

Chlorido[1-(2-ethoxyphenyl)3-(4-nitrophenyl)triazenido]mercury(II)

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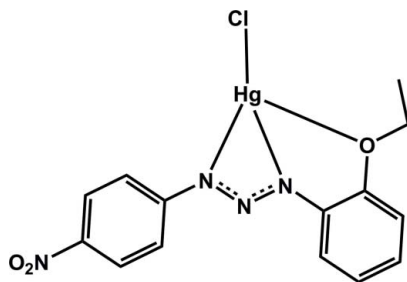
Received 6 June 2010; accepted 13 July 2010

Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.022; wR factor = 0.047; data-to-parameter ratio = 26.9.

In the title compound, $[\text{Hg}(\text{C}_{14}\text{H}_{13}\text{N}_4\text{O}_3)\text{Cl}]$, the Hg^{II} atom is four-coordinated by one O atom and two N atoms from a tridentate 1-(2-ethoxyphenyl)-3-(4-nitrophenyl)triazenido ligand and one terminal chloride ion in a distorted square-planar geometry. In the crystal structure, the mononuclear complexes are linked into pairs through $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds as well as $\pi-\pi$ and $\text{C}-\text{H}\cdots\pi$ stacking interactions. In addition, weak $\text{Hg}-\mu^6$ -arene π -interactions [mean distance of 3.667 (2) Å] are present between these dimers. The $\pi-\pi$ stacking interactions are between aromatic rings with a centroid-centroid distance of 3.884 (2) Å. Moreover, edge-to-face interactions are present between ethoxy CH groups and aromatic rings with $\text{H}\cdots\pi$ distances of 2.81 Å.

Related literature

For transition-metal complexes containing 1,3-diaryltriazenido ligands, see: Moore & Robinson (1986); Vrieze & Van Koten, (1987); Horner *et al.* (2006). For related structures, see: Melardi *et al.* (2007, 2009); Rofouei *et al.* (2009).



Experimental

Crystal data

$[\text{Hg}(\text{C}_{14}\text{H}_{13}\text{N}_4\text{O}_3)\text{Cl}]$

$M_r = 521.32$

Monoclinic, Cc
 $a = 13.4829$ (5) Å
 $b = 15.5746$ (6) Å
 $c = 7.7545$ (3) Å
 $\beta = 107.6355$ (6)°
 $V = 1551.84$ (10) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 10.11$ mm⁻¹
 $T = 120$ K
 $0.44 \times 0.10 \times 0.08$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\text{min}} = 0.142$, $T_{\text{max}} = 0.618$

11603 measured reflections
 5612 independent reflections
 5130 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.047$
 $S = 0.76$
 5612 reflections
 209 parameters
 2 restraints

H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.87$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.73$ e Å⁻³
 Absolute structure: Flack (1983),
 2739 Friedel pairs
 Flack parameter: 0.003 (5)

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the C1–C6 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C3}-\text{H3}\cdots\text{O3}^{\text{i}}$	0.95	2.54	3.489 (5)	174
$\text{C5}-\text{H5}\cdots\text{O2}^{\text{ii}}$	0.95	2.55	3.390 (5)	147
$\text{C9}-\text{H9}\cdots\text{Cl1}^{\text{iii}}$	0.95	2.80	3.738 (4)	169
$\text{C13}-\text{H13A}\cdots\text{O3}^{\text{iv}}$	0.99	2.47	3.431 (5)	162
$\text{C13}-\text{H13B}\cdots\text{Cg2}^{\text{v}}$	0.99	2.81	3.570 (4)	134

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; 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.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2293).

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supporting information

Acta Cryst. (2010). E66, m975 [https://doi.org/10.1107/S1600536810027819]

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S1. Comment

Triazene compounds characterized by having a diazoamino group ($-N=NN-$) commonly adopt a trans configuration in the ground state. The study of transition-metal complexes containing 1,3-diaryltriazene ligands has greatly increased in the past few years because of the versatility of their coordination forms, yielding a variety of coordination compounds with large structural diversity (Moore & Robinson, 1986; Vrieze & Van Koten, 1987; Horner *et al.*, 2006). The crystal structures of a few complexes related to the title compound have been reported recently (Melardi *et al.*, 2007; Rofouei *et al.*, 2009).

