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Crystal structure of di-μ-chlorido-bis(chlorido-{N^1,N^1-diethyl-N^4-[(pyridin-2-yl-κN)methylidene]-benzene-1,4-diamine-κN^4}mercury(II))

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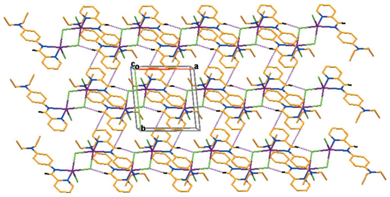
The title dinuclear mercury(II) complex, $[Hg_2Cl_4(C_{16}H_{19}N_3)_2]$, synthesized from the pyridine-derived Schiff base (*E*)-N^1,N^1-diethyl-N^4-[(pyridin-2-yl)methylidene]benzene-1,4-diamine (DPMBD), has inversion symmetry. The five-coordinated Hg^{II} atoms have distorted square-pyramidal stereochemistry comprising two N-atom donors from bidentate chelate BPMBD ligands and three Cl-atom donors, two bridging and one monodentate. The dihedral angle between the benzene and the pyridine rings in the BPMBD ligand is 7.55 (4)°. In the crystal, the dinuclear molecules are linked by weak C—H···Cl hydrogen bonds, forming zigzag ribbons lying parallel to [001]. Also present in the structure are π–π interactions between benzene and pyridine rings [minimum ring-centroid separation = 3.698 (8) Å].

