

Crystal structure of an Hg^{II} coordination polymer with an unsymmetrical dipyrindyl ligand: *catena*-poly[[[dichloridomercury(II)]- μ -*N*-(pyridin-4-ylmethyl)pyridin-3-amine- κ^2 N:N'] chloroform hemisolvate]

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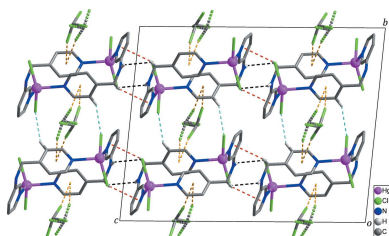
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Keywords: crystal structure; Hg^{II} compound; unsymmetrical dipyrindyl ligand; zigzag coordination polymer.**CCDC reference:** 1507232**Supporting information:** this article has supporting information at journals.iucr.org/e

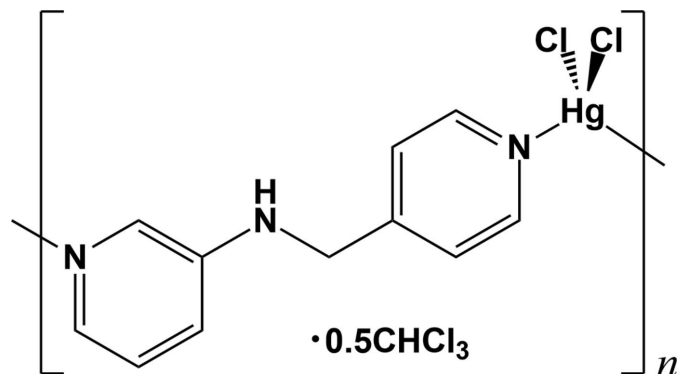
The asymmetric unit of the title compound, $\{[\text{Hg}L\text{Cl}_2] \cdot 0.5\text{CHCl}_3\}_n$ ($L = N$ -(pyridin-4-ylmethyl)pyridin-3-amine, $\text{C}_{11}\text{H}_{11}\text{N}_3$), contains one Hg^{II} ion, one bridging L ligand, two chloride ligands and a chloroform solvent molecule with half-occupancy that is disordered about a crystallographic twofold rotation axis. Each Hg^{II} ion is coordinated by two pyridine N atoms from two symmetry-related L ligands and two chloride anions in a highly distorted tetrahedral geometry with bond angles falling in the range 99.05 (17)–142.96 (7)°. Each L ligand bridges two Hg^{II} ions, forming polymeric zigzag chains propagating in [010]. In the crystal, the chains are linked by intermolecular N/C–H···Cl hydrogen bonds together with weak C–H··· π interactions, resulting in the formation of a three-dimensional supramolecular network, which is further stabilized by C–Cl··· π interactions between the solvent chloroform molecules and the pyridine rings of L [chloride-to-centroid distances = 3.442 (11) and 3.626 (13) Å]. In addition, weak Cl···Cl contacts [3.320 (5) Å] between the chloroform solvent molecules and the coordinating chloride anions are also observed.

1. Chemical context

A variety of coordination polymers have been explored extensively over the last two decades because of their fascinating architectures and their useful applications in materials chemistry (Silva *et al.*, 2015; Furukawa *et al.*, 2014; Robson, 2008; Leong & Vittal, 2011). In this area of research, symmetrical dipyrindyl ligands composed of two terminal pyridines with same substituted nitrogen positions have been used mainly for the design and construction of the coordination polymers. By contrast, investigations based on unsymmetrical dipyrindyl ligands, with the nitrogen atoms in different positions on each of the two terminal pyridines, are still rare (Uemura *et al.*, 2008; Khlobystov *et al.*, 2003). Recently, our group and that of Gao have already reported Ag^I coordination polymers with some unsymmetrical dipyrindyl ligands such as N -(pyridine-3-ylmethyl)pyridine-2-amine (Lee *et al.*, 2013; Zhang *et al.*, 2013), N -(pyridine-2-ylmethyl)pyridine-3-amine (Ju *et al.*, 2014; Moon & Park, 2014; Moon *et al.*, 2014; Zhang *et al.*, 2013) and N -(pyridine-4-ylmethyl)pyridine-3-amine (Lee *et al.*, 2015; Moon *et al.*, 2015; Zhang *et al.*, 2013). As a part of our ongoing efforts to construct coordination polymers with