In the title complex (Fig. 1), the [1-(2-ethoxyphenyl)3-(4-nitrophenyl)]triazene ion is coordinated to the central atom Hg(II) through two N atoms [Hg1—N1 = 2.070 (3) Å and Hg1—N3 = 2.711 (3) Å] and one O atom [Hg1—O1 = 2.662 (2) Å]. In addition, a Cl⁻ ion is coordinated to Hg(II) atom with the bond distance Hg1—Cl1 = 2.269 (9) Å. These bond distances agree very well with the corresponding distances reported in related structures (Melardi *et al.*, 2007; Rofouei *et al.*, 2009). The atoms of the ligand and lie in a plane (maximum deviation from coplanarity being 0.115 (4) Å for O2 while Cl1 and Hg1 lie 1.402 (3) and 0.606 (2) Å, respectively, out of this plane. The molecules of the title complex are linked to form pairs through non-classical C—H \cdots O and C—H \cdots Cl hydrogen bond, as well as π - π and C—H \cdots π stacking interactions.

There are π - π stacking interactions present between aromatic rings with centroid-centroid distance of 3.884 (2) Å for Cg1 \cdots Cg1 (Cg1 = C7—C12, $x, 1 - y, z - 1/2$), and also edge-to-face interactions are present between CH group of ethoxy with aromatic rings with H \cdots π distance of 2.81 Å for C13—H13B \cdots Cg2 (Cg2 = C1—C6, $x, 1 - y, z - 1/2$). In addition, weak Hg- μ^6 -arene π -interactions (mean distance 3.667 (2) Å) are present between these dimers. The secondary Hg- μ^6 -arene π -interactions involve carbon atoms of the C1—C6 phenyl rings (Table 1, Fig. 2). The weak non-covalent interactions seem to play important role in the crystal packing and the formation of a desired framework. The unit cell packing of the title compound is shown in Fig. 3.

S2. Experimental

A methanol solution of 1-(2-ethoxyphenyl)-3-(4-nitrophenyl)triazene (0.286 g, 1 mmol) was added to a solution of mercury(II) chloride (0.270 g, 1 mmol). After mixing for 30 minutes at room temperature, solution of sodium acetate in water was added to adjust the pH at 6–6.2. After 2 h, a red solid was readily precipitated out. It was filtered off, washed with methanol and dried in vacuum. The orange crude material was dissolved in 10 ml of dichloromethane (CH₂Cl₂), and placed in a freezer without covering. After two weeks beautiful orange and air-stable crystals of the title complex were obtained by slow evaporation of the solvent; m.p. 460–462 K.

S3. Refinement

An absolute structure was established using Flack (1983) method. The H-atoms were placed in calculated positions with C—H = 0.95, 0.98 and 0.99 Å for aryl, methyl and methylene type H-atoms, respectively, and included in the refinement in riding mode with fixed isotropic displacement parameters ($U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the CH₃-groups and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the other groups). The highest positive residual electron density peak of 0.87 eÅ³ was localized at a distance of 0.91 Å from the Hg1 atom and was meaningless.

