

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# Diiodido(1,10-phenanthroline-5,6-dione- $\kappa^2N,N'$ )mercury(II)

 Akbar Ghaemi,<sup>a‡</sup> Rezvan Shojaiean,<sup>a</sup> Seik Weng Ng<sup>b,c</sup> and Edward R. T. Tiekink<sup>b\*</sup>
<sup>a</sup>Department of Chemistry, Saveh Branch, Islamic Azad University, Saveh, Iran,

<sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and <sup>c</sup>Chemistry Department, Faculty of, Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia

Correspondence e-mail: Edward.Tiekink@gmail.com

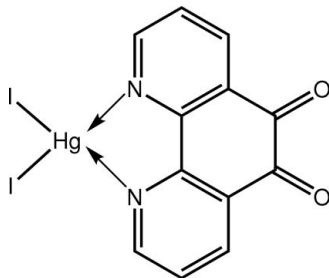
Received 21 September 2011; accepted 21 September 2011

 Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.022;  $wR$  factor = 0.049; data-to-parameter ratio = 18.7.

The Hg<sup>II</sup> atom in the title complex, [HgI<sub>2</sub>(C<sub>12</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>)], is tetrahedrally coordinated by the N atoms of the chelating 1,10-phenanthroline-5,6-dione ligand and two I atoms. The range of tetrahedral angles is broad, *viz.* 68.94 (17)° for the chelate angle to a wide 132.627 (15)° for the I—Hg—I angle. The ligand molecule is non-planar with the O atoms lying 0.422 (5) and −0.325 (5) Å out of the plane through the remaining atoms [r.m.s. deviation = 0.068 Å]. Molecules are consolidated in the crystal packing by C—H···O interactions.

## Related literature

For the ligand synthesis and the crystal structure of 1,10-phenanthroline-5,6-dione, see: Calderazzo *et al.* (1999). For an evaluation of the different coordinating ability of the two sets of donor atoms in the ligand, see: Fujihara *et al.* (2003). For the structure of the dichlorido analogue with two 1,10-phenanthroline-5,6-dione ligands, see: Figueiras *et al.* (2009). For the crystallization procedure, see: Harrowfield *et al.* (1996).



## Experimental

### Crystal data

[HgI<sub>2</sub>(C<sub>12</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>)]  
 $M_r = 664.58$   
 Monoclinic,  $Cc$   
 $a = 11.7941$  (3) Å  
 $b = 8.1725$  (1) Å  
 $c = 15.3982$  (3) Å  
 $\beta = 108.298$  (2)°

$V = 1409.14$  (5) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 15.30$  mm<sup>−1</sup>  
 $T = 100$  K  
 $0.15 \times 0.15 \times 0.15$  mm

### Data collection

Agilent SuperNova Dual diffractometer with Atlas detector  
 Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2010)  
 $T_{\min} = 0.586$ ,  $T_{\max} = 1.000$

15631 measured reflections  
 3209 independent reflections  
 3155 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.041$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.049$   
 $S = 1.03$   
 3209 reflections  
 172 parameters  
 2 restraints

H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.51$  e Å<sup>−3</sup>  
 $\Delta\rho_{\text{min}} = -0.79$  e Å<sup>−3</sup>  
 Absolute structure: Flack (1983),  
 1579 Friedel pairs  
 Flack parameter: −0.005 (3)

**Table 1**

Selected bond lengths (Å).

Hg1—N1	2.411 (5)	Hg1—I1	2.6637 (4)
Hg1—N2	2.416 (5)	Hg1—I2	2.6739 (4)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1···O2 <sup>i</sup>	0.95	2.58	3.077 (8)	113
C12—H12···O1 <sup>ii</sup>	0.95	2.40	3.248 (7)	148

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

Data collection: CrysAlis PRO (Agilent, 2010); cell refinement: CrysAlis PRO; data reduction: CrysAlis PRO; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: publCIF (Westrip, 2010).