such unsymmetrical dipyriddy ligands, we prepared the title compound obtained by the reaction of mercury(II) chloride with an unsymmetrical dipyriddy ligand, namely *N*-(pyridine-4-ylmethyl)pyridine-3-amine, synthesized according to a literature procedure (Lee *et al.*, 2013). Herein, we report the crystal structure of the title compound.



2. Structural commentary

The asymmetric unit of the title compound, $\{[\text{HgCl}_2] \cdot 0.5\text{CHCl}_3\}_n$, $L = N$ -(pyridine-4-ylmethyl)pyridine-3-amine, $\text{C}_{11}\text{H}_{11}\text{N}_3$, comprises one Hg^{II} ion, one L ligand, two chloride anions and one half-molecule of chloroform. The solvent molecule is disordered over two orientations of equal occupancy about the crystallographic twofold rotation axis. As shown in Fig. 1, the coordination geometry of each Hg^{II} ion is highly distorted tetrahedral with two coordination sites being occupied by two pyridine N atoms from two symmetry-related L ligands. The geometry of the Hg^{II} ion is completed by the coordination of two chloride ions. The tetrahedral angles around the Hg^{II} ion fall in the range of 99.05 (17)–142.96 (7) $^\circ$ (Table 1).

Each L ligand bridges two Hg^{II} ions into an infinite zigzag chain propagating along the b axis (Fig. 2). The separation

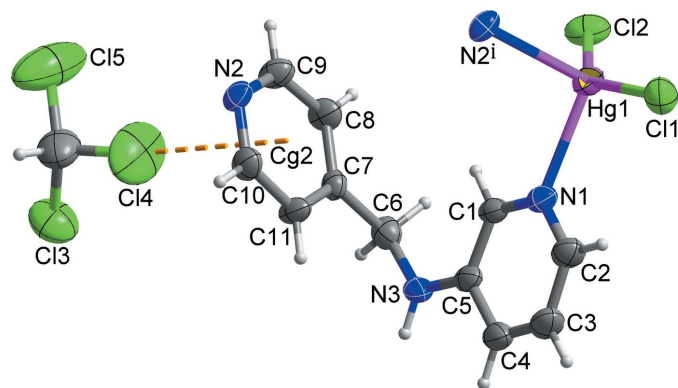


Figure 1

A view of the molecular structure of the title compound, showing the atom-numbering scheme [symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$]. Displacement ellipsoids are drawn at the 30% probability level. Only one component of the disordered chloroform molecule is shown. The dashed line represents the intermolecular $\text{C}-\text{Cl} \cdots \pi$ interaction [$\text{Cl}4 \cdots \text{Cg}2 = 3.442$ (11) Å; $\text{Cg}2$ is the centroid of the $\text{N}2/\text{C}7-\text{C}11$ ring].

Table 1
Selected geometric parameters (Å, $^\circ$).

Hg1–N1	2.367 (5)	Hg1–Cl1	2.3759 (18)
Hg1–Cl2	2.3718 (19)	Hg1–N2 ⁱ	2.385 (5)
N1–Hg1–Cl2	103.82 (14)	N1–Hg1–N2 ⁱ	99.05 (17)
N1–Hg1–Cl1	102.31 (14)	Cl2–Hg1–N2 ⁱ	101.20 (14)
Cl2–Hg1–Cl1	142.96 (7)	Cl1–Hg1–N2 ⁱ	100.11 (13)

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

Table 2
Hydrogen-bond geometry (Å, $^\circ$).

$\text{Cg}1$ is the centroid of the $\text{N}1/\text{C}1-\text{C}5$ ring.