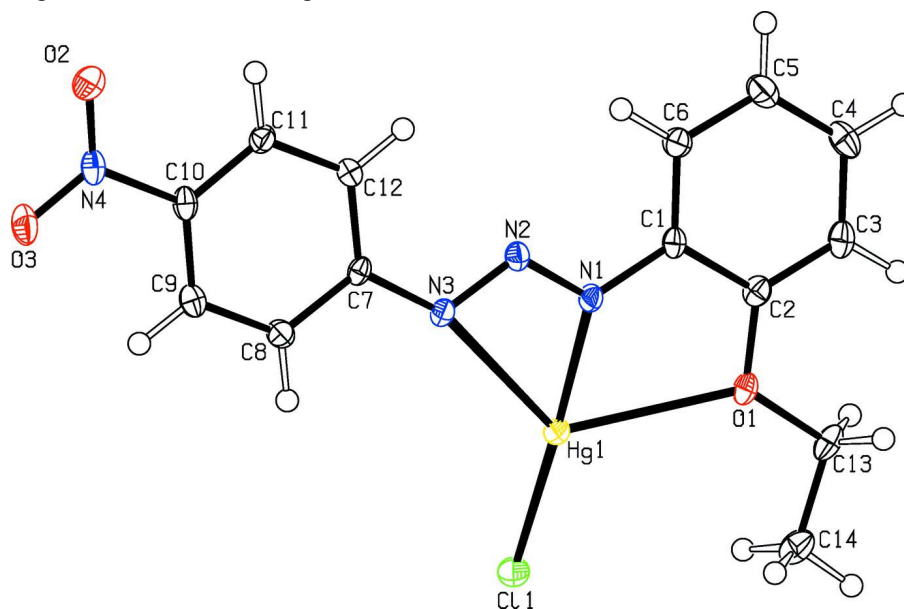


Figure 1

Molecular structure of the title compound, with ellipsoids drawn at 50% probability level.

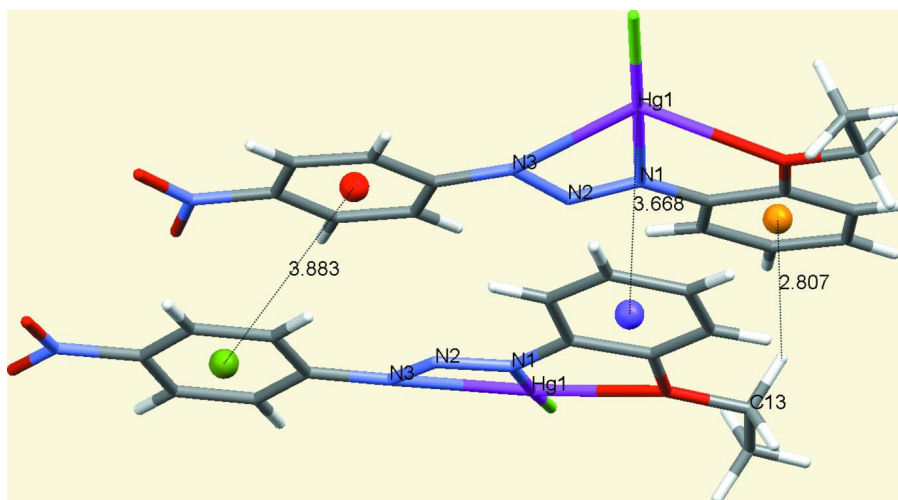


Figure 2

π - π , C—H \cdots π and weak Hg- μ^6 -arene stacking interactions between two [Hg(C₁₄H₁₃N₄O₃)Cl] moieties.