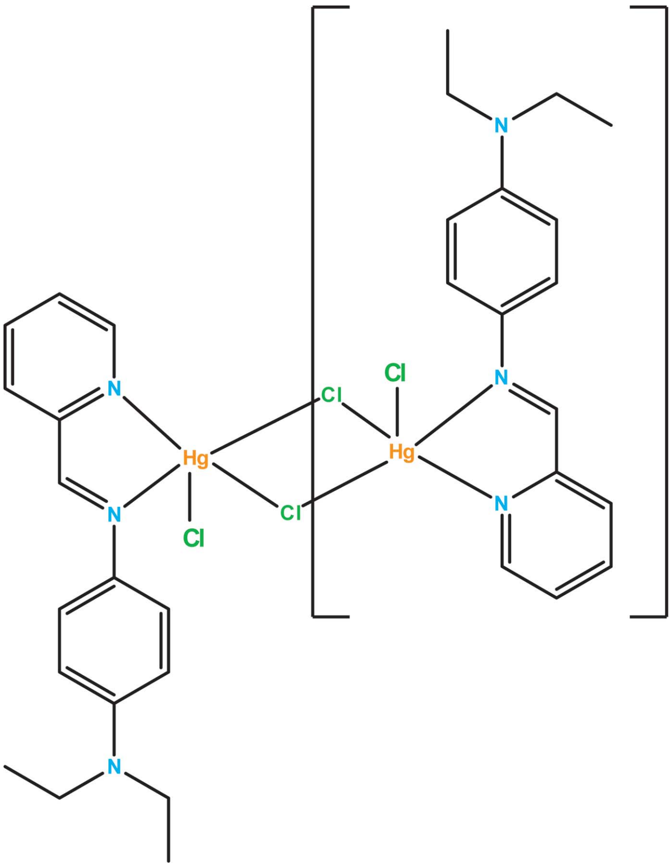


1. Chemical context

Mercury is one of the most prevalent toxic metals in the environment and gains access to the body orally or dermally, causing cell dysfunction that consequently leads to health problems (Mandal *et al.*, 2012). Schiff base complexes of 2-pyridinecarboxaldehyde and its derivatives have been found to be good herbicides, used for the protection of plants (Hughes & Prince, 1978). Transition metal complexes of pyridyl Schiff bases have found applications in catalysis (Kasselouri *et al.*, 1993). Pyridyl derivatives of Schiff bases are important building blocks for many important compounds, widely used in biological applications such as antioxidative, anticancer agents, as fluorescent probes in industry, in coordination chemistry and in catalysis (Jursic *et al.*, 2002; Song *et al.*, 2011; Motswainyana *et al.*, 2013; Das *et al.*, 2013). Our research interest focuses on a study of Schiff bases derived from N^1,N^1-diethyl-*p*-phenylenediamine and their metal complexes (Faizi & Hussain, 2014; Faizi *et al.*, 2015). We report herein the synthesis and the crystal structure of a new complex of mercury(II), $[Hg_2Cl_4(C_{16}H_{19}N_3)_2]$, with the pyridine-derived Schiff base (*E*)-N^1,N^1-diethyl-N^4-[(pyridin-2-yl)-methylidene]benzene-1,4-diamine (DPMBD).

2. Structural commentary

The dinuclear molecule of the title complex is generated by inversion symmetry (Fig. 1). The Schiff base-derived ligand (DPMBD) coordinates to the Hg^{II} atom in a bidentate chelating mode through the N atoms of the pyridine ring (N1) and the imine group (N2) [Hg1—N = 2.317 (9) and 2.437 (8) Å, respectively].



The five-coordinated Hg^{2+} ion has a distorted square-pyramidal geometry completed by three Hg—Cl bonds, one monodentate [Hg1—Cl2 = 2.402 (4) Å] and two bridging Hg1—Cl1 [2.459 (3) Å] and $Hg1—Cl1^{i}$ [2.999 (3) Å; symmetry code: (i) $-x + 2, -y + 1, -z + 1$]. The environment of a five-coordinated mercuric ion is common among Hg^{2+} complexes (Baul *et al.*, 2004). The longest Hg—Cl distance bridges across the centre of inversion, giving an $Hg\cdots Hg^{i}$ separation of 4.1985 (16) Å. The observed Hg—Cl and Hg—N bond lengths and bond angles are considered normal for this type of Hg^{II} complex (Faizi & Prisyazhnaya, 2015; Faizi & Sen, 2014). The benzene and pyridine rings of the DPMBD ligand form a dihedral angle of 7.55 (4)°.

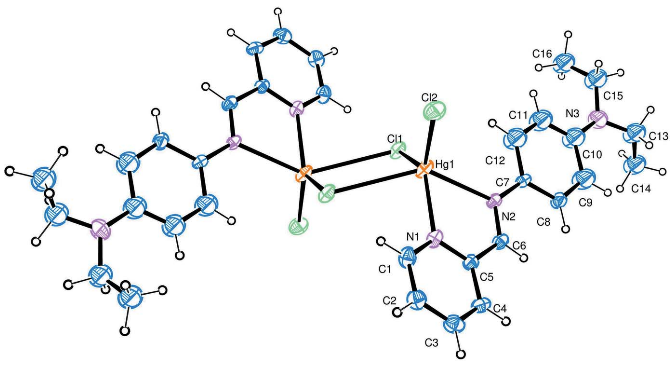


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 40% probability level. The unlabelled atoms are related to the labelled atoms by inversion symmetry (symmetry operation: $-x + 2, -y + 1, -z + 1$).

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
$C6—H6\cdots Cl1^{i}$	0.93	2.74	3.578 (9)	151
$C1—H1\cdots Cl1^{ii}$	0.93	2.89	3.471 (12)	122
$C1—H1\cdots Cl2^{iii}$	0.93	2.97	3.623 (11)	129

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

3. Supramolecular features

In the crystal, molecules are linked by C—H$\cdots$Cl hydrogen bonds, forming a sheet like arrangement parallel to [001] (see Table 1 and Fig. 2 for details). The centroid-to-centroid distance between inversion-related benzene rings ($-x + 1, -y + 2, -z + 1$) is 3.879 (6) Å, indicating a weak π–π interaction along the *c* axis (Fig. 2). Also present is a benzene–pyridine ring interaction with $Cg\cdots Cg$ ($-x+1, -y+1, -z+1$) = 3.698 (8) Å (Fig. 3).