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N}3-\text{H}3 \cdots \text{Cl}2^{\text{ii}}$	0.86	2.78	3.467 (5)	138
$\text{C}8-\text{H}8 \cdots \text{Cl}1^{\text{iii}}$	0.93	2.80	3.654 (6)	153
$\text{C}6-\text{H}6 \cdots \text{Cg}1^{\text{ii}}$	0.97	2.71	3.465 (7)	135

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

between the Hg^{II} ions through a L ligand in the chain is 8.1033 (6) Å. In the L ligand, the $\text{C}_{\text{py}}-\text{N}-\text{C}-\text{C}_{\text{py}}$ torsion angle is -70.9 (7) $^\circ$ while the dihedral angle between two terminal pyridine ring planes is 85.0 (2) $^\circ$. The conformation of the L ligand, along with the the $\text{N}_{\text{py}}-\text{Hg}-\text{N}_{\text{py}}$ coordination angle [99.05 (17) $^\circ$], may induce the zigzag topology of the chain.

3. Supramolecular features

In the crystal, adjacent zigzag chains are linked by intermolecular $\text{N}-\text{H} \cdots \text{Cl}$ hydrogen bonds and weak intermolecular $\text{C}-\text{H} \cdots \pi$ interactions (Table 2), forming a layer extending parallel to the bc plane (Figs. 2 and 3). Furthermore,

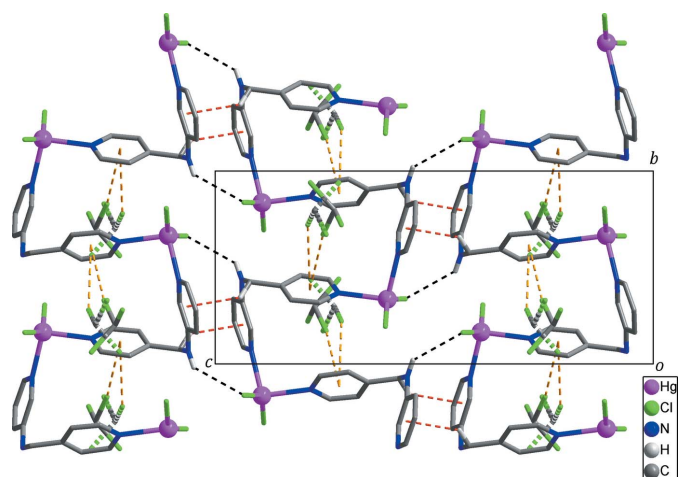
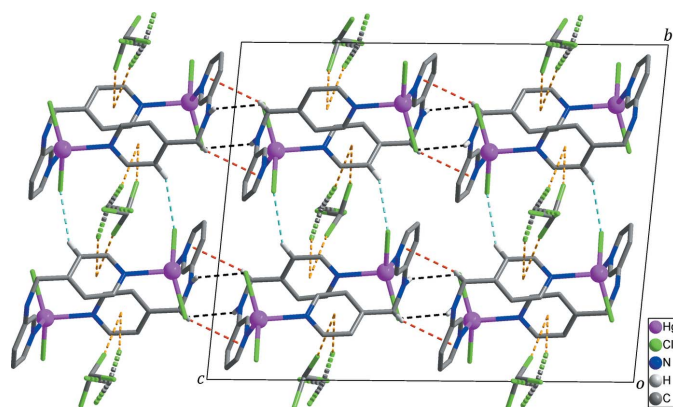


Figure 2

The layer formed through intermolecular $\text{N}-\text{H} \cdots \text{Cl}$ hydrogen bonds (black dashed lines) and weak $\text{C}-\text{H} \cdots \pi$ interactions (red dashed lines). Disordered chloroform molecules and intermolecular $\text{C}-\text{Cl} \cdots \pi$ interactions are shown as two-colored dashed lines and yellow dashed lines, respectively. H atoms not involved in intermolecular interactions have been omitted for clarity.