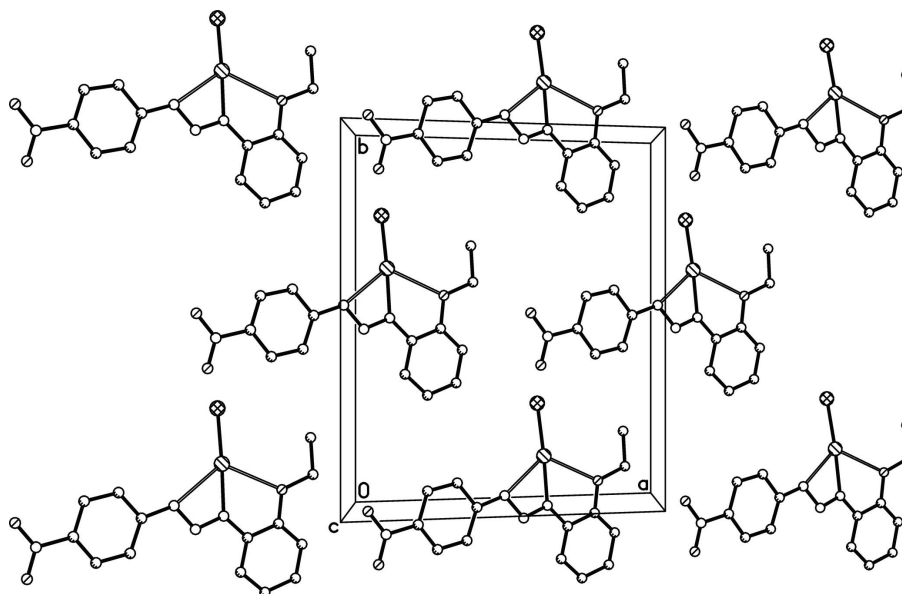


Figure 3

The unit cell packing diagram of the title compound along the *c* axis.

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Monoclinic, *Cc*

Hall symbol: C -2yc

a = 13.4829 (5) Å

b = 15.5746 (6) Å

c = 7.7545 (3) Å

β = 107.6355 (6)°

V = 1551.84 (10) Å³

Z = 4

F(000) = 984

D_x = 2.231 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 5899 reflections

θ = 2.6–32.6°

μ = 10.11 mm⁻¹

T = 120 K

Needle, red

0.44 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

T_{min} = 0.142, *T_{max}* = 0.618

11603 measured reflections

5612 independent reflections

5130 reflections with *I* > 2σ(*I*)

R_{int} = 0.031

θ_{\max} = 32.8°, θ_{\min} = 2.1°

h = -20→20

k = -23→23

l = -11→11

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.022

wR(*F*²) = 0.047

S = 0.76

5612 reflections

209 parameters

2 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

$w = 1/[\sigma^2(F_o^2)]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.87 \text{ e } \text{\AA}^{-3}$

$$\Delta\rho_{\min} = -0.73 \text{ e } \text{\AA}^{-3}$$

Absolute structure: Flack (1983), 2739 Friedel
 pairs

Absolute structure parameter: 0.003 (5)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.12017 (2)	0.366861 (6)	0.01531 (2)	0.01598 (3)
Cl1	0.09959 (7)	0.22761 (6)	-0.07489 (13)	0.02390 (18)
O1	0.29846 (19)	0.43726 (16)	0.0064 (3)	0.0186 (5)
O2	-0.3935 (2)	0.61872 (18)	0.3415 (5)	0.0284 (6)
O3	-0.4252 (2)	0.48304 (18)	0.3448 (4)	0.0251 (6)
N1	0.1308 (2)	0.49607 (17)	0.0809 (4)	0.0139 (5)
N2	0.0536 (2)	0.52465 (18)	0.1369 (4)	0.0143 (5)
N3	-0.0072 (2)	0.46291 (18)	0.1493 (4)	0.0135 (5)
N4	-0.3717 (2)	0.5440 (2)	0.3237 (4)	0.0178 (6)
C1	0.1976 (2)	0.5559 (2)	0.0397 (4)	0.0141 (6)
C2	0.2875 (3)	0.5247 (2)	0.0013 (4)	0.0158 (6)
C3	0.3560 (3)	0.5818 (2)	-0.0381 (5)	0.0207 (7)
H3	0.4169	0.5612	-0.0620	0.025*
C4	0.3359 (3)	0.6695 (3)	-0.0427 (5)	0.0240 (8)
H4	0.3840	0.7086	-0.0675	0.029*
C5	0.2464 (3)	0.7004 (2)	-0.0112 (5)	0.0240 (7)
H5	0.2326	0.7604	-0.0169	0.029*
C6	0.1767 (3)	0.6436 (2)	0.0287 (5)	0.0177 (6)
H6	0.1149	0.6646	0.0484	0.021*
C7	-0.0947 (2)	0.4891 (2)	0.1988 (4)	0.0126 (6)
C8	-0.1560 (3)	0.4226 (2)	0.2309 (5)	0.0162 (6)
H8	-0.1348	0.3647	0.2252	0.019*
C9	-0.2472 (3)	0.4396 (2)	0.2710 (5)	0.0169 (6)
H9	-0.2888	0.3943	0.2931	0.020*
C10	-0.2762 (3)	0.5245 (2)	0.2780 (5)	0.0158 (6)
C11	-0.2170 (3)	0.5921 (2)	0.2465 (5)	0.0155 (6)
H11	-0.2385	0.6498	0.2531	0.019*
C12	-0.1261 (3)	0.5744 (2)	0.2052 (5)	0.0155 (6)
H12	-0.0853	0.6200	0.1813	0.019*
C13	0.3904 (3)	0.4016 (3)	-0.0273 (5)	0.0206 (7)

