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## Structure Reports

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# Dichlorido[methyl 2-(quinolin-8-yloxy- $\kappa^2N,O$ )acetate- $\kappa O$ ]mercury(II)

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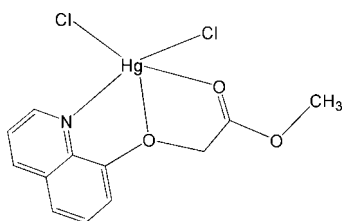
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 Key indicators: single-crystal X-ray study;  $T = 223$  K; mean  $\sigma(C-C) = 0.013$  Å;  $R$  factor = 0.052;  $wR$  factor = 0.142; data-to-parameter ratio = 14.0.

In the neutral title complex,  $[HgCl_2(C_{12}H_{11}NO_3)]$ , the  $Hg^{II}$  ion is pentacoordinated by two Cl atoms, one N atom and two weakly coordinating O atoms from the methyl 2-(quinolin-8-yloxy)acetate ligand. The coordination around the  $Hg^{II}$  ion may be described as highly distorted trigonal-bipyramidal. Centrosymmetric dimers are formed by an additional weak  $Hg \cdots Cl$  interaction, leading to a distorted octahedral coordination geometry around the  $Hg^{II}$  ion.

## Related literature

For the use of quinolin-8-yloxy acetic acid and its derivatives as ligands in transition metal complexes, see: Cheng *et al.* (2007); Song *et al.* (2004); Wang *et al.* (2005, 2008).



## Experimental

### Crystal data

$[HgCl_2(C_{12}H_{11}NO_3)]$   
 $M_r = 488.71$   
 Triclinic,  $P\bar{1}$

$a = 7.2644$  (4) Å  
 $b = 9.7607$  (2) Å  
 $c = 10.8411$  (6) Å

$\alpha = 71.317$  (7)°  
 $\beta = 75.453$  (7)°  
 $\gamma = 69.816$  (8)°  
 $V = 674.87$  (5) Å<sup>3</sup>  
 $Z = 2$

Mo  $K\alpha$  radiation  
 $\mu = 11.80$  mm<sup>-1</sup>  
 $T = 223$  K  
 $0.50 \times 0.25 \times 0.10$  mm

### Data collection

Rigaku Saturn diffractometer  
 Absorption correction: multi-scan  
 (REQAB; Jacobson, 1998)  
 $T_{min} = 0.067$ ,  $T_{max} = 0.385$

5090 measured reflections  
 2432 independent reflections  
 2330 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.050$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.142$   
 $S = 1.07$   
 2432 reflections

174 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 3.58$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -2.39$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Hg1—Cl1	2.340 (2)	Hg1—O1	2.746 (6)
Hg1—Cl2	2.350 (2)	Hg1—O3	2.876 (6)
Hg1—N1	2.463 (6)	Hg1—Cl1 <sup>i</sup>	3.204 (2)

 Symmetry code: (i)  $-x + 1, -y, -z + 2$ .

Data collection: *CrystalClear* (Rigaku/MSC, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2385).

## References

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## supporting information

*Acta Cryst.* (2012). E68, m951 [https://doi.org/10.1107/S1600536812026591]

**Dichlorido[methyl 2-(quinolin-8-yloxy- $\kappa^2N,O$ )acetate- $\kappa O$ ]mercury(II)****Yu-Hong Wang, Xue-Hua Zhu and Rui-Feng Song****S1. Comment**

Quinolin-8-yloxy acetic acid and its derivatives are well known ligands in transition metal coordination compounds (Cheng *et al.*, 2007; Song *et al.*, 2004; Wang *et al.*, 2005; Wang *et al.*, 2008). Some metal complexes with such ligands are being prepared because of their intriguing structural diversity and potential uses as functional materials (Cheng *et al.*, 2007; Song *et al.*, 2004; Wang *et al.*, 2005; Wang *et al.*, 2008). So, we prepared the title Hg<sup>II</sup> complex with methyl-2-(quinoline-8-yloxy)-acetate ligand, (I).