4. Database survey

A search of the Cambridge Structure Database (Version 5.37 with updates May 2016; Groom *et al.*, 2016) reveals that there is no entry in the literature for a dichloridomercury(II) complex with (*E*)-N^1,N^1-diethyl-*N*4-(pyridin-2-ylmethylene)-benzene-1,4-diamine that has been structurally characterized. A dihalomercury(II) complex has been reported by Baul *et al.* (2013) in which the Hg^{II} atom is coordinated by the bis-chelating *N*-heterocyclic ligand [(*E*)-*N*-(pyridin-2-ylmethylidene)arylamine)], two bridging Cl ligands and one terminal Cl ligand. Similar Hg^{II} complexes have also been reported with a slight modification of the ligand (Nejad *et al.*, 2010), *viz.* di-μ-chlorido-bis{chlorido[2-(phenyliminomethyl)-pyridine-κ^2N,N']mercury(II)} (Salehzadeh *et al.*, 2011) di-μ-chlorido-

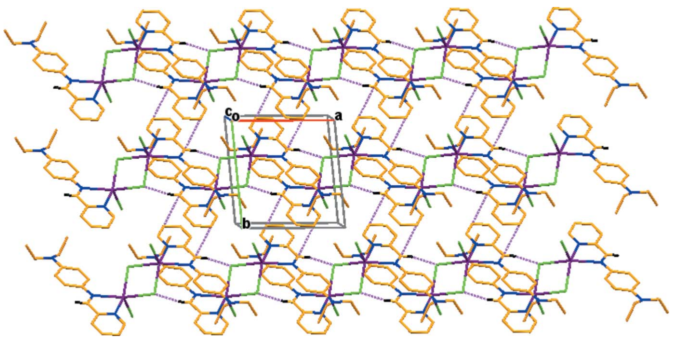


Figure 2
The crystal packing of the title compound, viewed along the *c* axis, with hydrogen bonds (Table 1) shown as dashed lines.

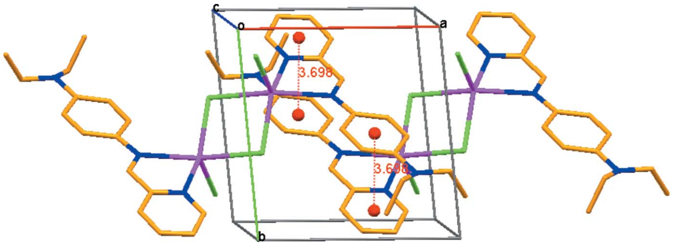


Figure 3
The crystal packing of the title compound, viewed approximately along the *c* axis. The π–π interactions between the benzene and pyridine rings are shown as dotted lines.

bis{chlorido[4-nitro-*N*-(pyridin-2-ylmethylidene-κN)aniline-κN]mercury(II)} (Hoseyni *et al.*, 2012), di-μ-chlorido-bis-{chlorido[2,3-dimethyl-*N*-(pyridin-2-ylmethylidene)aniline-$\kappa^2 N,N'$]mercury(II)} (Faizi & Prisyazhnaya, 2015) and di-μ-chlorido-bis-(chlorido{N^1-phenyl-N^4)-[(pyridin-2-yl-κN)methylidene]benzene-1,4-diamine-κN^4} mercury(II)). All of the above compounds show the Hg$^{\rm II}$ ion in a distorted square-pyramidal coordination environment formed by the N atoms of the diimine ligand, two bridging Cl atoms and one monodentate Cl atom, as found in the title compound, one of the bridging Hg—Cl bonds being significantly longer than the other.