Figure 3

The three-dimensional supramolecular network constructed through intermolecular C—H...Cl hydrogen bonds (light-blue dashed lines) and C—Cl... π interactions (yellow dashed lines) between the layers formed through N—H...Cl (black dashed lines) and C—H... π (red dashed lines) interactions. Disordered chloroform molecules are shown as two-colored dashed lines. H atoms not involved in intermolecular interactions have been omitted for clarity.

neighboring layers are packed by C—H...Cl hydrogen bonds (Table 2), resulting in the formation of a three-dimensional supramolecular network (Fig. 3). This three-dimensional network is further stabilized by C—Cl... π interactions (Chifotides & Dunbar, 2013; Matter *et al.*, 2009) between the solvent chloroform molecules and the pyridine rings of *L* with $\text{Cl4}\cdots\text{Cg2} = 3.442(11)\text{ \AA}$, $\text{Cl14}\cdots\text{Cg2} = 170.7(8)^\circ$, $\text{Cl5}\cdots\text{Cg2}^{\text{iv}} = 3.626(13)\text{ \AA}$ and $\text{Cl12}\cdots\text{Cg2}^{\text{iv}} = 144.1(8)^\circ$ [yellow dashed lines in Figs. 1, 2 and 3; Cg2 is the centroid of the N2/C7—C11 ring; symmetry code: (iv) $-x, y, -z + \frac{1}{2}$]. In addition, weak intermolecular Cl...Cl contacts between the solvent chloroform molecule and the coordinating chloride anion [$\text{Cl1}\cdots\text{Cl3}^{\text{v}} = 3.320(5)\text{ \AA}$, $\text{Hg1}\cdots\text{Cl1}\cdots\text{Cl3}^{\text{v}} = 126.70(14)$ and $\text{Cl1}\cdots\text{Cl3}^{\text{v}}\cdots\text{Cl2}^{\text{v}} = 169.2(8)^\circ$; symmetry code: (v) $x + \frac{1}{2}, y + \frac{3}{2}, z$] are observed.

4. Synthesis and crystallization

The *L* ligand was synthesized according to a literature method (Lee *et al.*, 2013). X-ray-quality single crystals of the title compound were obtained by slow diffusion of a methanol solution of HgCl_2 into a chloroform solution of the *L* ligand.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. A reflection affected by the beamstop was omitted from the final refinement. The chloroform molecule is disordered over two sets of sites about a twofold rotation axis with equal occupancy. The C—Cl bond lengths were restrained using the DFIX instructions in *SHELXL2014/7* (Sheldrick, 2015). All H atoms were positioned geometrically with $d(\text{C—H}) = 0.93\text{ \AA}$ for $\text{Csp}^2\text{—H}$, 0.97 \AA for methylene C—H, 0.98 \AA for methine C—H, and

Table 3

Experimental details.

Crystal data	
Chemical formula	$[\text{HgCl}_2(\text{C}_{11}\text{H}_{11}\text{N}_3)]\cdot 0.5\text{CHCl}_3$
M_r	516.40
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	298
a, b, c (Å)	16.6906 (14), 9.1942 (8), 21.0159 (17)
β (°)	95.501 (2)
V (Å ³)	3210.2 (5)
Z	8
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	10.16
Crystal size (mm)	$0.4 \times 0.3 \times 0.3$
Data collection	
Diffractometer	Bruker APEXII CCD area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2014)
$T_{\text{min}}, T_{\text{max}}$	0.521, 0.928
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8852, 3151, 2189
R_{int}	0.044
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.033, 0.074, 0.99
No. of reflections	3151
No. of parameters	190
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.58, -0.83

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *DIAMOND* (Brandenburg, 2010).