We acknowledge financial support of this work by the Islamic Azad University, Saveh Branch, and thank the University of Malaya for support of the crystallographic facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5098).

<sup>‡</sup> Additional correspondence author, e-mail: akbarghaemi@yahoo.com.

## References

- Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
- Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Calderazzo, F., Marchetti, F., Pampaloni, G. & Passarelli, V. (1999). *J. Chem. Soc. Dalton Trans.* pp. 4389–4396.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Figueiras, C. A. L., Bomfim, J. A. S., Howie, R. A., Tiekink, E. R. T. & Wardell, J. L. (2009). *Acta Cryst.* **E65**, m1645.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Fujihara, T., Okamura, R., Wada, T. & Tanaka, K. (2003). *J. Chem. Soc. Dalton Trans.* pp. 3221–3226.
- Harrowfield, J. M., Miyamae, H., Skelton, B. W., Soudi, A. A. & White, A. H. (1996). *Aust. J. Chem.* **49**, 1165–1169.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

## supporting information

*Acta Cryst.* (2011). E67, m1449–m1450 [https://doi.org/10.1107/S1600536811038748]

**Diiodido(1,10-phenanthroline-5,6-dione- $\kappa^2N,N'$ )mercury(II)****Akbar Ghaemi, Rezvan Shojaiean, Seik Weng Ng and Edward R. T. Tiekink****S1. Comment**

1,10-Phenanthroline-5,6-dione (Calderazzo *et al.*, 1999) has attracted our attention due to the presence of two coordinating functionalities within the same molecule, *i.e.* the quinonoid and the diimine residues. Moreover, the presence of two types of basic centres, *i.e.* nitrogen and oxygen, both  $sp^2$ -hybridized, makes this molecule an ideal system to study the different coordinating ability of the two sets of donor atoms (Calderazzo *et al.*, 1999; Fujihara *et al.*, 2003). In connection with a recent structure determination of the related mercury(II)dichlorido structure with two 1,10-phenanthroline-5,6-dione ligands (Figueiras *et al.*, 2009), the structure of the title compound, (I), was determined.

The Hg atom in (I), Fig. 1 and Table 1, is chelated by the 1,10-phenanthroline-5,6-dione ligand and the distorted tetrahedral  $I_2N_2$  donor set is completed by two I atoms. The range of tetrahedral angles is from a narrow  $68.94$  ( $17$ ) $^\circ$ , for the chelate angle, to a wide  $132.627$  ( $15$ ) $^\circ$ , for the angle subtended at Hg by the I atoms. The 1,10-phenanthroline-5,6-dione ligand is planar with the r.m.s. deviation for the 14 C and N atoms being  $0.068$  Å with the maximum deviations from the least-squares plane being  $0.146$  ( $6$ ) Å for atom C7 and  $-0.116$  ( $7$ ) for atom C6; the O1 and O2 atoms lie  $-0.325$  ( $5$ ) and  $0.422$  ( $5$ ) Å out of this plane, respectively.

