Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

[1,3-Bis(2-ethoxyphenyl)triazenido]bromidomercury(II)

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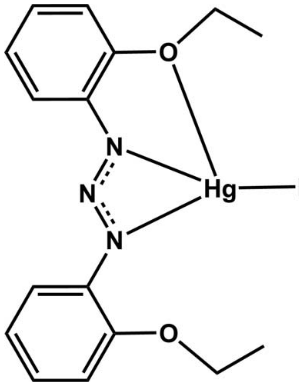
Received 20 August 2009; accepted 24 September 2009

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.029; wR factor = 0.062; data-to-parameter ratio = 23.5.

To the central atom of the title compound, [HgBr($C_{16}H_{18}N_3O_2$)], is attached one bromide ion and a 1,3-bis(2-ethoxyphenyl)triazenide ligand through one O and two N atoms, forming a distorted square-planar geometry around the Hg^{II} atom. The mononuclear complexes are linked into centrosymmetric dimers by non-classical intermolecular C—H⋯N hydrogen bonds and by weak Hg–η^3-arene π-interactions [mean distance = 3.434 (3) Å]. The resulting dimeric units are assembled into zigzag chains by translation along the crystallographic c axis through secondary C—H⋯π edge-to-face benzene ring interactions.

Related literature

For aryl triazenes, their structural properties and metal complexes see: Vrieze & Van Koten (1987); Hörner *et al.* (2002, 2004, 2006). For the different coordination modes of the triazenide ligand, see: Moore & Robinson (1986). For the synthesis and molecular structure of similar structures with cyano, methoxy and ethoxy groups, see: Melardi *et al.* (2008); Rofouei *et al.* (2006); Rofouei, Melardi, Salemi *et al.* (2009). For the synthesis and crystal structures of Hg^{II} complexes with [1,3-bis(2-methoxyphenyl)]triazene by using $HgCl_2$, $HgBr_2$, $Hg(CH_3COO)_2$ and $Hg(SCN)_2$ salts as starting materials, see: Melardi *et al.* (2007); Hematyar & Rofouei (2008); Rofouei, Hematyar *et al.* (2009). For the synthesis and crystal structures of cadmium(II) and silver(I) complexes with 1,3-bis(2-methoxyphenyl)triazene, see: Rofouei, Melardi, Khalili Ghaydari *et al.* (2009) and Payehghadr *et al.* (2007), respectively. For the synthesis and characterization of an isomorphous Hg^{II} structure with [1,3-bis(2-ethoxyphenyl)]triazene by using $HgCl_2$ instead of $HgBr_2$, see: Melardi *et al.* (2009).



Experimental

Crystal data

[HgBr($C_{16}H_{18}N_3O_2$)]
M_r = 564.83
Monoclinic, $P2_1/n$
a = 10.2359 (7) Å
b = 7.4659 (5) Å
c = 22.4123 (14) Å
β = 98.860 (6)°
V = 1692.32 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 11.47 mm^{-1}
T = 100 K
0.28 × 0.12 × 0.03 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998) T_{min} = 0.221, T_{max} = 0.709
20759 measured reflections
4943 independent reflections
4081 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.062
S = 1.00
4943 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.33 e Å^{-3}
$\Delta\rho_{min}$ = −1.43 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C13—H13B⋯N2^{i}	0.99	2.60	3.496 (5)	151
C12—H12⋯Cg1^{ii}	0.95	2.85	3.559 (4)	132
C13—H13A⋯Cg1^{iii}	0.99	2.72	3.523 (4)	139

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x, -y+1, -z$. Cg1 is the centroid of the C7–C12 aromatic ring.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *Mercury* (Macrae *et al.*, 2006), *PLATON* (Spek, 2009) and *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: OM2271).