0.86 \AA for amine N—H, and were refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

Acknowledgements

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supporting information

Acta Cryst. (2016). E72, 1513-1516 [https://doi.org/10.1107/S2056989016015310]

Crystal structure of an Hg^{II} coordination polymer with an unsymmetrical di-pyridyl ligand: *catena*-poly[[[dichloridomercury(II)]- μ -*N*-(pyridin-4-ylmethyl)-pyridin-3-amine- κ^2 *N:N'*] chloroform hemisolvate]

Suk-Hee Moon, Donghyun Kang and Ki-Min Park

Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINTE* (Bruker, 2014); data reduction: *SAINTE* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

catena-Poly[[[dichloridomercury(II)]- μ -*N*-(pyridin-4-ylmethyl)pyridin-3-amine- κ^2 *N:N'*] chloroform hemisolvate]

Crystal data

[HgCl₂(C₁₁H₁₁N₃)]·0.5CHCl₃

$M_r = 516.40$

Monoclinic, *C2/c*

$a = 16.6906$ (14) Å

$b = 9.1942$ (8) Å

$c = 21.0159$ (17) Å

$\beta = 95.501$ (2)°

$V = 3210.2$ (5) Å³

$Z = 8$

$F(000) = 1928$

$D_x = 2.137$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3870 reflections

$\theta = 2.0$ – 28.3 °

$\mu = 10.16$ mm⁻¹

$T = 298$ K

Block, colorless

$0.4 \times 0.3 \times 0.3$ mm

Data collection

Bruker APEXII CCD area detector
diffractometer

phi and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2014)

$T_{\min} = 0.521$, $T_{\max} = 0.928$

8852 measured reflections

3151 independent reflections

2189 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 26.0$ °, $\theta_{\min} = 2.5$ °

$h = -12 \rightarrow 20$

$k = -11 \rightarrow 10$

$l = -24 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.074$

$S = 0.99$

3151 reflections

190 parameters

3 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.034P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.58$ e Å⁻³

$\Delta\rho_{\min} = -0.83$ e Å⁻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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Hg1	0.32126 (2)	0.66479 (3)	0.10699 (2)	0.06180 (11)	
Cl1	0.44104 (11)	0.8055 (2)	0.11123 (9)	0.0766 (5)	
Cl2	0.18389 (11)	0.6629 (2)	0.06581 (9)	0.0839 (6)	
N1	0.3676 (3)	0.4300 (6)	0.0825 (2)	0.0548 (13)	
N2	0.1898 (3)	0.1323 (5)	0.2816 (2)	0.0568 (13)	
N3	0.2853 (4)	0.0648 (6)	0.0611 (2)	0.0641 (15)	
H3	0.3015	-0.0182	0.0486	0.077*	
C1	0.3176 (4)	0.3179 (7)	0.0811 (3)	0.0522 (15)	
H1	0.2663	0.3330	0.0938	0.063*	
C2	0.4398 (4)	0.4134 (8)	0.0648 (3)	0.0693 (18)	
H2	0.4749	0.4922	0.0662	0.083*	
C3	0.4649 (5)	0.2790 (10)	0.0439 (4)	0.080 (2)	
H3A	0.5163	0.2687	0.0310	0.096*	
C4	0.4152 (5)	0.1641 (8)	0.0423 (3)	0.075 (2)	
H4	0.4322	0.0742	0.0284	0.090*	
C5	0.3372 (4)	0.1798 (7)	0.0618 (3)	0.0562 (16)	
C6	0.2052 (4)	0.0749 (7)	0.0800 (3)	0.0615 (17)	
H6A	0.1761	-0.0130	0.0667	0.074*	
H6B	0.1780	0.1559	0.0576	0.074*	
C7	0.2007 (4)	0.0955 (7)	0.1513 (2)	0.0499 (15)	
C8	0.1386 (4)	0.1686 (7)	0.1738 (3)	0.0636 (17)	
H8	0.0986	0.2093	0.1454	0.076*	
C9	0.1348 (4)	0.1821 (7)	0.2375 (3)	0.0664 (18)	
H9	0.0904	0.2298	0.2512	0.080*	
C10	0.2502 (4)	0.0629 (7)	0.2600 (3)	0.0677 (19)	
H10	0.2895	0.0249	0.2897	0.081*	
C11	0.2594 (4)	0.0424 (7)	0.1953 (3)	0.0618 (18)	
H11	0.3040	-0.0060	0.1825	0.074*	
C12	0.0095 (13)	-0.2965 (16)	0.2726 (7)	0.128 (8)	0.5
H12	0.0355	-0.3356	0.3128	0.153*	0.5
Cl3	-0.0016 (4)	-0.4392 (6)	0.2177 (3)	0.1288 (19)	0.5
Cl4	0.0705 (7)	-0.1706 (11)	0.2464 (6)	0.201 (5)	0.5
Cl5	-0.0803 (8)	-0.2208 (14)	0.2885 (6)	0.230 (7)	0.5