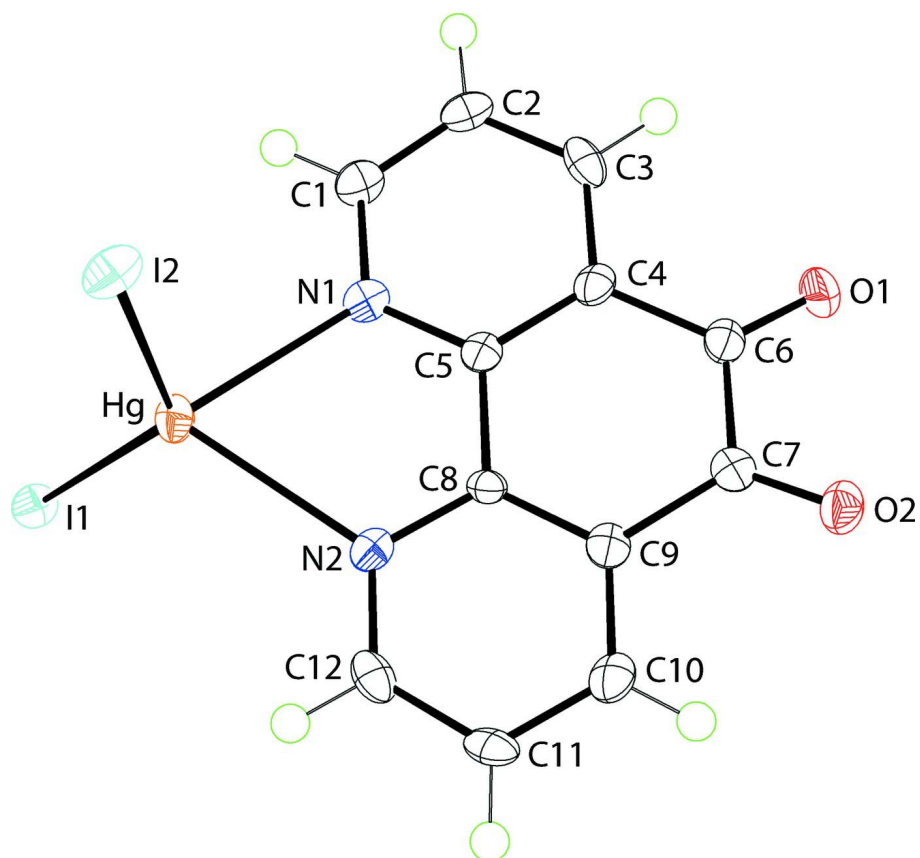
The molecules of (I) are consolidated in the crystal packing *via* weak C—H $\cdots$ O interactions involving both O atoms, Table 2 and Fig. 2.

**S2. Experimental**

The title complex was obtained by the branched tube method (Harrowfield *et al.*, 1996). 1,10-Phenanthroline-5,6-dione (0.136 g, 0.648 mmol) and  $HgI_2$  (0.294 g, 0.648 mmol) were placed at the bottom of main arm of a branched tube. Methanol was carefully added to fill both arms. The tube was sealed and the main arm immersed in a bath at 333 K while the other was kept at ambient temperature. After five days, red crystals were deposited in the cooler arm. These were filtered off, washed with acetone and ether, and air dried; Yield: 60%; *M.pt.* 524–526 K. Anal. Calc for  $C_{12}H_6HgI_2N_2O_2$ ; C, 21.7, H, 0.60, N, 4.2%; Found: C, 21.89, H, 0.69, N, 4.24%. Selected FT—IR data,  $\nu$ ( $cm^{-1}$ ): 1687 (C=O).  $^1H$  NMR ( $\delta$ ): 7.85–7.89 (dd, 2H, H3,8), 8.53–8.56 (dd, 2H, H2,9), 9.01–9.03 (dd, 2H, H4,7) p.p.m..

**S3. Refinement**

The H-atoms were placed in calculated positions (C—H  $0.95$  Å) and were included in the refinement in the riding model approximation, with  $U_{iso}(H)$  set to  $1.2U_{equiv}(C)$ . A number of reflections, *i.e.*  $4\ 0\ -10$ ,  $1\ 3\ -10$ ,  $6\ 0\ -10$ ,  $0\ 0\ \bar{8}$ ,  $2\ 4\ -11$ ,  $6\ 0\ \bar{8}$ ,  $5\ 3\ -14$  and  $3\ 3\ -12$ , were omitted from the final refinement owing to poor agreement.