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supplementary materials

Acta Cryst. (2009). E**65**, m1259-m1260 [**doi:10.1107/S1600536809038732**]

[1,3-Bis(2-ethoxyphenyl)triazenido]bromidomercury(II)

M. K. Rofouei, A. Beiza and J. Attar Gharamaleki

Comment

Transition metal complexes containing 1,3-diaryltriazenide ligands have been the object of numerous structural studies in the past few years because of their diverse range of coordination geometries. The uncoordinated –NN–N– compounds commonly adopt a *trans* configuration in the ground state. As ligands they exhibit versatile coordination geometries: with single or twofold nitrogen chains, neutral or anionic (triazenides) donor sets; they can be monodentate, (N1, N3)-chelating towards one metal atom or (N1, N3)-bridging over two metal atoms (Moore & Robinson, 1986), and they show a remarkable ability to support the stereochemical requisites of a wide variety of transition metal complexes (Hörner *et al.*, 2002, 2004). In these compounds, secondary bonds, or interactions such as hydrogen bonds and metal π-aryl interactions, can play an important role in their structures (Vrieze & Van Koten, 1987; Hörner *et al.*, 2006). We have previously reported the synthesis of the ligands, 1,3-bis(2-methoxyphenyl)]triazene (Rofouei *et al.*, 2006), [1,3-bis(2-ethoxyphenyl)]triazene (Rofouei, Melardi, Salemi *et al.*, 2009), and [1,3-bis(2-cyanophenyl)]triazene (Melardi *et al.*, 2008). Representative metal complexes include the Hg^{II} complex with [1,3-bis(2-methoxyphenyl)]triazene by using $HgCl_2$ (Melardi *et al.*, 2007), $HgBr_2$ (Hematyar & Rofouei 2008), $Hg(CH_3COO)_2$ and $Hg(SCN)_2$ (Rofouei, Hematyar *et al.*, 2009) salts as starting materials. In addition, Ag(I) and Cd(II) complexes with this ligand are known (Payehghadr *et al.*, 2007; Rofouei, Melardi, Khalili Ghaydari *et al.*, 2009). More recently, a Hg^{II} complex with [1,3-bis(2-ethoxyphenyl)]triazene as ligand was reported in which $HgCl_2$ was used as the starting salt (Melardi *et al.*, 2009). In this paper, a Hg^{II} complex using $HgBr_2$ as a starting material is reported. It is isomorphous to the latter chloride complex.

The molecular structure of $HgBr(C_{16}H_{18}N_3O_2)$ is presented in Fig. 1. The Hg^{II} atom is coordinated by one triazenide and one bromide ion. The 1,3-bis(2-ethoxyphenyl)triazenide is coordinated to the central atom through two N atoms [Hg1–N1 = 2.086 (3) Å and Hg1–N3 = 2.660 (3) Å] and one O atom [Hg1–O1 = 2.722 (3) Å] at a relatively long distance. The Hg1–Br1 distance of 2.4014 (4) Å is shorter than the corresponding distance in 1,3-bis(2-methoxyphenyl) with Hg1–Br1 = 2.5175 (11) Å (Hematyar & Rofouei, 2008). The Hg–Cl, Hg–O and Hg–N bonds distances in the isomorphous chloride, $HgCl(C_{16}H_{18}N_3O_2)$, are 2.284 (8), 2.721 (2), 2.074 (2) and 2.674 (2) Å, respectively. The atoms of the ligand and the bromide ion generate a plane (maximum deviation from coplanarity of 0.037 Å).