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.06149 (17)	0.07271 (18)	0.05193 (16)	0.00720 (15)	0.00918 (12)	-0.00275 (14)
Cl1	0.0576 (10)	0.0833 (12)	0.0887 (13)	0.0035 (9)	0.0056 (10)	0.0198 (10)

Cl2	0.0639 (11)	0.1104 (15)	0.0748 (11)	0.0191 (11)	-0.0065 (9)	-0.0262 (11)
N1	0.052 (3)	0.069 (3)	0.044 (3)	0.012 (3)	0.006 (3)	-0.001 (2)
N2	0.053 (3)	0.078 (4)	0.040 (3)	0.007 (3)	0.009 (3)	0.006 (2)
N3	0.096 (4)	0.052 (3)	0.047 (3)	0.018 (3)	0.019 (3)	-0.004 (2)
C1	0.053 (4)	0.063 (4)	0.041 (3)	0.017 (3)	0.007 (3)	-0.001 (3)
C2	0.056 (4)	0.083 (5)	0.070 (4)	0.019 (4)	0.011 (4)	0.008 (4)
C3	0.065 (5)	0.097 (6)	0.083 (6)	0.030 (5)	0.026 (4)	0.020 (5)
C4	0.099 (6)	0.072 (5)	0.057 (4)	0.032 (5)	0.027 (4)	0.010 (4)
C5	0.070 (4)	0.066 (4)	0.034 (3)	0.023 (4)	0.010 (3)	0.007 (3)
C6	0.074 (5)	0.061 (4)	0.047 (4)	0.002 (4)	-0.004 (4)	0.001 (3)
C7	0.061 (4)	0.053 (3)	0.036 (3)	0.000 (3)	0.002 (3)	0.006 (3)
C8	0.052 (4)	0.082 (4)	0.053 (4)	0.017 (4)	-0.011 (3)	0.007 (4)
C9	0.052 (4)	0.089 (5)	0.059 (4)	0.015 (4)	0.005 (3)	-0.002 (4)
C10	0.065 (4)	0.083 (5)	0.055 (4)	0.018 (4)	0.004 (4)	0.017 (3)
C11	0.061 (4)	0.083 (5)	0.042 (3)	0.029 (4)	0.008 (3)	0.003 (3)
C12	0.18 (2)	0.108 (14)	0.098 (18)	0.000 (18)	0.04 (2)	-0.024 (10)
Cl3	0.147 (5)	0.100 (3)	0.135 (4)	-0.006 (4)	-0.011 (5)	-0.026 (3)
Cl4	0.208 (10)	0.167 (7)	0.234 (11)	-0.120 (7)	0.051 (8)	-0.057 (7)
Cl5	0.184 (9)	0.242 (12)	0.281 (15)	-0.077 (9)	0.110 (10)	-0.150 (11)

Geometric parameters (Å, °)