**Figure 1**

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

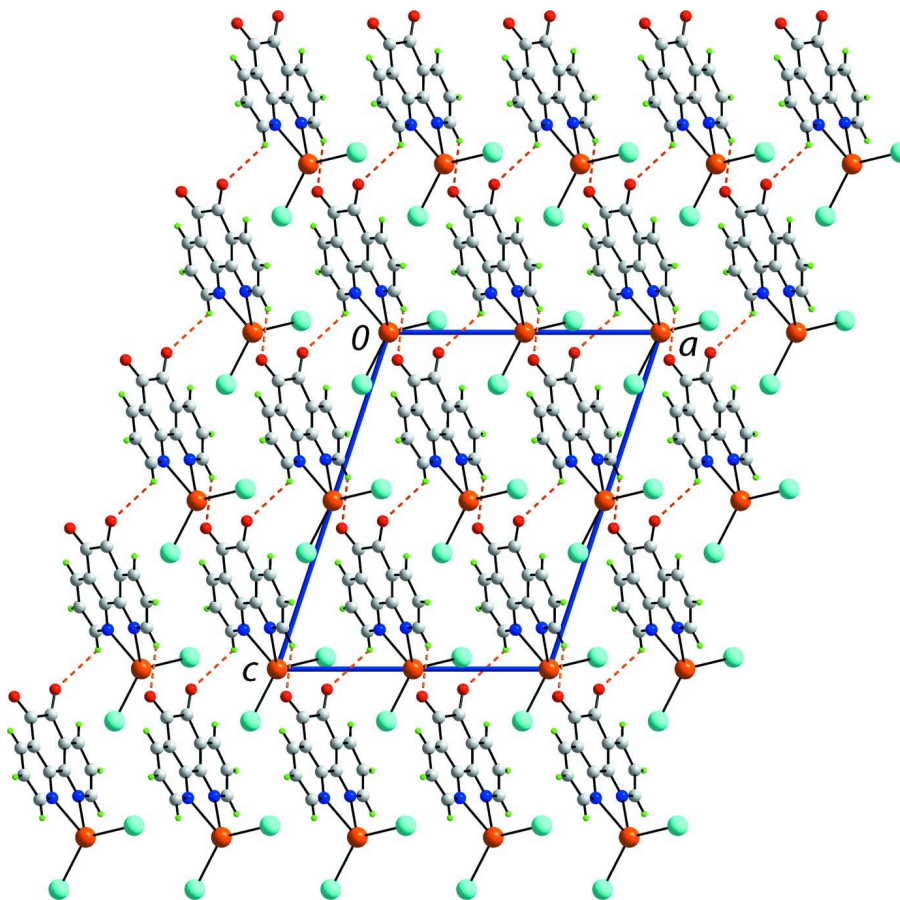


Figure 2

A view in projection down the  $b$  axis of the unit-cell contents of (I). The C—H...O interactions are shown as orange dashed lines.

### Diiodido(1,10-phenanthroline-5,6-dione- $\kappa^2N,N'$ )mercury(II)

#### Crystal data

[HgI<sub>2</sub>(C<sub>12</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>)]

$M_r = 664.58$

Monoclinic,  $Cc$

Hall symbol:  $C -2yc$

$a = 11.7941(3) \text{ \AA}$

$b = 8.1725(1) \text{ \AA}$

$c = 15.3982(3) \text{ \AA}$

$\beta = 108.298(2)^\circ$

$V = 1409.14(5) \text{ \AA}^3$

$Z = 4$

$F(000) = 1176$

$D_x = 3.133 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 11298 reflections

$\theta = 2.8\text{--}29.3^\circ$

$\mu = 15.30 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Block, red

$0.15 \times 0.15 \times 0.15 \text{ mm}$

#### Data collection

Agilent SuperNova Dual

diffractometer with Atlas detector

Radiation source: SuperNova (Mo) X-ray

Source

Mirror monochromator

Detector resolution:  $10.4041 \text{ pixels mm}^{-1}$

$\omega$  scan

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2010)