H13A	0.4541	0.4228	0.0641	0.025*
H13B	0.3930	0.4188	-0.1487	0.025*
C14	0.3835 (3)	0.3054 (2)	-0.0161 (6)	0.0251 (8)
H14A	0.4450	0.2792	-0.0368	0.038*
H14B	0.3207	0.2851	-0.1083	0.038*
H14C	0.3802	0.2891	0.1042	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.01404 (5)	0.01342 (4)	0.02179 (5)	0.00069 (9)	0.00741 (3)	-0.00111 (10)
C11	0.0207 (4)	0.0148 (4)	0.0376 (5)	0.0004 (3)	0.0109 (4)	-0.0046 (3)
O1	0.0137 (11)	0.0211 (12)	0.0250 (13)	0.0020 (9)	0.0117 (10)	-0.0003 (10)
O2	0.0230 (14)	0.0235 (14)	0.0441 (18)	0.0042 (11)	0.0182 (13)	0.0018 (12)
O3	0.0175 (13)	0.0306 (15)	0.0307 (15)	-0.0056 (11)	0.0127 (12)	-0.0014 (12)
N1	0.0124 (12)	0.0148 (12)	0.0164 (12)	-0.0001 (10)	0.0070 (11)	-0.0015 (10)
N2	0.0123 (12)	0.0168 (13)	0.0144 (13)	-0.0011 (10)	0.0048 (10)	0.0009 (10)
N3	0.0111 (12)	0.0162 (13)	0.0133 (12)	0.0012 (10)	0.0040 (10)	0.0011 (10)
N4	0.0134 (13)	0.0239 (15)	0.0179 (14)	-0.0031 (11)	0.0074 (11)	-0.0009 (11)
C1	0.0115 (14)	0.0188 (15)	0.0127 (14)	-0.0012 (11)	0.0048 (11)	-0.0004 (12)
C2	0.0161 (15)	0.0196 (16)	0.0132 (14)	0.0017 (12)	0.0067 (12)	0.0004 (12)
C3	0.0151 (15)	0.0282 (19)	0.0209 (17)	-0.0013 (13)	0.0088 (13)	-0.0001 (14)
C4	0.0261 (19)	0.0242 (18)	0.0256 (18)	-0.0077 (15)	0.0134 (16)	0.0024 (15)
C5	0.0248 (19)	0.0191 (17)	0.0308 (19)	-0.0043 (14)	0.0123 (16)	0.0012 (15)
C6	0.0188 (16)	0.0169 (15)	0.0203 (16)	0.0005 (12)	0.0100 (13)	-0.0003 (12)
C7	0.0103 (13)	0.0176 (15)	0.0103 (13)	0.0016 (11)	0.0037 (11)	0.0007 (11)
C8	0.0168 (15)	0.0148 (14)	0.0180 (15)	-0.0013 (12)	0.0067 (12)	-0.0005 (12)
C9	0.0163 (15)	0.0197 (16)	0.0157 (15)	-0.0036 (12)	0.0065 (12)	-0.0010 (12)
C10	0.0138 (15)	0.0221 (16)	0.0135 (14)	-0.0028 (12)	0.0070 (13)	-0.0010 (12)
C11	0.0129 (14)	0.0161 (15)	0.0181 (15)	0.0012 (12)	0.0055 (12)	-0.0014 (12)
C12	0.0142 (15)	0.0144 (14)	0.0180 (15)	-0.0023 (11)	0.0053 (12)	0.0004 (12)
C13	0.0144 (15)	0.0272 (18)	0.0211 (16)	0.0060 (14)	0.0069 (13)	-0.0027 (15)
C14	0.0222 (18)	0.0262 (19)	0.0289 (19)	0.0072 (15)	0.0107 (16)	-0.0008 (15)