5. Synthesis and crystallization

The iminopyridyl compound (*E*)-N^1,N^1-diethyl-N^4-[(pyridin-2-yl)methylidene]benzene-1,4-diamine (DPMBD) was prepared by adding portionwise pyridine-2-carbaldehyde (0.29 g, 2.71 mmol) to a methanolic solution (50 ml) of N^1,N^1-diethyl-*p*-phenylenediamine (0.50 g, 2.71 mmol). The reaction mixture was stirred for 3 h at room temperature and filtered. The resulting yellow powder was washed with methanol (2 × 3 ml) and hexane (3 × 10 ml). The compound was recrystallized from hot MeOH to give yellow crystals, which were dried in a vacuum desiccator to give the pure product (yield: 0.60 g, 80%).

The title compound was prepared by reacting DPMBD (0.10 g, 0.39 mmol) with mercury(II) chloride (0.05 g, 0.18 mmol) in methanol (5 ml), with vigorous stirring for 2 h at room temperature. The red precipitate that formed was filtered off and redissolved in dimethylformamide. Crystals of the red title complex (yield: 0.31 g, 76%) suitable for X-ray analysis were obtained within 3 d by slow evaporation of the dimethylformamide.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to C atoms were placed in calculated positions with C—H = 0.93–0.97 Å and included in the refinement in a riding-model approximation with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) (for methyl H) and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) (for other H atoms).

Table 2
Experimental details.

Crystal data	
Chemical formula	[$Hg_2Cl_4(C_{16}H_{19}N_3)_2$]
M_r	1049.66
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	8.329 (3), 8.565 (3), 12.936 (4)
α, β, γ (°)	89.043 (8), 81.107 (7), 84.206 (7)
V (Å^3)	907.1 (5)
Z	1
Radiation type	Mo *K*α
μ (mm^{-1})	8.78
Crystal size (mm)	0.20 × 0.15 × 0.12
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2003)
$T_{\rm min}$, $T_{\rm max}$	0.944, 0.981
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6272, 3303, 2779
$R_{\rm int}$	0.037
(sin θ/λ)$_{\rm max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.054, 0.156, 1.06
No. of reflections	3303
No. of parameters	158
No. of restraints	57
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	2.56, −2.43

Computer programs: *APEX2* and *SAINT* (Bruker, 2003), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *DIAMOND* (Brandenburg & Putz, 2006).

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Acta Cryst. (2017). E**73**, 809–812 Faizi *et al.* • [$Hg_2Cl_4(C_{16}H_{19}N_3)_2$] **811**

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supporting information

Acta Cryst. (2017). E**73**, 809-812 [https://doi.org/10.1107/S2056989017005874]

Crystal structure of di-μ-chlorido-bis(chlorido{N^1,N^1-diethyl-N^4-[(pyridin-2-yl-κN)methylidene]benzene-1,4-diamine-κN^4}mercury(II))

Md. Serajul Haque Faizi, Necmi Dege and Kateryna Goleva

Computing details

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenberg & Putz, 2006); software used to prepare material for publication: *DIAMOND* (Brandenberg & Putz, 2006).

Di-μ-chlorido-bis(chlorido{N^1,N^1-diethyl-N^4-[(pyridin-2-yl-κN)methylidene]benzene-1,4-diamine-κN^4}mercury(II))

Crystal data

$[Hg_2Cl_4(C_{16}H_{19}N_3)_2]$
$M_r = 1049.66$
Triclinic, $P\bar{1}$
$a = 8.329$ (3) Å
$b = 8.565$ (3) Å
$c = 12.936$ (4) Å
$\alpha = 89.043$ (8)°
$\beta = 81.107$ (7)°
$\gamma = 84.206$ (7)°
$V = 907.1$ (5) Å^3

$Z = 1$
$F(000) = 500$
$D_x = 1.921$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3407 reflections
$\theta = 2.7$–26.6°
$\mu = 8.78$ mm^{-1}
$T = 100$ K
Needle, red
0.20 × 0.15 × 0.12 mm