$T_{\min} = 0.586$ ,  $T_{\max} = 1.000$

15631 measured reflections

3209 independent reflections

3155 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.041$  $\theta_{\text{max}} = 27.5^\circ$ ,  $\theta_{\text{min}} = 2.8^\circ$  $h = -15 \rightarrow 15$  $k = -10 \rightarrow 10$  $l = -19 \rightarrow 19$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.022$  $wR(F^2) = 0.049$  $S = 1.03$ 

3209 reflections

172 parameters

2 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0292P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} = 0.001$  $\Delta\rho_{\text{max}} = 0.51 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\text{min}} = -0.79 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack (1983), 1579 Friedel  
pairsAbsolute structure parameter:  $-0.005(3)$ *Special details*

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.499993 (19)	0.48034 (2)	0.500006 (16)	0.01421 (6)
I1	0.46538 (3)	0.38365 (4)	0.65496 (2)	0.01434 (9)
I2	0.66399 (3)	0.67286 (5)	0.46534 (3)	0.01911 (10)
O1	0.0663 (4)	0.5129 (5)	0.0820 (3)	0.0211 (10)
O2	0.2083 (4)	0.2572 (5)	0.0607 (3)	0.0174 (9)
N1	0.3288 (4)	0.5884 (6)	0.3831 (3)	0.0132 (10)
N2	0.4235 (4)	0.2848 (6)	0.3779 (3)	0.0120 (10)
C1	0.2862 (5)	0.7383 (7)	0.3878 (4)	0.0154 (12)
H1	0.3175	0.7988	0.4428	0.018*
C2	0.1973 (6)	0.8101 (7)	0.3152 (4)	0.0160 (12)
H2	0.1679	0.9164	0.3208	0.019*
C3	0.1537 (5)	0.7221 (8)	0.2351 (4)	0.0156 (12)
H3	0.0938	0.7673	0.1842	0.019*
C4	0.1990 (6)	0.5657 (7)	0.2299 (4)	0.0132 (11)
C5	0.2882 (6)	0.5030 (6)	0.3057 (4)	0.0111 (11)
C6	0.1530 (6)	0.4715 (7)	0.1439 (4)	0.0142 (12)
C7	0.2238 (5)	0.3175 (7)	0.1356 (4)	0.0115 (11)
C8	0.3413 (5)	0.3392 (7)	0.3019 (4)	0.0100 (11)
C9	0.3084 (5)	0.2485 (7)	0.2209 (4)	0.0130 (12)
C10	0.3582 (5)	0.0953 (7)	0.2196 (4)	0.0156 (12)