In the title compound, the Hg<sup>II</sup> atom is five-coordinated by two Cl atoms, one N atom and two O atoms from methyl-2-(quinoline-8-yloxy)-acetate ligand, forming a highly distorted trigonal bipyramidal geometry (Fig. 1). Hg—Cl bond lengths are 2.340 (2) and 2.350 (2) Å, and Hg—N bond lengths are 2.463 (6) Å. The weak coordinative Hg—O bond lengths are 2.746 (6) Å and 2.876 (6) Å. Angles around Hg are in a range of 56.55 (16)–153.41 (8)° (Table 1). If these are considered to be chemically significant interactions, two mononuclear Hg complexes are formed into the centrosymmetric dimers by weak Hg—Cl interactions (Fig. 1). So, the coordination around Hg atom can act as a distorted octahedral geometry.

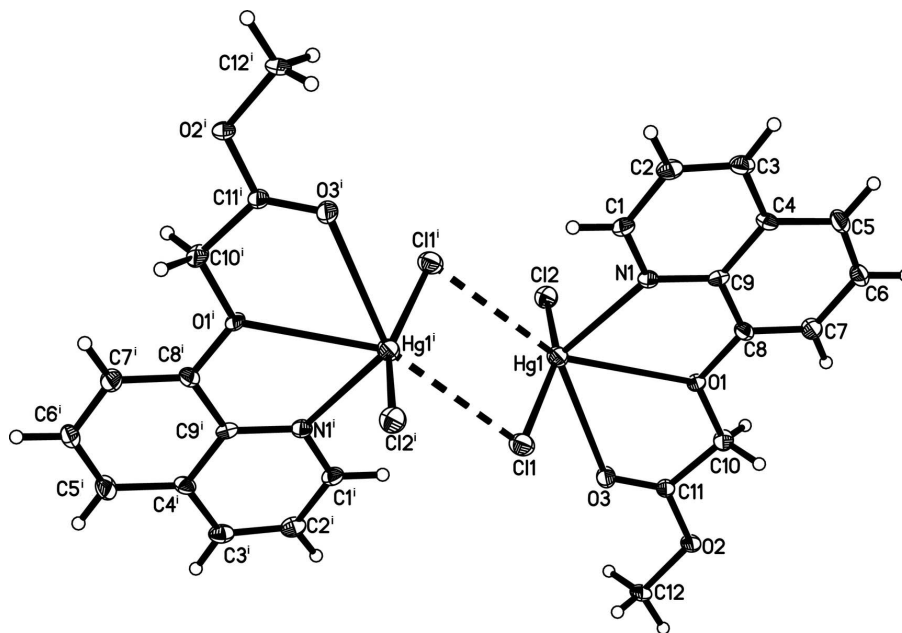
The molecular packing is controlled by these dimers and intermolecular  $\pi$ - $\pi$  interactions; the quinoline rings are separated by 3.527 (1) and 3.813 (1) Å (Fig. 2).