Data collection

Bruker APEXII CCD
diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 2003)
$T_{min} = 0.944$, $T_{max} = 0.981$

6272 measured reflections
3303 independent reflections
2779 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.4°$
$h = -10 \rightarrow 10$
$k = -7 \rightarrow 10$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.156$
$S = 1.06$
3303 reflections
158 parameters

57 restraints
Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0936P)^2 + 2.7873P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 2.56 e Å^{-3}
$\Delta\rho_{min}$ = −2.43 e Å^{-3}

Extinction correction: SHELXL2016 (Sheldrick, 2015), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0154 (18)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.81436 (5)	0.66012 (4)	0.57709 (3)	0.0580 (3)
Cl1	0.8912 (3)	0.3764 (3)	0.5896 (2)	0.0565 (6)
Cl2	0.8896 (4)	0.8431 (4)	0.6955 (3)	0.0756 (8)
N2	0.5206 (9)	0.6438 (8)	0.5996 (6)	0.0418 (16)
N1	0.7065 (10)	0.8114 (9)	0.4494 (7)	0.0486 (18)
C5	0.5464 (11)	0.8065 (10)	0.4459 (7)	0.0425 (19)
C7	0.4285 (19)	0.564 (2)	0.6811 (12)	0.0965 (13)
C6	0.4541 (11)	0.7127 (10)	0.5239 (7)	0.045 (2)
H6	0.345407	0.701618	0.519674	0.054*
C4	0.4711 (14)	0.8919 (12)	0.3733 (8)	0.054 (2)
H4	0.361040	0.884616	0.371099	0.064*
C8	0.2645 (12)	0.5445 (14)	0.6857 (8)	0.060 (3)
H8	0.207736	0.588526	0.634069	0.072*
C2	0.7167 (15)	0.9953 (13)	0.3116 (9)	0.062 (3)
H2	0.776639	1.064049	0.268772	0.075*
C10	0.266 (2)	0.389 (2)	0.8458 (13)	0.1012 (7)
C1	0.7883 (14)	0.9042 (13)	0.3803 (10)	0.062 (3)
H1	0.899938	0.905612	0.379875	0.075*
C12	0.505 (2)	0.498 (2)	0.7587 (12)	0.1012 (7)
H12	0.613677	0.512565	0.760116	0.121*
N3	0.1794 (12)	0.3036 (16)	0.9288 (8)	0.1012 (9)
C3	0.5551 (16)	0.9872 (13)	0.3044 (9)	0.063 (3)
H3	0.505047	1.044522	0.254433	0.075*
C9	0.186 (2)	0.462 (2)	0.7646 (13)	0.1012 (7)
H9	0.075706	0.452541	0.766178	0.121*
C11	0.424 (2)	0.409 (2)	0.8348 (13)	0.1012 (7)
H11	0.484613	0.359696	0.882884	0.121*
C15	0.2584 (16)	0.2780 (17)	1.0150 (10)	0.1012 (7)
H15A	0.182347	0.272105	1.079438	0.121*
H15B	0.331868	0.357020	1.021477	0.121*
C16	0.3500 (18)	0.1193 (16)	0.9831 (12)	0.1012 (7)
H16A	0.413710	0.082530	1.036072	0.152*
H16B	0.273224	0.045619	0.975182	0.152*
H16C	0.420937	0.129507	0.917922	0.152*
C13	0.0131 (13)	0.3113 (19)	0.9350 (12)	0.1012 (7)