In the title compound, the monomeric $HgBr(C_{16}H_{18}N_3O_2)$ moieties are linked to pairs through non-classical C13–H13B···N2 hydrogen bond (C13···N2 = 3.496 (5) Å and <C13–H13B···N2 = 151 °, symmetry code (-*x*, 2 - *y*, -*z*). Also, weak Hg-η^3-arene π-interactions (mean distance of 3.434 (3) Å) are present between these dimers. The secondary Hg-η^3-arene π-interactions involving three carbon atoms of the C1–C6 phenyl ring. These metal-π interactions involve the Hg1 atom and C4 [3.461 (5) Å], C5 [3.254 (5) Å] and C6 [3.515 (5) Å] atoms with related symmetry code (-*x*, 2 - *y*, -*z*) (Fig. 2). The resulted dimeric units are assembled into zigzag chains by translation along the crystallographic *c* axis through secondary C–H···π stacking interactions. These edge-to-face interactions are present between CH group of phenyl rings and aromatic rings with H···π distances of 2.72 and 2.85 Å for C13–H13A···*Cg*1 [symmetry code: 1/2 - *x*, -1/2 + *y*, 1/2 - *z*] and C12–H12···*Cg*1 [symmetry code: -*x*, 1 - *y*, -*z*], respectively in which *Cg*1 is the centroid for C7—C12 aromatic ring (Fig. 3).

The sum of the weak non-covalent interactions seems to play an important role in the crystal packing. The unit cell packing diagram of the title compound is shown in Fig. 4.

Experimental

A methanol solution of 1,3-bis(2-ethoxyphenyl)triazene (0.2853 g, 1 mmol) was added to a methanol solution of mercury(II) bromide (0.3604 g, 1 mmol). After mixing for 1 h at room temperature, an orange solid was readily precipitated out. It was then filtered off, washed with methanol and dried in vacuum. The orange crude material was dissolved in 10 ml of THF, 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.

Refinement

Positions of the H(C) were calculated from geometry with C—H = 0.95 - 0.99 Å. All hydrogen atoms were refined by use of a riding model with U_{iso}(H) parameters equal to 1.5 U_{eq}(C) for methyl groups and to 1.2 U_{eq}(C) for other carbon atoms where U_{eq}(C) are the equivalent isotropic thermal parameters of the atoms to which the corresponding H atoms are bonded.

Figures

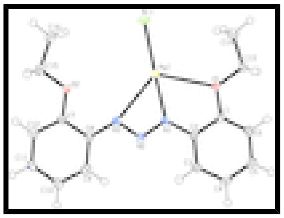

Fig. 1. Molecular structure of the title compound, with ellipsoids drawn at the 50% probability level.

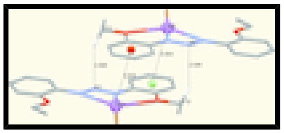

Fig. 2. Non-classical C13–H13B···N2 hydrogen bond with H13B···N2 distance of 2.60 Å and weak Hg-η^3-arene π-interactions (mean distance of 3.434 (3) Å) between dimers. The secondary Hg-η^3-arene π-interactions involve three carbon atoms of the C1–C6 phenyl ring.

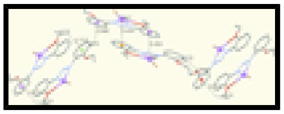

Fig. 3. C–H···π stacking interactions between CH group of phenyl rings and aromatic rings with H···π distances of 2.72 and 2.85 Å for C13–H13A···*Cg*1 and C12–H12···*Cg*1 (*Cg*1 is the centroid for the C7—C12 aromatic ring).

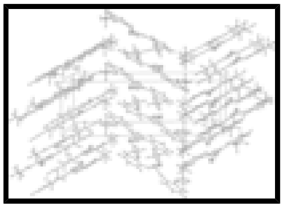

Fig. 4. The packing diagram of the title compound.