H10	0.3378	0.0324	0.1650	0.019*
C11	0.4383 (6)	0.0363 (7)	0.2996 (4)	0.0147 (12)
H11	0.4713	-0.0702	0.3019	0.018*
C12	0.4696 (6)	0.1365 (8)	0.3764 (4)	0.0155 (12)
H12	0.5267	0.0971	0.4307	0.019*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Hg1	0.01526 (11)	0.01650 (11)	0.01011 (10)	-0.00067 (10)	0.00290 (7)	-0.00105 (10)
I1	0.01624 (19)	0.01475 (19)	0.01394 (18)	-0.00041 (15)	0.00747 (15)	-0.00073 (14)
I2	0.0206 (2)	0.01604 (19)	0.0225 (2)	-0.00531 (16)	0.00937 (17)	-0.00433 (16)
O1	0.023 (3)	0.019 (2)	0.015 (2)	-0.0015 (18)	-0.0049 (19)	0.0022 (17)
O2	0.021 (2)	0.018 (2)	0.012 (2)	-0.0045 (18)	0.0053 (17)	-0.0010 (18)
N1	0.012 (2)	0.013 (2)	0.015 (2)	-0.001 (2)	0.007 (2)	-0.001 (2)
N2	0.014 (2)	0.012 (2)	0.012 (2)	-0.0029 (19)	0.0064 (19)	-0.0014 (19)
C1	0.017 (3)	0.015 (3)	0.016 (3)	0.000 (2)	0.009 (3)	-0.002 (2)
C2	0.017 (3)	0.011 (3)	0.021 (3)	-0.003 (2)	0.009 (3)	-0.002 (2)
C3	0.013 (3)	0.021 (3)	0.012 (3)	0.000 (2)	0.004 (2)	0.006 (2)
C4	0.015 (3)	0.012 (3)	0.013 (3)	-0.005 (2)	0.005 (2)	-0.001 (2)
C5	0.013 (3)	0.011 (3)	0.011 (3)	-0.004 (2)	0.006 (2)	0.001 (2)
C6	0.018 (3)	0.014 (3)	0.011 (3)	-0.005 (2)	0.005 (3)	0.001 (2)
C7	0.009 (3)	0.013 (3)	0.014 (3)	-0.004 (2)	0.005 (2)	0.002 (2)
C8	0.010 (3)	0.008 (2)	0.012 (3)	0.000 (2)	0.003 (2)	0.001 (2)
C9	0.015 (3)	0.013 (3)	0.012 (3)	-0.005 (2)	0.006 (2)	0.002 (2)
C10	0.018 (3)	0.014 (3)	0.015 (3)	-0.007 (2)	0.005 (2)	-0.001 (2)
C11	0.014 (3)	0.009 (3)	0.021 (3)	-0.001 (2)	0.006 (3)	0.005 (2)
C12	0.014 (3)	0.019 (3)	0.012 (3)	-0.001 (2)	0.004 (2)	0.006 (2)

*Geometric parameters (Å, °)*

Hg1—N1	2.411 (5)	C3—C4	1.398 (9)
Hg1—N2	2.416 (5)	C3—H3	0.9500
Hg1—I1	2.6637 (4)	C4—C5	1.400 (9)
Hg1—I2	2.6739 (4)	C4—C6	1.479 (8)
O1—C6	1.207 (8)	C5—C8	1.487 (8)
O2—C7	1.215 (7)	C6—C7	1.538 (8)
N1—C5	1.333 (8)	C7—C9	1.488 (8)
N1—C1	1.335 (8)	C8—C9	1.396 (8)
N2—C8	1.341 (7)	C9—C10	1.386 (9)
N2—C12	1.331 (8)	C10—C11	1.382 (9)
C1—C2	1.399 (9)	C10—H10	0.9500
C1—H1	0.9500	C11—C12	1.390 (9)
C2—C3	1.380 (9)	C11—H11	0.9500
C2—H2	0.9500	C12—H12	0.9500
N2—Hg1—N1	68.94 (17)	N1—C5—C4	121.3 (5)
N2—Hg1—I1	112.07 (11)	N1—C5—C8	118.0 (5)