H13A	−0.023986	0.413409	0.909047	0.121*
H13B	−0.033164	0.307139	1.008496	0.121*
C14	−0.059 (2)	0.1883 (19)	0.8782 (12)	0.1012 (7)
H14A	−0.176271	0.208254	0.889439	0.152*
H14B	−0.019235	0.192811	0.804657	0.152*
H14C	−0.028458	0.086028	0.904586	0.152*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0436 (3)	0.0551 (3)	0.0792 (4)	−0.00681 (18)	−0.0217 (2)	0.0087 (2)
Cl1	0.0404 (12)	0.0548 (13)	0.0761 (16)	−0.0047 (10)	−0.0161 (11)	0.0139 (11)
Cl2	0.0711 (19)	0.0739 (18)	0.089 (2)	−0.0146 (15)	−0.0278 (16)	−0.0072 (15)
N2	0.039 (4)	0.037 (4)	0.052 (4)	−0.007 (3)	−0.010 (3)	0.000 (3)
N1	0.042 (4)	0.041 (4)	0.065 (5)	−0.007 (3)	−0.012 (4)	−0.004 (3)
C5	0.040 (5)	0.039 (4)	0.049 (5)	−0.001 (4)	−0.012 (4)	−0.010 (4)
C7	0.080 (2)	0.124 (2)	0.089 (2)	−0.025 (2)	−0.018 (2)	0.032 (2)
C6	0.039 (5)	0.042 (4)	0.057 (5)	−0.005 (4)	−0.018 (4)	−0.007 (4)
C4	0.056 (6)	0.054 (6)	0.053 (5)	0.000 (5)	−0.022 (5)	0.002 (4)
C8	0.038 (5)	0.087 (8)	0.058 (6)	−0.011 (5)	−0.012 (4)	0.020 (5)
C2	0.073 (8)	0.052 (6)	0.060 (6)	−0.010 (5)	−0.003 (5)	0.007 (5)
C10	0.0849 (13)	0.1288 (13)	0.0928 (13)	−0.0231 (13)	−0.0184 (12)	0.0329 (13)
C1	0.046 (6)	0.056 (6)	0.083 (7)	−0.009 (5)	−0.005 (5)	0.009 (5)
C12	0.0849 (13)	0.1288 (13)	0.0928 (13)	−0.0231 (13)	−0.0184 (12)	0.0329 (13)
N3	0.0848 (16)	0.1290 (17)	0.0927 (15)	−0.0230 (16)	−0.0183 (15)	0.0330 (16)
C3	0.077 (8)	0.049 (5)	0.064 (6)	0.003 (5)	−0.018 (6)	0.002 (5)
C9	0.0849 (13)	0.1288 (13)	0.0928 (13)	−0.0231 (13)	−0.0184 (12)	0.0329 (13)
C11	0.0849 (13)	0.1288 (13)	0.0928 (13)	−0.0231 (13)	−0.0184 (12)	0.0329 (13)
C15	0.0849 (13)	0.1288 (13)	0.0928 (13)	−0.0231 (13)	−0.0184 (12)	0.0329 (13)
C16	0.0849 (13)	0.1288 (13)	0.0928 (13)	−0.0231 (13)	−0.0184 (12)	0.0329 (13)
C13	0.0849 (13)	0.1288 (13)	0.0928 (13)	−0.0231 (13)	−0.0184 (12)	0.0329 (13)
C14	0.0849 (13)	0.1288 (13)	0.0928 (13)	−0.0231 (13)	−0.0184 (12)	0.0329 (13)

Geometric parameters (Å, º)

Hg1—Cl1	2.459 (3)	C11—C12	1.37 (2)
Hg1—Cl2	2.402 (4)	C13—C14	1.52 (2)
Hg1—N1	2.317 (9)	C15—C16	1.52 (2)
Hg1—N2	2.437 (8)	C1—H1	0.9300
Hg1—Cl1^{i}	2.999 (3)	C2—H2	0.9300
N1—C1	1.339 (15)	C3—H3	0.9300
N1—C5	1.346 (13)	C4—H4	0.9300
N2—C6	1.302 (12)	C6—H6	0.9300
N2—C7	1.414 (18)	C8—H8	0.9300
N3—C10	1.43 (2)	C9—H9	0.9300
N3—C13	1.370 (15)	C11—H11	0.9300
N3—C15	1.384 (17)	C12—H12	0.9300
C1—C2	1.342 (17)	C13—H13A	0.9700