**S2. Experimental**

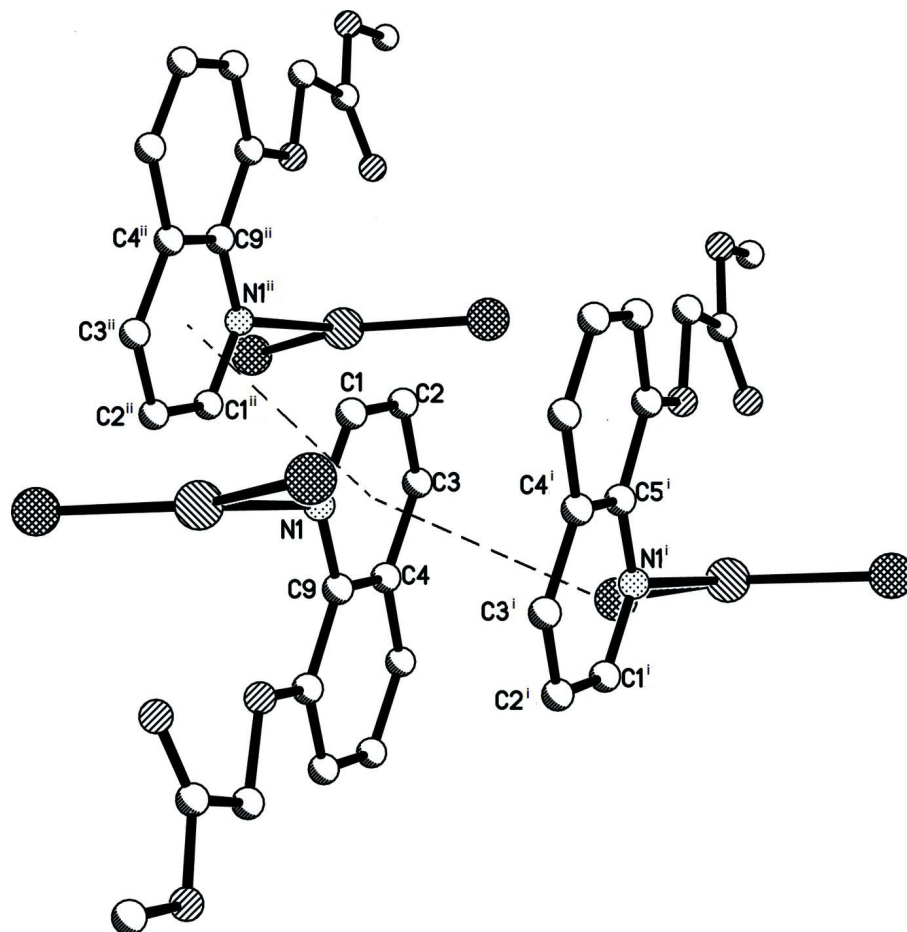
Quinolin-8-yloxy acetic acid (0.0203 g, 0.1 mmol), HgCl<sub>2</sub> (0.0272 g, 0.1 mmol), methanol (3 ml) and triethylamine (0.0101 g, 0.1 mmol) were placed in a thick Pyrex tube and heated to 130 °C for 5 days. After cooling at a rate of 5 °C/h to ambient temperature, yellow prismatic crystals were collected, washed with anhydrous ethanol, and dried at room temperature. The yield is 51% based on quinolin-8-yloxy acetic acid. Analysis found: C, 29.91; H, 2.30; N, 2.87%; calculated for C<sub>12</sub>H<sub>11</sub>Cl<sub>2</sub>HgNO<sub>3</sub>: C, 29.49; H, 2.27; N, 2.87%.

**S3. Refinement**

H atoms were included in calculated positions and refined as riding, with C—H distances of 0.94 (aromatic), 0.98 (methylene) and 0.97 Å (methyl), and with  $U_{\text{iso}}(\text{aromatic and ethyl}) = 1.2U_{\text{eq}}(\text{C})$  and  $U_{\text{iso}}(\text{methylene}) = 1.5U_{\text{eq}}(\text{C})$ .

**Figure 1**

The molecular structure of (I), with 30% probability displacement ellipsoids [symmetry codes: (i)  $1 - x, -y, 2 - z$ ]. The dashed line indicates the weak  $\text{Hg}\cdots\text{Cl}$  interaction.



**Figure 2**

A view of intermolecular  $\pi$ - $\pi$  interactions, interactions between the parallel quinoline rings of neighbouring complexes [symmetry codes: (i)  $1 - x, 1 - y, 2 - z$ ; (ii)  $-x, 1 - y, 2 - z$ ].

### Dichlorido[methyl 2-(quinolin-8-yloxy- $\kappa^2N,O$ )acetate- $\kappa O$ ]mercury(II)

#### Crystal data

[HgCl<sub>2</sub>(C<sub>12</sub>H<sub>11</sub>NO<sub>3</sub>)]

$M_r = 488.71$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.2644$  (4) Å

$b = 9.7607$  (2) Å

$c = 10.8411$  (6) Å

$\alpha = 71.317$  (7)°

$\beta = 75.453$  (7)°

$\gamma = 69.816$  (8)°

$V = 674.87$  (5) Å<sup>3</sup>

$Z = 2$

$F(000) = 456$

$D_x = 2.405$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71075$  Å

Cell parameters from 3438 reflections

$\theta = 3.0$ – $27.5$ °

$\mu = 11.80$  mm<sup>-1</sup>

$T = 223$  K

Prism, yellow

$0.50 \times 0.25 \times 0.10$  mm

#### Data collection

Rigaku Saturn  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 14.63 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan  
(REQAB; Jacobson, 1998)  
 $T_{\min} = 0.067$ ,  $T_{\max} = 0.385$   
5090 measured reflections  
2432 independent reflections  
2330 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$   
 $\theta_{\max} = 25.5^\circ$ ,  $\theta_{\min} = 3.0^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -11 \rightarrow 9$   
 $l = -13 \rightarrow 10$

#### Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.142$   
 $S = 1.07$   
2432 reflections  
174 parameters  
0 restraints  
Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map  
Hydrogen site location: inferred from  
neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.114P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 3.58 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -2.39 \text{ e } \text{\AA}^{-3}$

#### 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.

**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  $F^2 > 2\sigma(F^2)$  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	0.48080 (4)	0.17195 (3)	0.82524 (2)	0.0283 (2)
Cl1	0.7584 (4)	0.0079 (3)	0.9214 (2)	0.0343 (5)
Cl2	0.2251 (4)	0.2330 (3)	0.7032 (2)	0.0328 (5)
O1	0.5887 (9)	0.4276 (6)	0.6794 (5)	0.0267 (12)
O2	0.9795 (10)	0.3004 (7)	0.4386 (6)	0.0293 (13)
O3	0.7782 (11)	0.1803 (7)	0.5930 (6)	0.0350 (15)
N1	0.3624 (11)	0.3914 (8)	0.9197 (6)	0.0229 (14)
C1	0.2572 (13)	0.3719 (9)	1.0411 (8)	0.0250 (17)
H1	0.2485	0.2744	1.0883	0.030*
C2	0.1591 (14)	0.4918 (11)	1.1008 (8)	0.0291 (19)
H2	0.0929	0.4727	1.1882	0.035*
C3	0.1596 (13)	0.6348 (10)	1.0327 (8)	0.0280 (18)
H3	0.0892	0.7160	1.0707	0.034*
C4	0.2680 (12)	0.6597 (9)	0.9034 (7)	0.0229 (16)
C5	0.2793 (15)	0.8066 (10)	0.8262 (9)	0.032 (2)
H5	0.2102	0.8915	0.8595	0.038*
C6	0.3906 (15)	0.8224 (9)	0.7043 (9)	0.0306 (19)
H6	0.3995	0.9189	0.6541	0.037*
C7	0.4920 (14)	0.6985 (10)	0.6522 (8)	0.0288 (19)

H7	0.5649	0.7133	0.5665	0.035*
C8	0.4873 (13)	0.5564 (9)	0.7230 (8)	0.0232 (16)
C9	0.3727 (12)	0.5317 (9)	0.8506 (7)	0.0226 (16)
C10	0.7341 (16)	0.4428 (10)	0.5679 (8)	0.030 (2)
H10A	0.8339	0.4787	0.5842	0.037*
H10B	0.6737	0.5164	0.4927	0.037*
C11	0.8301 (13)	0.2914 (9)	0.5380 (7)	0.0221 (16)
C12	1.0873 (14)	0.1595 (10)	0.3990 (9)	0.0313 (19)
H12A	1.1489	0.0841	0.4717	0.047*
H12B	1.1890	0.1780	0.3236	0.047*
H12C	0.9953	0.1234	0.3756	0.047*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Hg1	0.0304 (3)	0.0247 (3)	0.0247 (3)	-0.00519 (19)	-0.00101 (17)	-0.00514 (17)
C11	0.0304 (12)	0.0320 (12)	0.0350 (11)	-0.0028 (10)	-0.0050 (9)	-0.0083 (9)
C12	0.0360 (13)	0.0344 (11)	0.0255 (10)	-0.0096 (10)	-0.0038 (9)	-0.0057 (8)
O1	0.027 (3)	0.025 (3)	0.022 (3)	-0.011 (3)	0.017 (2)	-0.009 (2)
O2	0.030 (3)	0.025 (3)	0.028 (3)	-0.006 (3)	0.010 (3)	-0.012 (2)
O3	0.041 (4)	0.025 (3)	0.034 (3)	-0.013 (3)	0.014 (3)	-0.012 (2)
N1	0.027 (4)	0.023 (3)	0.019 (3)	-0.008 (3)	0.002 (3)	-0.009 (3)
C1	0.024 (4)	0.030 (4)	0.021 (4)	-0.007 (4)	0.000 (3)	-0.009 (3)
C2	0.029 (5)	0.039 (5)	0.019 (4)	-0.012 (4)	0.005 (4)	-0.012 (3)
C3	0.018 (4)	0.038 (5)	0.030 (4)	-0.005 (4)	0.003 (3)	-0.019 (4)
C4	0.020 (4)	0.024 (4)	0.022 (4)	-0.001 (3)	0.002 (3)	-0.011 (3)
C5	0.041 (6)	0.025 (4)	0.034 (4)	-0.012 (4)	0.000 (4)	-0.014 (4)
C6	0.034 (5)	0.017 (4)	0.034 (5)	-0.004 (4)	-0.003 (4)	-0.003 (3)
C7	0.035 (5)	0.028 (4)	0.022 (4)	-0.009 (4)	-0.002 (4)	-0.005 (3)
C8	0.021 (4)	0.020 (4)	0.024 (4)	-0.003 (3)	0.003 (3)	-0.009 (3)
C9	0.018 (4)	0.030 (4)	0.020 (3)	-0.006 (3)	-0.001 (3)	-0.009 (3)
C10	0.041 (6)	0.032 (5)	0.018 (4)	-0.015 (4)	0.010 (4)	-0.012 (3)
C11	0.023 (4)	0.024 (4)	0.019 (4)	-0.009 (3)	0.005 (3)	-0.008 (3)
C12	0.023 (5)	0.029 (5)	0.035 (5)	-0.002 (4)	0.011 (4)	-0.018 (4)