N1—Hg1—I1	116.72 (11)	C4—C5—C8	120.7 (5)
N2—Hg1—I2	110.55 (11)	O1—C6—C4	122.9 (6)
N1—Hg1—I2	97.13 (12)	O1—C6—C7	120.7 (5)
I1—Hg1—I2	132.627 (15)	C4—C6—C7	116.4 (5)
C5—N1—C1	119.5 (5)	O2—C7—C9	123.0 (5)
C5—N1—Hg1	117.2 (4)	O2—C7—C6	119.2 (5)
C1—N1—Hg1	122.5 (4)	C9—C7—C6	117.9 (5)
C8—N2—C12	118.3 (5)	N2—C8—C9	121.7 (5)
C8—N2—Hg1	116.8 (4)	N2—C8—C5	117.5 (5)
C12—N2—Hg1	124.1 (4)	C9—C8—C5	120.7 (5)
N1—C1—C2	122.8 (6)	C10—C9—C8	119.5 (6)
N1—C1—H1	118.6	C10—C9—C7	120.0 (5)
C2—C1—H1	118.6	C8—C9—C7	120.5 (5)
C3—C2—C1	118.1 (6)	C9—C10—C11	118.5 (6)
C3—C2—H2	120.9	C9—C10—H10	120.8
C1—C2—H2	120.9	C11—C10—H10	120.8
C2—C3—C4	119.1 (6)	C10—C11—C12	118.5 (6)
C2—C3—H3	120.5	C10—C11—H11	120.8
C4—C3—H3	120.5	C12—C11—H11	120.8
C5—C4—C3	119.1 (6)	N2—C12—C11	123.4 (6)
C5—C4—C6	121.6 (5)	N2—C12—H12	118.3
C3—C4—C6	119.2 (6)	C11—C12—H12	118.3
N2—Hg1—N1—C5	-9.4 (4)	C5—C4—C6—C7	-11.3 (8)
I1—Hg1—N1—C5	-114.3 (4)	C3—C4—C6—C7	167.7 (5)
I2—Hg1—N1—C5	99.9 (4)	O1—C6—C7—O2	15.4 (8)
N2—Hg1—N1—C1	-179.3 (5)	C4—C6—C7—O2	-163.1 (5)
I1—Hg1—N1—C1	75.8 (5)	O1—C6—C7—C9	-164.2 (6)
I2—Hg1—N1—C1	-69.9 (4)	C4—C6—C7—C9	17.3 (7)
N1—Hg1—N2—C8	10.8 (4)	C12—N2—C8—C9	-3.4 (8)
I1—Hg1—N2—C8	122.1 (4)	Hg1—N2—C8—C9	167.0 (4)
I2—Hg1—N2—C8	-79.1 (4)	C12—N2—C8—C5	178.2 (5)
N1—Hg1—N2—C12	-179.4 (5)	Hg1—N2—C8—C5	-11.3 (6)
I1—Hg1—N2—C12	-68.1 (5)	N1—C5—C8—N2	2.7 (8)
I2—Hg1—N2—C12	90.8 (5)	C4—C5—C8—N2	-177.9 (5)
C5—N1—C1—C2	1.7 (9)	N1—C5—C8—C9	-175.7 (5)
Hg1—N1—C1—C2	171.3 (4)	C4—C5—C8—C9	3.8 (8)
N1—C1—C2—C3	-0.9 (9)	N2—C8—C9—C10	2.5 (8)
C1—C2—C3—C4	0.4 (9)	C5—C8—C9—C10	-179.2 (5)
C2—C3—C4—C5	-0.6 (9)	N2—C8—C9—C7	-175.3 (5)
C2—C3—C4—C6	-179.6 (5)	C5—C8—C9—C7	3.0 (8)
C1—N1—C5—C4	-1.8 (8)	O2—C7—C9—C10	-10.9 (8)
Hg1—N1—C5—C4	-172.0 (4)	C6—C7—C9—C10	168.7 (5)
C1—N1—C5—C8	177.6 (5)	O2—C7—C9—C8	166.9 (5)
Hg1—N1—C5—C8	7.4 (6)	C6—C7—C9—C8	-13.6 (8)
C3—C4—C5—N1	1.3 (9)	C8—C9—C10—C11	0.9 (9)
C6—C4—C5—N1	-179.7 (5)	C7—C9—C10—C11	178.6 (5)
C3—C4—C5—C8	-178.1 (5)	C9—C10—C11—C12	-3.0 (9)



C6—C4—C5—C8	0.8 (9)	C8—N2—C12—C11	1.1 (9)
C5—C4—C6—O1	170.3 (6)	Hg1—N2—C12—C11	-168.6 (4)
C3—C4—C6—O1	-10.8 (9)	C10—C11—C12—N2	2.1 (9)

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C1—H1...O2 <sup>i</sup>	0.95	2.58	3.077 (8)	113
C12—H12...O1 <sup>ii</sup>	0.95	2.40	3.248 (7)	148

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