

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

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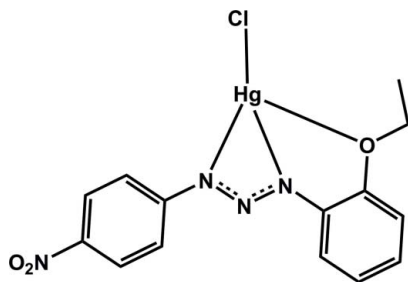
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Key indicators: single-crystal X-ray study;  $T = 120$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.022;  $wR$  factor = 0.047; data-to-parameter ratio = 26.9.

In the title compound,  $[\text{Hg}(\text{C}_{14}\text{H}_{13}\text{N}_4\text{O}_3)\text{Cl}]$ , the  $\text{Hg}^{\text{II}}$  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  $\pi$ -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) Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 10.11$  mm<sup>-1</sup>  
 $T = 120$  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<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.73$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 2739 Friedel pairs  
 Flack parameter: 0.003 (5)

**Table 1**

Hydrogen-bond geometry (Å, °).

$\text{Cg}_2$  is the centroid of the C1–C6 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}3-\text{H}3\cdots\text{O}3^{\text{i}}$	0.95	2.54	3.489 (5)	174
$\text{C}5-\text{H}5\cdots\text{O}2^{\text{ii}}$	0.95	2.55	3.390 (5)	147
$\text{C}9-\text{H}9\cdots\text{Cl}^{\text{iii}}$	0.95	2.80	3.738 (4)	169
$\text{C}13-\text{H}13\text{A}\cdots\text{O}3^{\text{iv}}$	0.99	2.47	3.431 (5)	162
$\text{C}13-\text{H}13\text{B}\cdots\text{Cg}2^{\text{v}}$	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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**supplementary materials**

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

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### 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<sup>-</sup> 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  $\pi$ - $\pi$  and C—H $\cdots$  $\pi$  stacking interactions.

There are  $\pi$ - $\pi$  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 $\cdots$  $\pi$  distance of 2.81 Å for C13—H13B $\cdots$ Cg2 (Cg2 = C1—C6,  $x, 1 - y, z - 1/2$ ). In addition, weak Hg- $\mu^6$ -arene  $\pi$ -interactions (mean distance 3.667 (2) Å) are present between these dimers. The secondary Hg- $\mu^6$ -arene  $\pi$ -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.

### 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 (CH<sub>2</sub>Cl<sub>2</sub>), 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.

### 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

## supplementary materials

riding mode with fixed isotropic displacement parameters ( $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for the  $\text{CH}_3$ -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  $0.87 \text{ e}\text{\AA}^3$  was localized at a distance of  $0.91 \text{ \AA}$  from the Hg1 atom and was meaningless.

### Figures

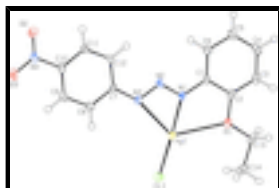


Fig. 1. Molecular structure of the title compound, with ellipsoids drawn at 50% probability level.

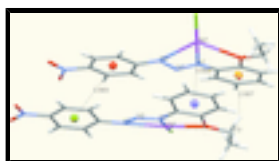


Fig. 2.  $\pi$ - $\pi$ , C—H $\cdots$  $\pi$  and weak Hg- $\mu^6$ -arene stacking interactions between two  $[\text{Hg}(\text{C}_{14}\text{H}_{13}\text{N}_4\text{O}_3)\text{Cl}]$  moieties.

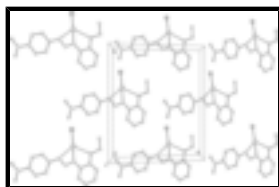


Fig. 3. The unit cell packing diagram of the title compound along the  $c$  axis.

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

#### Crystal data

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$M_r = 521.32$

Monoclinic,  $Cc$

Hall symbol:  $C -2yc$

$a = 13.4829 (5) \text{ \AA}$

$b = 15.5746 (6) \text{ \AA}$

$c = 7.7545 (3) \text{ \AA}$

$\beta = 107.6355 (6)^\circ$

$V = 1551.84 (10) \text{ \AA}^3$

$Z = 4$

$F(000) = 984$

$D_x = 2.231 \text{ Mg m}^{-3}$

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

Cell parameters from 5899 reflections

$\theta = 2.6\text{--}32.6^\circ$

$\mu = 10.11 \text{ mm}^{-1}$

$T = 120 \text{ K}$

Needle, red

$0.44 \times 0.10 \times 0.08 \text{ mm}$

#### Data collection

Bruker APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube  
graphite

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)

5612 independent reflections

5130 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\text{max}} = 32.8^\circ$ ,  $\theta_{\text{min}} = 2.1^\circ$

$h = -20 \rightarrow 20$

$T_{\min} = 0.142$ ,  $T_{\max} = 0.618$   
11603 measured reflections

$k = -23 \rightarrow 23$   
 $l = -11 \rightarrow 11$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.047$	$w = 1/[\sigma^2(F_o^2)]$
$S = 0.76$	where $P = (F_o^2 + 2F_c^2)/3$
5612 reflections	$(\Delta/\sigma)_{\max} = 0.002$
209 parameters	$\Delta\rho_{\max} = 0.87 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\min} = -0.73 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2739 Friedel pairs Flack 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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*

