917 (5)	0.0218 (13)
H4	0.773405	0.404774	0.435526	0.026*
C5	0.7931 (8)	0.2981 (3)	0.4560 (5)	0.0233 (14)
H5	0.760912	0.287104	0.375152	0.028*
C6	0.8351 (8)	0.2437 (3)	0.5370 (5)	0.0204 (13)
H6	0.832653	0.195319	0.512429	0.024*
C7	0.6611 (7)	0.4561 (3)	0.8435 (4)	0.0156 (11)
C8	0.5189 (8)	0.4097 (3)	0.8070 (5)	0.0207 (13)
H8	0.542666	0.360651	0.796344	0.025*
C9	0.3408 (8)	0.4351 (3)	0.7860 (5)	0.0261 (14)
H9	0.240770	0.403667	0.760625	0.031*
C10	0.3099 (8)	0.5073 (3)	0.8024 (5)	0.0264 (14)
H10	0.188027	0.525256	0.788713	0.032*
C11	0.4533 (8)	0.5521 (3)	0.8379 (5)	0.0231 (13)
H11	0.431858	0.601379	0.848200	0.028*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Hg1	0.01884 (11)	0.01544 (11)	0.02109 (11)	0.00085 (10)	0.00505 (8)	0.00204 (9)
I1	0.0205 (2)	0.0230 (2)	0.01644 (18)	0.00366 (16)	0.00510 (14)	0.00259 (15)
I2	0.0291 (2)	0.0186 (2)	0.02230 (19)	0.00029 (17)	-0.00105 (16)	0.00206 (16)
S1	0.0211 (8)	0.0141 (7)	0.0146 (7)	0.0020 (5)	0.0016 (5)	0.0001 (5)
S2	0.0179 (7)	0.0155 (7)	0.0204 (7)	-0.0002 (6)	0.0017 (6)	-0.0037 (6)
O1	0.020 (2)	0.014 (2)	0.019 (2)	0.0012 (16)	0.0052 (16)	0.0031 (16)

O2	0.019 (2)	0.014 (2)	0.021 (2)	-0.0039 (16)	0.0034 (16)	-0.0005 (16)
N1	0.019 (3)	0.017 (3)	0.014 (2)	0.001 (2)	0.0071 (18)	0.0011 (19)
N2	0.022 (3)	0.014 (3)	0.018 (2)	-0.003 (2)	0.0044 (19)	0.0054 (19)
C2	0.011 (3)	0.016 (3)	0.014 (3)	-0.001 (2)	0.003 (2)	-0.002 (2)
C3	0.025 (3)	0.020 (3)	0.015 (3)	0.000 (2)	0.005 (2)	0.000 (2)
C4	0.019 (3)	0.026 (4)	0.021 (3)	0.000 (3)	0.007 (2)	0.007 (2)
C5	0.020 (3)	0.036 (4)	0.014 (3)	-0.006 (3)	0.006 (2)	-0.003 (3)
C6	0.020 (3)	0.025 (3)	0.019 (3)	-0.002 (2)	0.010 (2)	-0.007 (2)
C7	0.016 (3)	0.013 (3)	0.017 (3)	0.001 (2)	0.003 (2)	0.002 (2)
C8	0.020 (3)	0.017 (3)	0.025 (3)	-0.004 (2)	0.005 (2)	-0.004 (2)
C9	0.018 (3)	0.024 (4)	0.038 (4)	-0.008 (3)	0.010 (3)	-0.004 (3)
C10	0.016 (3)	0.024 (4)	0.041 (4)	-0.001 (3)	0.009 (3)	0.006 (3)
C11	0.023 (3)	0.012 (3)	0.033 (3)	0.002 (2)	0.004 (3)	0.004 (2)