[1,3-Bis(2-ethoxyphenyl)triazenido]bromidomercury(II)

Crystal data

[HgBr($C_{16}H_{18}N_3O_2$)]

F_{000} = 1064

M_r = 564.83

D_x = 2.217 Mg m^{-3}

Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.2359 (7) Å
b = 7.4659 (5) Å
c = 22.4123 (14) Å
β = 98.860 (6)°
V = 1692.32 (19) Å^3
Z = 4

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4844 reflections
θ = 2.3–29.5°
μ = 11.47 mm^{-1}
T = 100 K
Plate, orange
0.28 × 0.12 × 0.03 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 100 K
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1998)
$T_{\min}$ = 0.221, $T_{\max}$ = 0.709
20759 measured reflections

4943 independent reflections
4081 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
$\theta_{\max}$ = 30.0°
$\theta_{\min}$ = 2.1°
$h = -14 \rightarrow 14$
$k = -10 \rightarrow 10$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.062
S = 1.00
4943 reflections
210 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.01P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 1.33 e Å^{-3}
$\Delta\rho_{\min}$ = −1.43 e Å^{-3}
Extinction correction: none

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. The maximum and minimum difference map peaks are within 1.21 Å of Hg1.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Hg1	−0.152069 (14)	0.681795 (19)	0.053806 (7)	0.01739 (5)
Br1	−0.36007 (4)	0.63210 (6)	0.08813 (2)	0.02803 (10)
O1	−0.1764 (2)	0.8602 (3)	−0.05325 (12)	0.0160 (5)
O2	0.0190 (3)	0.4368 (3)	0.20087 (13)	0.0175 (6)
N1	0.0246 (3)	0.7115 (4)	0.01922 (15)	0.0148 (6)
N2	0.1262 (3)	0.6390 (4)	0.05569 (15)	0.0140 (6)
N3	0.0888 (3)	0.5769 (4)	0.10309 (15)	0.0147 (6)
C1	−0.0555 (3)	0.8727 (5)	−0.07197 (17)	0.0127 (7)
C2	0.0503 (4)	0.7918 (4)	−0.03385 (17)	0.0133 (7)
C3	0.1769 (4)	0.7992 (5)	−0.05036 (18)	0.0170 (8)
H3	0.2493	0.7441	−0.0254	0.020*
C4	0.1972 (4)	0.8862 (5)	−0.1028 (2)	0.0202 (8)
H4	0.2834	0.8906	−0.1136	0.024*
C5	0.0928 (4)	0.9665 (5)	−0.13943 (18)	0.0182 (8)
H5	0.1073	1.0270	−0.1751	0.022*
C6	−0.0331 (4)	0.9589 (5)	−0.12414 (18)	0.0168 (8)
H6	−0.1048	1.0134	−0.1497	0.020*
C7	0.1494 (3)	0.4203 (5)	0.19634 (18)	0.0143 (7)
C8	0.1896 (3)	0.4974 (5)	0.14479 (17)	0.0136 (7)
C9	0.3235 (4)	0.4931 (5)	0.13872 (18)	0.0172 (8)
H9	0.3514	0.5475	0.1045	0.021*
C10	0.4158 (4)	0.4114 (5)	0.18149 (19)	0.0187 (8)
H10	0.5066	0.4105	0.1770	0.022*
C11	0.3744 (4)	0.3301 (5)	0.23141 (19)	0.0183 (8)
H11	0.4371	0.2716	0.2606	0.022*