## supplementary materials

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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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Hg1	0.01404 (5)	0.01342 (4)	0.02179 (5)	0.00069 (9)	0.00741 (3)	-0.00111 (10)
Cl1	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—Cl1	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—Cl1	175.95 (8)	C1—C6—C5	120.0 (3)
N1—Hg1—O1	67.07 (9)	C1—C6—H6	120.0
Cl1—Hg1—O1	114.37 (6)	C5—C6—H6	120.0
N1—Hg1—N3	51.23 (10)	C8—C7—C12	119.8 (3)
Cl1—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

## supplementary materials

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)
Cl1—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)
Cl1—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)
Cl1—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)
Cl1—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 <sup>i</sup>	0.95	2.54	3.489 (5)	174
C5—H5...O2 <sup>ii</sup>	0.95	2.55	3.390 (5)	147
C9—H9...Cl1 <sup>iii</sup>	0.95	2.80	3.738 (4)	169
C13—H13A...O3 <sup>iv</sup>	0.99	2.47	3.431 (5)	162
C13—H13B...Cg2 <sup>v</sup>	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)  $x, -y+1, z-1/2$ .



Fig. 1

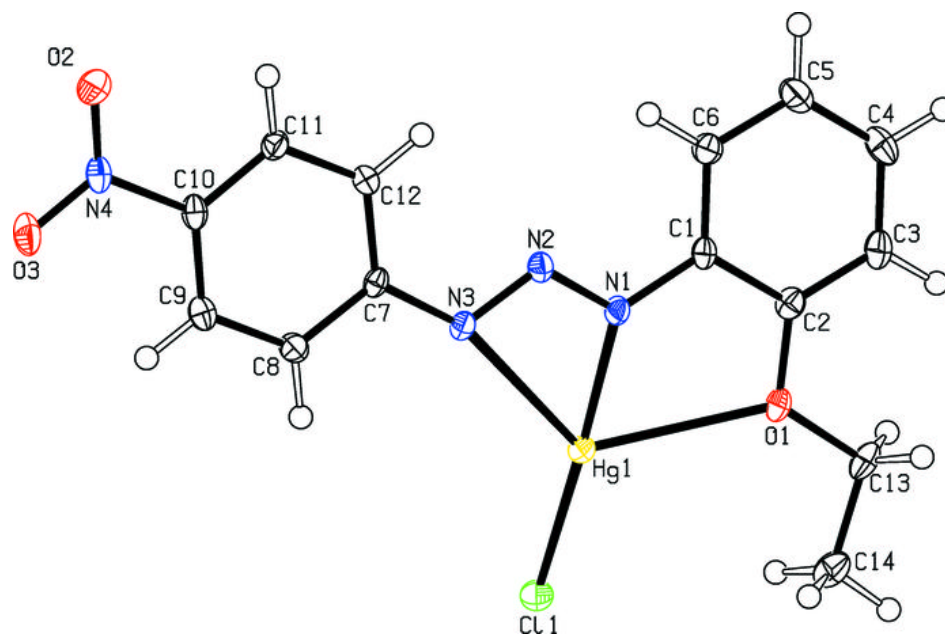


Fig. 2

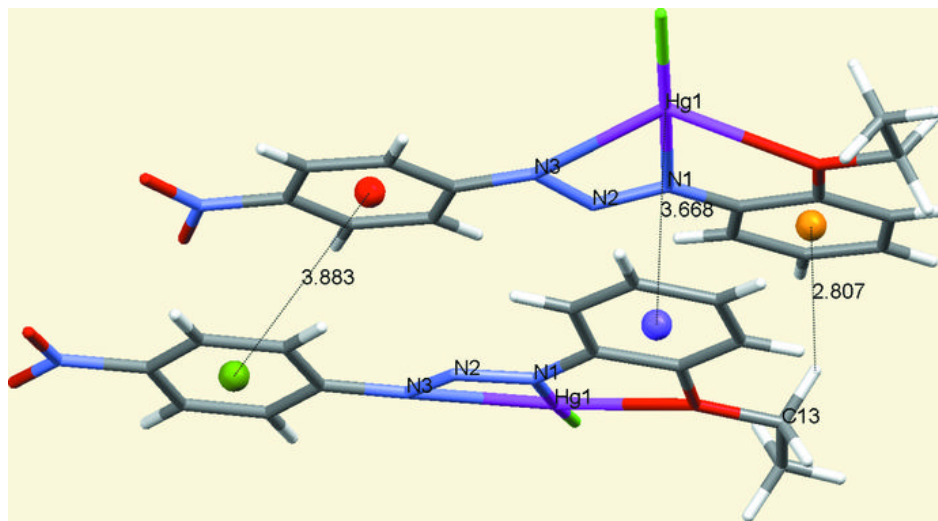


Fig. 3