*Geometric parameters (Å, °)*

Hg1—C11	2.340 (2)	C3—C4	1.416 (12)
Hg1—C12	2.350 (2)	C3—H3	0.9400
Hg1—N1	2.463 (6)	C4—C9	1.432 (11)
Hg1—O1	2.746 (6)	C4—C5	1.428 (12)
Hg1—O3	2.876 (6)	C5—C6	1.357 (13)
Hg1—C11 <sup>i</sup>	3.204 (2)	C5—H5	0.9400
O1—C8	1.383 (10)	C6—C7	1.392 (13)
O1—C10	1.396 (10)	C6—H6	0.9400
O2—C11	1.329 (10)	C7—C8	1.361 (12)
O2—C12	1.468 (10)	C7—H7	0.9400
O3—C11	1.195 (10)	C8—C9	1.418 (11)

N1—C1	1.337 (11)	C10—C11	1.502 (12)
N1—C9	1.352 (11)	C10—H10A	0.9800
C1—C2	1.405 (12)	C10—H10B	0.9800
C1—H1	0.9400	C12—H12A	0.9700
C2—C3	1.355 (14)	C12—H12B	0.9700
C2—H2	0.9400	C12—H12C	0.9700
C11—Hg1—C12	153.41 (8)	C3—C4—C5	122.3 (7)
C11—Hg1—N1	106.61 (17)	C9—C4—C5	119.5 (7)
C12—Hg1—N1	99.30 (17)	C6—C5—C4	119.5 (8)
C11—Hg1—O1	105.43 (15)	C6—C5—H5	120.3
C12—Hg1—O1	91.75 (15)	C4—C5—H5	120.3
N1—Hg1—O1	62.08 (19)	C5—C6—C7	121.3 (8)
C11—Hg1—O3	80.81 (15)	C5—C6—H6	119.4
C12—Hg1—O3	92.53 (16)	C7—C6—H6	119.4
N1—Hg1—O3	117.7 (2)	C8—C7—C6	121.2 (8)
O1—Hg1—O3	56.55 (16)	C8—C7—H7	119.4
C11—Hg1—C11 <sup>i</sup>	83.50 (8)	C6—C7—H7	119.4
C12—Hg1—C11 <sup>i</sup>	90.92 (7)	C7—C8—O1	124.5 (7)
N1—Hg1—C11 <sup>i</sup>	89.63 (16)	C7—C8—C9	120.5 (7)
O1—Hg1—C11 <sup>i</sup>	151.64 (12)	O1—C8—C9	115.1 (7)
O3—Hg1—C11 <sup>i</sup>	151.45 (13)	N1—C9—C8	120.7 (7)
C8—O1—C10	116.4 (6)	N1—C9—C4	121.2 (7)
C8—O1—Hg1	115.6 (4)	C8—C9—C4	118.0 (7)
C10—O1—Hg1	128.0 (5)	O1—C10—C11	108.5 (7)
C11—O2—C12	115.3 (7)	O1—C10—H10A	110.0
C11—O3—Hg1	121.0 (5)	C11—C10—H10A	110.0
C1—N1—C9	119.1 (7)	O1—C10—H10B	110.0
C1—N1—Hg1	116.1 (5)	C11—C10—H10B	110.0
C9—N1—Hg1	124.1 (5)	H10A—C10—H10B	108.4
N1—C1—C2	122.4 (8)	O3—C11—O2	124.9 (8)
N1—C1—H1	118.8	O3—C11—C10	125.5 (8)
C2—C1—H1	118.8	O2—C11—C10	109.6 (7)
C3—C2—C1	120.2 (8)	O2—C12—H12A	109.5
C3—C2—H2	119.9	O2—C12—H12B	109.5
C1—C2—H2	119.9	H12A—C12—H12B	109.5
C2—C3—C4	118.8 (8)	O2—C12—H12C	109.5
C2—C3—H3	120.6	H12A—C12—H12C	109.5
C4—C3—H3	120.6	H12B—C12—H12C	109.5
C3—C4—C9	118.2 (7)		
C11—Hg1—O1—C8	-113.6 (5)	C3—C4—C5—C6	178.0 (9)
C12—Hg1—O1—C8	86.9 (5)	C9—C4—C5—C6	-0.6 (13)
N1—Hg1—O1—C8	-12.7 (5)	C4—C5—C6—C7	0.9 (15)
O3—Hg1—O1—C8	178.8 (6)	C5—C6—C7—C8	-1.8 (15)
C11 <sup>i</sup> —Hg1—O1—C8	-8.3 (7)	C6—C7—C8—O1	-178.0 (8)
C11—Hg1—O1—C10	65.7 (7)	C6—C7—C8—C9	2.2 (14)
C12—Hg1—O1—C10	-93.8 (7)	C10—O1—C8—C7	13.2 (13)