C2—C3	1.372 (19)	C13—H13B	0.9700
C3—C4	1.360 (16)	C14—H14A	0.9600
C4—C5	1.370 (14)	C14—H14B	0.9600
C5—C6	1.453 (13)	C14—H14C	0.9600
C7—C8	1.385 (19)	C15—H15A	0.9700
C7—C12	1.36 (2)	C15—H15B	0.9700
C8—C9	1.35 (2)	C16—H16A	0.9600
C9—C10	1.43 (2)	C16—H16B	0.9600
C10—C11	1.33 (2)	C16—H16C	0.9600

Cl1—Hg1—Cl2	121.69 (10)	N1—C1—H1	118.00
Cl1—Hg1—N1	131.9 (2)	C2—C1—H1	118.00
Cl1—Hg1—N2	96.06 (17)	C1—C2—H2	120.00
Cl1—Hg1—Cl1^{i}	79.90 (8)	C3—C2—H2	120.00
Cl2—Hg1—N1	105.7 (2)	C2—C3—H3	121.00
Cl2—Hg1—N2	112.60 (19)	C4—C3—H3	121.00
Cl1^{i}—Hg1—Cl2	102.68 (10)	C3—C4—H4	120.00
N1—Hg1—N2	71.2 (3)	C5—C4—H4	120.00
Cl1^{i}—Hg1—N1	82.2 (2)	N2—C6—H6	119.00
Cl1^{i}—Hg1—N2	140.17 (19)	C5—C6—H6	119.00
Hg1—Cl1—Hg1^{i}	100.10 (8)	C7—C8—H8	120.00
Hg1—N1—C1	125.9 (7)	C9—C8—H8	120.00
Hg1—N1—C5	116.6 (6)	C8—C9—H9	119.00
C1—N1—C5	117.5 (9)	C10—C9—H9	119.00
Hg1—N2—C6	112.2 (6)	C10—C11—H11	118.00
Hg1—N2—C7	125.9 (8)	C12—C11—H11	117.00
C6—N2—C7	121.8 (10)	C7—C12—H12	120.00
C10—N3—C13	117.2 (12)	C11—C12—H12	120.00
C10—N3—C15	114.4 (11)	N3—C13—H13A	108.00
C13—N3—C15	123.0 (11)	N3—C13—H13B	108.00
N1—C1—C2	123.0 (11)	C14—C13—H13A	108.00
C1—C2—C3	120.1 (11)	C14—C13—H13B	108.00
C2—C3—C4	117.3 (11)	H13A—C13—H13B	107.00
C3—C4—C5	120.9 (11)	C13—C14—H14A	109.00
N1—C5—C4	121.0 (9)	C13—C14—H14B	110.00
N1—C5—C6	118.1 (8)	C13—C14—H14C	110.00
C4—C5—C6	120.8 (9)	H14A—C14—H14B	109.00
N2—C6—C5	121.3 (8)	H14A—C14—H14C	109.00
N2—C7—C8	124.1 (13)	H14B—C14—H14C	110.00
N2—C7—C12	118.6 (14)	N3—C15—H15A	112.00
C8—C7—C12	117.2 (14)	N3—C15—H15B	112.00
C7—C8—C9	120.6 (12)	C16—C15—H15A	112.00
C8—C9—C10	122.8 (15)	C16—C15—H15B	112.00
N3—C10—C9	121.5 (14)	H15A—C15—H15B	110.00
N3—C10—C11	125.2 (15)	C15—C16—H16A	109.00
C9—C10—C11	113.3 (15)	C15—C16—H16B	109.00
C10—C11—C12	125.2 (16)	C15—C16—H16C	109.00
C7—C12—C11	120.7 (16)	H16A—C16—H16B	109.00