Geometric parameters (Å, °)

Hg1—N1	2.070 (3)	C5—C6	1.392 (5)
Hg1—C11	2.2699 (9)	C5—H5	0.9500
Hg1—O1	2.662 (2)	C6—H6	0.9500
Hg1—N3	2.711 (3)	C7—C8	1.394 (4)
O1—C2	1.370 (4)	C7—C12	1.401 (5)
O1—C13	1.453 (4)	C8—C9	1.382 (5)
O2—N4	1.218 (4)	C8—H8	0.9500
O3—N4	1.233 (4)	C9—C10	1.385 (5)
N1—N2	1.320 (4)	C9—H9	0.9500
N1—C1	1.399 (4)	C10—C11	1.387 (5)
N2—N3	1.286 (4)	C11—C12	1.385 (5)
N3—C7	1.406 (4)	C11—H11	0.9500

N4—C10	1.467 (4)	C12—H12	0.9500
C1—C6	1.392 (4)	C13—C14	1.505 (6)
C1—C2	1.419 (4)	C13—H13A	0.9900
C2—C3	1.382 (5)	C13—H13B	0.9900
C3—C4	1.390 (6)	C14—H14A	0.9800
C3—H3	0.9500	C14—H14B	0.9800
C4—C5	1.389 (6)	C14—H14C	0.9800
C4—H4	0.9500		
N1—Hg1—C11	175.95 (8)	C1—C6—C5	120.0 (3)
N1—Hg1—O1	67.07 (9)	C1—C6—H6	120.0
C11—Hg1—O1	114.37 (6)	C5—C6—H6	120.0
N1—Hg1—N3	51.23 (10)	C8—C7—C12	119.8 (3)
C11—Hg1—N3	127.80 (6)	C8—C7—N3	115.2 (3)
O1—Hg1—N3	117.69 (8)	C12—C7—N3	124.9 (3)
C2—O1—C13	117.8 (3)	C9—C8—C7	120.9 (3)
C2—O1—Hg1	108.66 (19)	C9—C8—H8	119.5
C13—O1—Hg1	132.3 (2)	C7—C8—H8	119.5
N2—N1—C1	118.5 (3)	C8—C9—C10	118.3 (3)
N2—N1—Hg1	114.0 (2)	C8—C9—H9	120.9
C1—N1—Hg1	126.3 (2)	C10—C9—H9	120.9
N3—N2—N1	110.9 (3)	C9—C10—C11	122.2 (3)
N2—N3—C7	114.2 (3)	C9—C10—N4	119.1 (3)
N2—N3—Hg1	83.78 (18)	C11—C10—N4	118.7 (3)
C7—N3—Hg1	161.0 (2)	C12—C11—C10	119.1 (3)
O2—N4—O3	123.4 (3)	C12—C11—H11	120.4
O2—N4—C10	119.0 (3)	C10—C11—H11	120.4
O3—N4—C10	117.6 (3)	C11—C12—C7	119.7 (3)
C6—C1—N1	122.4 (3)	C11—C12—H12	120.2
C6—C1—C2	119.5 (3)	C7—C12—H12	120.2
N1—C1—C2	118.1 (3)	O1—C13—C14	107.4 (3)
O1—C2—C3	124.9 (3)	O1—C13—H13A	110.2
O1—C2—C1	115.2 (3)	C14—C13—H13A	110.2
C3—C2—C1	119.8 (3)	O1—C13—H13B	110.2
C2—C3—C4	120.0 (3)	C14—C13—H13B	110.2
C2—C3—H3	120.0	H13A—C13—H13B	108.5
C4—C3—H3	120.0	C13—C14—H14A	109.5
C5—C4—C3	120.7 (3)	C13—C14—H14B	109.5
C5—C4—H4	119.7	H14A—C14—H14B	109.5
C3—C4—H4	119.7	C13—C14—H14C	109.5
C4—C5—C6	119.9 (4)	H14A—C14—H14C	109.5
C4—C5—H5	120.0	H14B—C14—H14C	109.5
C6—C5—H5	120.0		
N1—Hg1—O1—C2	-16.5 (2)	N1—C1—C2—O1	0.9 (4)
C11—Hg1—O1—C2	159.32 (18)	C6—C1—C2—C3	3.1 (5)
N3—Hg1—O1—C2	-24.7 (2)	N1—C1—C2—C3	-179.3 (3)
N1—Hg1—O1—C13	176.7 (3)	O1—C2—C3—C4	178.8 (3)