C12	0.2414 (4)	0.3343 (5)	0.23868 (19)	0.0173 (8)
H12	0.2139	0.2781	0.2727	0.021*
C13	−0.2862 (4)	0.9515 (5)	−0.08961 (18)	0.0174 (8)
H13A	−0.3002	0.9034	−0.1313	0.021*
H13B	−0.2678	1.0814	−0.0914	0.021*
C14	−0.4070 (4)	0.9196 (6)	−0.0602 (2)	0.0233 (9)
H14A	−0.4809	0.9907	−0.0809	0.035*
H14B	−0.3885	0.9552	−0.0177	0.035*
H14C	−0.4303	0.7922	−0.0630	0.035*
C15	−0.0256 (4)	0.3651 (5)	0.25327 (19)	0.0213 (8)
H15A	0.0251	0.4179	0.2902	0.026*
H15B	−0.0132	0.2336	0.2548	0.026*
C16	−0.1692 (4)	0.4104 (6)	0.2491 (2)	0.0272 (10)
H16A	−0.2048	0.3543	0.2828	0.041*
H16B	−0.2173	0.3659	0.2108	0.041*
H16C	−0.1795	0.5406	0.2511	0.041*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.01495 (7)	0.01991 (8)	0.01826 (8)	−0.00083 (5)	0.00561 (5)	0.00169 (6)
Br1	0.01972 (19)	0.0300 (2)	0.0374 (3)	0.00079 (16)	0.01402 (18)	0.00757 (19)
O1	0.0130 (12)	0.0221 (13)	0.0132 (14)	0.0018 (10)	0.0027 (10)	0.0021 (11)
O2	0.0165 (13)	0.0211 (13)	0.0156 (14)	−0.0003 (10)	0.0042 (11)	0.0040 (11)
N1	0.0134 (14)	0.0167 (15)	0.0134 (16)	0.0014 (11)	−0.0006 (12)	0.0011 (12)
N2	0.0169 (15)	0.0129 (14)	0.0117 (16)	−0.0016 (11)	0.0006 (12)	−0.0013 (12)
N3	0.0156 (15)	0.0143 (14)	0.0138 (16)	−0.0030 (11)	0.0010 (12)	0.0007 (12)
C1	0.0149 (17)	0.0127 (15)	0.0103 (17)	−0.0005 (13)	0.0017 (14)	−0.0027 (14)
C2	0.0158 (17)	0.0123 (16)	0.0123 (18)	−0.0007 (12)	0.0043 (14)	−0.0009 (13)
C3	0.0142 (17)	0.0181 (18)	0.019 (2)	−0.0015 (13)	0.0032 (15)	0.0000 (15)
C4	0.0159 (18)	0.0242 (19)	0.022 (2)	−0.0039 (15)	0.0085 (16)	−0.0017 (17)
C5	0.0197 (19)	0.0212 (19)	0.0149 (19)	−0.0034 (15)	0.0061 (15)	0.0005 (16)
C6	0.0183 (18)	0.0148 (17)	0.017 (2)	−0.0002 (14)	0.0017 (15)	0.0008 (15)
C7	0.0141 (17)	0.0119 (16)	0.0168 (19)	0.0004 (13)	0.0028 (14)	0.0005 (14)
C8	0.0170 (17)	0.0123 (16)	0.0110 (18)	0.0001 (13)	0.0007 (14)	−0.0020 (14)
C9	0.0208 (19)	0.0146 (17)	0.017 (2)	−0.0034 (14)	0.0041 (15)	−0.0011 (15)
C10	0.0171 (18)	0.0187 (19)	0.019 (2)	−0.0005 (14)	−0.0001 (15)	−0.0015 (16)
C11	0.0183 (18)	0.0173 (17)	0.017 (2)	0.0004 (14)	−0.0035 (15)	−0.0022 (16)
C12	0.0215 (18)	0.0131 (17)	0.0167 (19)	−0.0001 (14)	0.0018 (15)	−0.0004 (15)
C13	0.0146 (17)	0.0189 (18)	0.017 (2)	−0.0005 (14)	−0.0018 (15)	0.0005 (16)
C14	0.0162 (19)	0.030 (2)	0.023 (2)	0.0012 (16)	0.0029 (16)	−0.0019 (18)
C15	0.029 (2)	0.0205 (19)	0.015 (2)	0.0008 (16)	0.0069 (17)	0.0025 (16)
C16	0.029 (2)	0.029 (2)	0.028 (3)	0.0044 (17)	0.0154 (19)	0.0074 (19)

Geometric parameters (Å, °)