*Geometric parameters (Å, °)*

Hg1—O1	2.432 (4)	C3—H3	0.9500
Hg1—O2 <sup>i</sup>	2.524 (4)	C4—C5	1.366 (8)
Hg1—I2	2.6100 (4)	C4—H4	0.9500
Hg1—I1	2.6236 (4)	C5—C6	1.385 (8)
S1—C2	1.771 (5)	C5—H5	0.9500
S1—S2	2.058 (2)	C6—H6	0.9500
S2—C7	1.764 (6)	C7—C8	1.372 (7)
O1—N1	1.336 (5)	C8—C9	1.383 (8)
O2—N2	1.333 (5)	C8—H8	0.9500
N1—C6	1.351 (6)	C9—C10	1.393 (8)
N1—C2	1.352 (7)	C9—H9	0.9500
N2—C11	1.356 (7)	C10—C11	1.357 (8)
N2—C7	1.358 (7)	C10—H10	0.9500
C2—C3	1.381 (7)	C11—H11	0.9500
C3—C4	1.389 (7)		
O1—Hg1—O2 <sup>i</sup>	81.13 (12)	C5—C4—H4	120.0
O1—Hg1—I2	97.24 (8)	C3—C4—H4	120.0
O2 <sup>i</sup> —Hg1—I2	101.01 (8)	C4—C5—C6	120.5 (5)
O1—Hg1—I1	100.48 (8)	C4—C5—H5	119.8
O2 <sup>i</sup> —Hg1—I1	98.87 (8)	C6—C5—H5	119.8
I2—Hg1—I1	155.113 (16)	N1—C6—C5	118.6 (5)
C2—S1—S2	102.39 (19)	N1—C6—H6	120.7
C7—S2—S1	102.3 (2)	C5—C6—H6	120.7
N1—O1—Hg1	112.8 (3)	N2—C7—C8	120.3 (5)
N2—O2—Hg1 <sup>ii</sup>	113.6 (3)	N2—C7—S2	110.4 (4)
O1—N1—C6	120.9 (5)	C8—C7—S2	129.3 (5)
O1—N1—C2	116.9 (4)	C7—C8—C9	119.4 (6)
C6—N1—C2	122.1 (5)	C7—C8—H8	120.3
O2—N2—C11	121.0 (5)	C9—C8—H8	120.3
O2—N2—C7	117.9 (5)	C8—C9—C10	119.1 (6)
C11—N2—C7	121.1 (5)	C8—C9—H9	120.4

N1—C2—C3	120.1 (5)	C10—C9—H9	120.4
N1—C2—S1	110.8 (4)	C11—C10—C9	120.3 (6)
C3—C2—S1	129.0 (4)	C11—C10—H10	119.9
C2—C3—C4	118.6 (5)	C9—C10—H10	119.9
C2—C3—H3	120.7	N2—C11—C10	119.9 (6)
C4—C3—H3	120.7	N2—C11—H11	120.1
C5—C4—C3	119.9 (5)	C10—C11—H11	120.1
Hg1—O1—N1—C6	-73.6 (5)	C2—N1—C6—C5	3.1 (8)
Hg1—O1—N1—C2	102.2 (4)	C4—C5—C6—N1	0.4 (9)
Hg1 <sup>ii</sup> —O2—N2—C11	-76.5 (5)	O2—N2—C7—C8	179.4 (5)
Hg1 <sup>ii</sup> —O2—N2—C7	103.9 (4)	C11—N2—C7—C8	-0.2 (8)
O1—N1—C2—C3	179.8 (5)	O2—N2—C7—S2	-0.6 (6)
C6—N1—C2—C3	-4.4 (8)	C11—N2—C7—S2	179.8 (4)
O1—N1—C2—S1	-3.7 (6)	S1—S2—C7—N2	-179.1 (3)
C6—N1—C2—S1	172.1 (4)	S1—S2—C7—C8	0.9 (6)
S2—S1—C2—N1	-180.0 (3)	N2—C7—C8—C9	-0.1 (8)
S2—S1—C2—C3	-3.9 (6)	S2—C7—C8—C9	179.9 (4)
N1—C2—C3—C4	2.3 (8)	C7—C8—C9—C10	0.0 (9)
S1—C2—C3—C4	-173.6 (4)	C8—C9—C10—C11	0.4 (9)
C2—C3—C4—C5	1.1 (9)	O2—N2—C11—C10	-179.0 (5)
C3—C4—C5—C6	-2.4 (9)	C7—N2—C11—C10	0.6 (8)
O1—N1—C6—C5	178.7 (5)	C9—C10—C11—N2	-0.7 (9)

Symmetry codes: (i)  $-x+3/2, y-1/2, -z+3/2$ ; (ii)  $-x+3/2, y+1/2, -z+3/2$ .

#### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 $\cdots$ I2 <sup>ii</sup>	0.95	3.00	3.776 (6)	140
C11—H11 $\cdots$ O1 <sup>ii</sup>	0.95	2.59	3.268 (7)	129

Symmetry code: (ii)  $-x+3/2, y+1/2, -z+3/2$ .