N3—C13—C14	118.6 (13)	H16A—C16—H16C	109.00
N3—C15—C16	98.2 (11)	H16B—C16—H16C	109.00

Cl2—Hg1—Cl1—Hg1^{i}	−98.74 (12)	C7—N2—C6—C5	174.3 (10)
N1—Hg1—Cl1—Hg1^{i}	69.9 (3)	Hg1—N2—C7—C8	−173.5 (10)
N2—Hg1—Cl1—Hg1^{i}	139.95 (19)	Hg1—N2—C7—C12	4.6 (19)
Cl1^{i}—Hg1—Cl1—Hg1^{i}	0.00 (7)	C6—N2—C7—C8	3 (2)
Cl1—Hg1—N1—C1	−104.6 (8)	C6—N2—C7—C12	−178.5 (12)
Cl1—Hg1—N1—C5	76.4 (7)	C13—N3—C10—C9	−8 (2)
Cl2—Hg1—N1—C1	65.4 (9)	C13—N3—C10—C11	172.1 (16)
Cl2—Hg1—N1—C5	−113.6 (6)	C15—N3—C10—C9	−162.9 (15)
N2—Hg1—N1—C1	174.4 (9)	C15—N3—C10—C11	17 (2)
N2—Hg1—N1—C5	−4.6 (6)	C10—N3—C13—C14	91.1 (18)
Cl1^{i}—Hg1—N1—C1	−35.7 (8)	C15—N3—C13—C14	−116.5 (16)
Cl1^{i}—Hg1—N1—C5	145.3 (7)	C10—N3—C15—C16	−92.0 (14)
Cl1—Hg1—N2—C6	−125.6 (6)	C13—N3—C15—C16	114.9 (15)
Cl1—Hg1—N2—C7	51.6 (10)	N1—C1—C2—C3	−5.1 (18)
Cl2—Hg1—N2—C6	106.4 (6)	C1—C2—C3—C4	4.0 (17)
Cl2—Hg1—N2—C7	−76.5 (10)	C2—C3—C4—C5	−0.7 (16)
N1—Hg1—N2—C6	6.7 (6)	C3—C4—C5—N1	−1.7 (15)
N1—Hg1—N2—C7	−176.1 (10)	C3—C4—C5—C6	175.9 (9)
Cl1^{i}—Hg1—N2—C6	−44.1 (7)	N1—C5—C6—N2	4.7 (13)
Cl1^{i}—Hg1—N2—C7	133.1 (9)	C4—C5—C6—N2	−173.0 (9)
Cl1—Hg1—Cl1^{i}—Hg1^{i}	0.00 (9)	N2—C7—C8—C9	177.8 (14)
Cl2—Hg1—Cl1^{i}—Hg1^{i}	120.45 (11)	C12—C7—C8—C9	0 (2)
N1—Hg1—Cl1^{i}—Hg1^{i}	−135.1 (2)	N2—C7—C12—C11	−174.8 (14)
N2—Hg1—Cl1^{i}—Hg1^{i}	−87.4 (3)	C8—C7—C12—C11	3 (2)
Hg1—N1—C1—C2	−176.5 (9)	C7—C8—C9—C10	−1 (2)
C5—N1—C1—C2	2.6 (16)	C8—C9—C10—N3	179.4 (14)
Hg1—N1—C5—C4	179.9 (7)	C8—C9—C10—C11	−1 (2)
Hg1—N1—C5—C6	2.3 (10)	N3—C10—C11—C12	−176.2 (16)
C1—N1—C5—C4	0.8 (14)	C9—C10—C11—C12	4 (3)
C1—N1—C5—C6	−176.9 (9)	C10—C11—C12—C7	−6 (3)
Hg1—N2—C6—C5	−8.5 (10)		

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Cl1^{ii}	0.93	2.74	3.578 (9)	151
C1—H1···Cl1^{i}	0.93	2.89	3.471 (12)	122
C1—H1···Cl2^{iii}	0.93	2.97	3.623 (11)	129

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