Hg1—N1	2.086 (3)	C7—C8	1.408 (5)
Hg1—Br1	2.4014 (4)	C8—C9	1.398 (5)
Hg1—N3	2.660 (3)	C9—C10	1.380 (5)
O1—C1	1.370 (4)	C9—H9	0.9500
O1—C13	1.452 (4)	C10—C11	1.395 (6)
O2—C7	1.359 (4)	C10—H10	0.9500
O2—C15	1.428 (5)	C11—C12	1.396 (5)
N1—N2	1.334 (4)	C11—H11	0.9500
N1—C2	1.393 (5)	C12—H12	0.9500
N2—N3	1.271 (4)	C13—C14	1.507 (5)
N3—C8	1.412 (5)	C13—H13A	0.9900
C1—C6	1.384 (5)	C13—H13B	0.9900
C1—C2	1.408 (5)	C14—H14A	0.9800
C2—C3	1.403 (5)	C14—H14B	0.9800
C3—C4	1.386 (6)	C14—H14C	0.9800
C3—H3	0.9500	C15—C16	1.497 (6)
C4—C5	1.381 (6)	C15—H15A	0.9900
C4—H4	0.9500	C15—H15B	0.9900
C5—C6	1.385 (5)	C16—H16A	0.9800

C5—H5	0.9500	C16—H16B	0.9800
C6—H6	0.9500	C16—H16C	0.9800
C7—C12	1.387 (5)		

N1—Hg1—Br1	175.94 (9)	C10—C9—C8	121.3 (4)
N1—Hg1—N3	52.01 (11)	C10—C9—H9	119.4
Br1—Hg1—N3	129.22 (7)	C8—C9—H9	119.4
C1—O1—C13	117.0 (3)	C9—C10—C11	119.3 (4)
C7—O2—C15	118.0 (3)	C9—C10—H10	120.4
N2—N1—C2	117.8 (3)	C11—C10—H10	120.4
N2—N1—Hg1	111.6 (2)	C10—C11—C12	120.4 (4)
C2—N1—Hg1	130.7 (2)	C10—C11—H11	119.8
N3—N2—N1	110.7 (3)	C12—C11—H11	119.8
N2—N3—C8	115.1 (3)	C7—C12—C11	120.1 (4)
N2—N3—Hg1	85.7 (2)	C7—C12—H12	119.9
C8—N3—Hg1	159.2 (3)	C11—C12—H12	119.9
O1—C1—C6	124.4 (3)	O1—C13—C14	107.3 (3)
O1—C1—C2	115.6 (3)	O1—C13—H13A	110.3
C6—C1—C2	120.0 (3)	C14—C13—H13A	110.3
N1—C2—C3	123.1 (3)	O1—C13—H13B	110.3
N1—C2—C1	118.3 (3)	C14—C13—H13B	110.3
C3—C2—C1	118.6 (3)	H13A—C13—H13B	108.5
C4—C3—C2	120.5 (4)	C13—C14—H14A	109.5
C4—C3—H3	119.7	C13—C14—H14B	109.5
C2—C3—H3	119.7	H14A—C14—H14B	109.5
C5—C4—C3	120.3 (4)	C13—C14—H14C	109.5
C5—C4—H4	119.9	H14A—C14—H14C	109.5
C3—C4—H4	119.9	H14B—C14—H14C	109.5
C4—C5—C6	120.0 (4)	O2—C15—C16	107.5 (3)
C4—C5—H5	120.0	O2—C15—H15A	110.2
C6—C5—H5	120.0	C16—C15—H15A	110.2
C1—C6—C5	120.6 (4)	O2—C15—H15B	110.2
C1—C6—H6	119.7	C16—C15—H15B	110.2
C5—C6—H6	119.7	H15A—C15—H15B	108.5
O2—C7—C12	124.2 (4)	C15—C16—H16A	109.5
O2—C7—C8	116.0 (3)	C15—C16—H16B	109.5
C12—C7—C8	119.8 (3)	H16A—C16—H16B	109.5
C9—C8—C7	119.0 (3)	C15—C16—H16C	109.5
C9—C8—N3	124.9 (3)	H16A—C16—H16C	109.5
C7—C8—N3	116.0 (3)	H16B—C16—H16C	109.5