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N1—Hg1—O1—C10	166.6 (8)	Hg1—O1—C8—C7	-167.4 (7)
O3—Hg1—O1—C10	-1.9 (7)	C10—O1—C8—C9	-167.0 (8)
C11 <sup>i</sup> —Hg1—O1—C10	171.0 (6)	Hg1—O1—C8—C9	12.4 (9)
C11—Hg1—O3—C11	-110.2 (7)	C1—N1—C9—C8	178.2 (8)
C12—Hg1—O3—C11	95.7 (7)	Hg1—N1—C9—C8	-11.9 (11)
N1—Hg1—O3—C11	-6.1 (8)	C1—N1—C9—C4	-2.1 (11)
O1—Hg1—O3—C11	5.3 (6)	Hg1—N1—C9—C4	167.8 (6)
C11 <sup>i</sup> —Hg1—O3—C11	-167.7 (5)	C7—C8—C9—N1	177.9 (8)
C11—Hg1—N1—C1	-78.3 (6)	O1—C8—C9—N1	-1.9 (11)
C12—Hg1—N1—C1	95.7 (6)	C7—C8—C9—C4	-1.8 (12)
O1—Hg1—N1—C1	-177.3 (7)	O1—C8—C9—C4	178.4 (7)
O3—Hg1—N1—C1	-166.5 (5)	C3—C4—C9—N1	2.7 (12)
C11 <sup>i</sup> —Hg1—N1—C1	4.8 (6)	C5—C4—C9—N1	-178.7 (8)
C11—Hg1—N1—C9	111.5 (6)	C3—C4—C9—C8	-177.6 (8)
C12—Hg1—N1—C9	-74.5 (6)	C5—C4—C9—C8	1.0 (11)
O1—Hg1—N1—C9	12.5 (6)	C8—O1—C10—C11	178.6 (7)
O3—Hg1—N1—C9	23.4 (7)	Hg1—O1—C10—C11	-0.7 (11)
C11 <sup>i</sup> —Hg1—N1—C9	-165.4 (6)	Hg1—O3—C11—O2	173.0 (6)
C9—N1—C1—C2	-1.0 (12)	Hg1—O3—C11—C10	-8.8 (12)
Hg1—N1—C1—C2	-171.7 (7)	C12—O2—C11—O3	-1.6 (12)
N1—C1—C2—C3	3.6 (14)	C12—O2—C11—C10	179.9 (7)
C1—C2—C3—C4	-2.9 (13)	O1—C10—C11—O3	6.4 (13)
C2—C3—C4—C9	-0.1 (12)	O1—C10—C11—O2	-175.1 (7)
C2—C3—C4—C5	-178.7 (9)		

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Symmetry code: (i)  $-x+1, -y, -z+2$ .