C11—Hg1—O1—C13	-7.4 (3)	C1—C2—C3—C4	-1.0 (5)
N3—Hg1—O1—C13	168.5 (3)	C2—C3—C4—C5	-1.2 (5)
O1—Hg1—N1—N2	-173.2 (2)	C3—C4—C5—C6	1.2 (6)
N3—Hg1—N1—N2	-2.54 (18)	N1—C1—C6—C5	179.4 (3)
O1—Hg1—N1—C1	19.7 (2)	C2—C1—C6—C5	-3.1 (5)
N3—Hg1—N1—C1	-169.6 (3)	C4—C5—C6—C1	0.9 (6)
C1—N1—N2—N3	172.7 (3)	N2—N3—C7—C8	-173.8 (3)
Hg1—N1—N2—N3	4.5 (3)	N2—N3—C7—C12	10.7 (4)
N1—N2—N3—C7	-176.7 (3)	C12—C7—C8—C9	-0.7 (5)
N1—N2—N3—Hg1	-3.1 (2)	N3—C7—C8—C9	-176.5 (3)
N1—Hg1—N3—N2	2.39 (17)	C7—C8—C9—C10	0.1 (5)
C11—Hg1—N3—N2	-172.60 (15)	C8—C9—C10—C11	0.0 (5)
O1—Hg1—N3—N2	12.1 (2)	C8—C9—C10—N4	-178.9 (3)
N1—Hg1—N3—C7	164.2 (7)	O2—N4—C10—C9	175.2 (3)
C11—Hg1—N3—C7	-10.8 (7)	O3—N4—C10—C9	-3.7 (5)
O1—Hg1—N3—C7	173.8 (6)	O2—N4—C10—C11	-3.6 (5)
N2—N1—C1—C6	-10.1 (5)	O3—N4—C10—C11	177.4 (3)
Hg1—N1—C1—C6	156.5 (3)	C9—C10—C11—C12	0.5 (5)
N2—N1—C1—C2	172.4 (3)	N4—C10—C11—C12	179.3 (3)
Hg1—N1—C1—C2	-21.0 (4)	C10—C11—C12—C7	-1.0 (5)
C13—O1—C2—C3	1.7 (5)	C8—C7—C12—C11	1.1 (5)
Hg1—O1—C2—C3	-167.2 (3)	N3—C7—C12—C11	176.5 (3)
C13—O1—C2—C1	-178.5 (3)	C2—O1—C13—C14	-179.4 (3)
Hg1—O1—C2—C1	12.6 (3)	Hg1—O1—C13—C14	-13.6 (4)
C6—C1—C2—O1	-176.7 (3)		

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C1—C6 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C3—H3...O3 ⁱ	0.95	2.54	3.489 (5)	174
C5—H5...O2 ⁱⁱ	0.95	2.55	3.390 (5)	147
C9—H9...C11 ⁱⁱⁱ	0.95	2.80	3.738 (4)	169
C13—H13A...O3 ^{iv}	0.99	2.47	3.431 (5)	162
C13—H13B...Cg2 ^v	0.99	2.81	3.570 (4)	134

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