N3—Hg1—N1—N2	1.4 (2)	C3—C4—C5—C6	−0.6 (6)
N3—Hg1—N1—C2	−178.7 (4)	O1—C1—C6—C5	179.5 (3)
C2—N1—N2—N3	177.6 (3)	C2—C1—C6—C5	0.1 (5)
Hg1—N1—N2—N3	−2.5 (3)	C4—C5—C6—C1	0.6 (6)
N1—N2—N3—C8	−179.9 (3)	C15—O2—C7—C12	1.7 (5)
N1—N2—N3—Hg1	1.8 (3)	C15—O2—C7—C8	−178.3 (3)
N1—Hg1—N3—N2	−1.37 (19)	O2—C7—C8—C9	176.9 (3)
Br1—Hg1—N3—N2	173.68 (16)	C12—C7—C8—C9	−3.1 (5)
N1—Hg1—N3—C8	−177.1 (7)	O2—C7—C8—N3	−2.1 (5)

Br1—Hg1—N3—C8	−2.1 (7)	C12—C7—C8—N3	177.9 (3)
C13—O1—C1—C6	−3.0 (5)	N2—N3—C8—C9	3.9 (5)
C13—O1—C1—C2	176.4 (3)	Hg1—N3—C8—C9	179.2 (5)
N2—N1—C2—C3	0.1 (5)	N2—N3—C8—C7	−177.2 (3)
Hg1—N1—C2—C3	−179.7 (3)	Hg1—N3—C8—C7	−1.9 (8)
N2—N1—C2—C1	−178.4 (3)	C7—C8—C9—C10	1.5 (5)
Hg1—N1—C2—C1	1.7 (5)	N3—C8—C9—C10	−179.6 (3)
O1—C1—C2—N1	−1.5 (5)	C8—C9—C10—C11	0.6 (6)
C6—C1—C2—N1	177.9 (3)	C9—C10—C11—C12	−1.2 (6)
O1—C1—C2—C3	179.8 (3)	O2—C7—C12—C11	−177.5 (3)
C6—C1—C2—C3	−0.7 (5)	C8—C7—C12—C11	2.5 (5)
N1—C2—C3—C4	−177.8 (3)	C10—C11—C12—C7	−0.3 (6)
C1—C2—C3—C4	0.7 (5)	C1—O1—C13—C14	−179.7 (3)
C2—C3—C4—C5	−0.1 (6)	C7—O2—C15—C16	176.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13B···N2^{i}	0.99	2.60	3.496 (5)	151
C12—H12···Cg1^{ii}	0.95	2.85	3.559 (4)	132
C13—H13A···Cg1^{iii}	0.99	2.72	3.523 (4)	139

Symmetry codes: (i) −*x*, −*y*+2, −*z*; (ii) −*x*+1/2, *y*−1/2, −*z*+1/2; (iii) −*x*, −*y*+1, −*z*.

Fig. 1

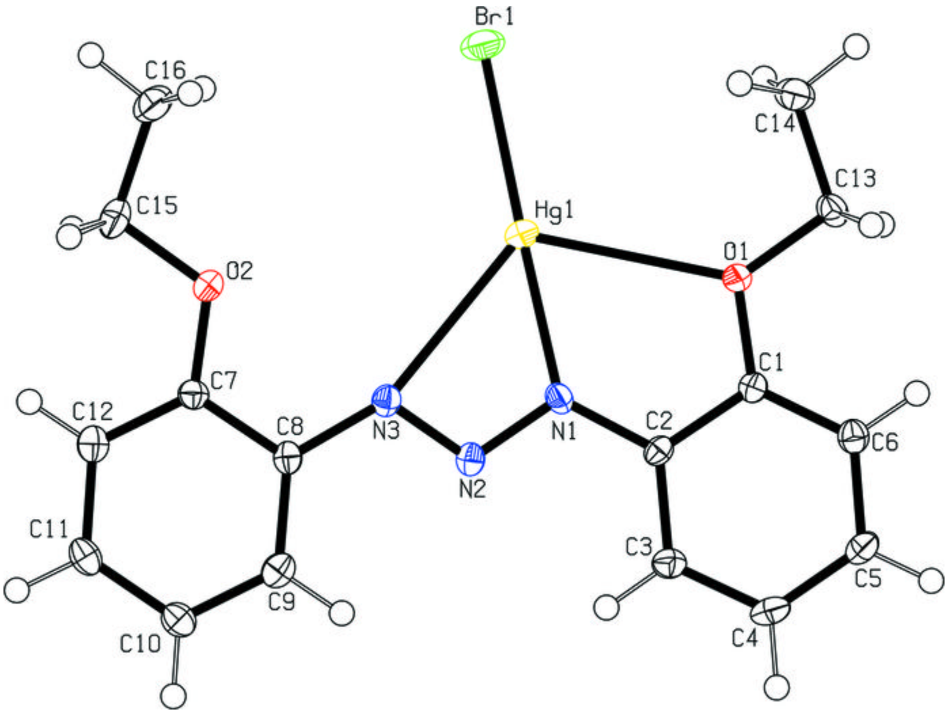
Br1
C16
C14
C13
Hg1
C15
O1
O2
C1
C7
C12
C8
N3
N1
C2
C6
N2
C11
C3
C9
C5
C10
C4

Fig. 2

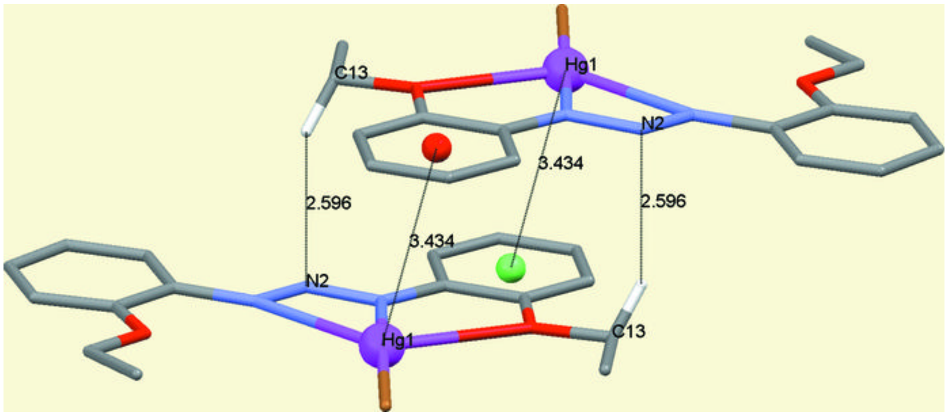

Fig. 3

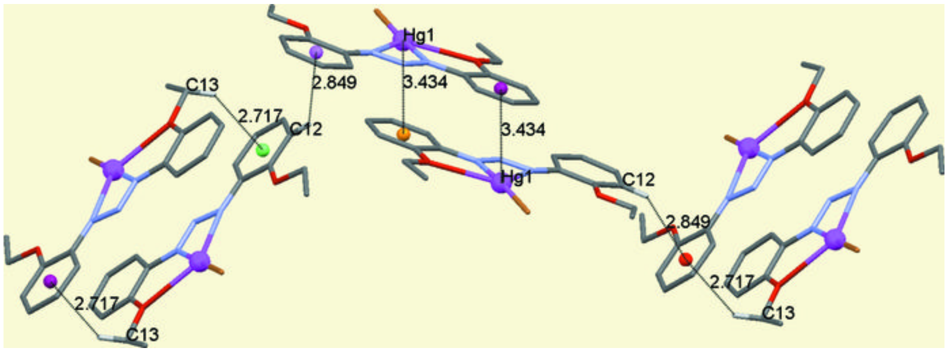

Fig. 4