Hg1—N1	2.367 (5)	C4—C5	1.409 (10)
Hg1—Cl2	2.3718 (19)	C4—H4	0.9300
Hg1—Cl1	2.3759 (18)	C6—C7	1.519 (7)
Hg1—N2 ⁱ	2.385 (5)	C6—H6A	0.9700
N1—C2	1.303 (8)	C6—H6B	0.9700
N1—C1	1.326 (8)	C7—C8	1.358 (8)
N2—C10	1.310 (8)	C7—C11	1.371 (8)
N2—C9	1.323 (8)	C8—C9	1.352 (9)
N2—Hg1 ⁱⁱ	2.386 (5)	C8—H8	0.9300
N3—C5	1.366 (8)	C9—H9	0.9300
N3—C6	1.434 (8)	C10—C11	1.394 (8)
N3—H3	0.8600	C10—H10	0.9300
C1—C5	1.382 (8)	C11—H11	0.9300
C1—H1	0.9300	C12—Cl4	1.670 (15)
C2—C3	1.389 (11)	C12—Cl5	1.713 (17)
C2—H2	0.9300	C12—Cl3	1.746 (13)
C3—C4	1.342 (10)	C12—H12	0.9800
C3—H3A	0.9300		
N1—Hg1—Cl2	103.82 (14)	C1—C5—C4	115.5 (7)
N1—Hg1—Cl1	102.31 (14)	N3—C6—C7	114.6 (5)
Cl2—Hg1—Cl1	142.96 (7)	N3—C6—H6A	108.6
N1—Hg1—N2 ⁱ	99.05 (17)	C7—C6—H6A	108.6
Cl2—Hg1—N2 ⁱ	101.20 (14)	N3—C6—H6B	108.6
Cl1—Hg1—N2 ⁱ	100.11 (13)	C7—C6—H6B	108.6
C2—N1—C1	120.0 (6)	H6A—C6—H6B	107.6

C2—N1—Hg1	120.0 (5)	C8—C7—C11	117.5 (5)
C1—N1—Hg1	119.7 (4)	C8—C7—C6	121.0 (5)
C10—N2—C9	115.6 (5)	C11—C7—C6	121.5 (6)
C10—N2—Hg1 ⁱⁱ	122.4 (4)	C9—C8—C7	119.9 (6)
C9—N2—Hg1 ⁱⁱ	122.0 (4)	C9—C8—H8	120.0
C5—N3—C6	123.7 (5)	C7—C8—H8	120.0
C5—N3—H3	118.2	N2—C9—C8	124.5 (6)
C6—N3—H3	118.2	N2—C9—H9	117.7
N1—C1—C5	123.7 (6)	C8—C9—H9	117.7
N1—C1—H1	118.2	N2—C10—C11	124.3 (6)
C5—C1—H1	118.2	N2—C10—H10	117.8
N1—C2—C3	120.6 (7)	C11—C10—H10	117.8
N1—C2—H2	119.7	C7—C11—C10	118.1 (6)
C3—C2—H2	119.7	C7—C11—H11	120.9
C4—C3—C2	120.3 (7)	C10—C11—H11	120.9
C4—C3—H3A	119.8	C14—C12—C15	110.8 (10)
C2—C3—H3A	119.8	C14—C12—C13	109.4 (9)
C3—C4—C5	119.9 (7)	C15—C12—C13	113.3 (11)
C3—C4—H4	120.1	C14—C12—H12	107.7
C5—C4—H4	120.1	C15—C12—H12	107.7
N3—C5—C1	123.1 (6)	C13—C12—H12	107.7
N3—C5—C4	121.4 (6)		
C2—N1—C1—C5	0.3 (9)	N3—C6—C7—C8	150.4 (6)
Hg1—N1—C1—C5	174.1 (4)	N3—C6—C7—C11	-29.1 (9)
C1—N1—C2—C3	0.6 (9)	C11—C7—C8—C9	-2.3 (10)
Hg1—N1—C2—C3	-173.3 (5)	C6—C7—C8—C9	178.2 (6)
N1—C2—C3—C4	-0.8 (11)	C10—N2—C9—C8	-1.6 (10)
C2—C3—C4—C5	0.1 (11)	Hg1 ⁱⁱ —N2—C9—C8	179.0 (5)
C6—N3—C5—C1	0.1 (9)	C7—C8—C9—N2	2.3 (11)
C6—N3—C5—C4	-179.6 (5)	C9—N2—C10—C11	1.1 (10)
N1—C1—C5—N3	179.5 (5)	Hg1 ⁱⁱ —N2—C10—C11	-179.5 (5)
N1—C1—C5—C4	-0.8 (9)	C8—C7—C11—C10	1.9 (10)
C3—C4—C5—N3	-179.7 (6)	C6—C7—C11—C10	-178.7 (6)
C3—C4—C5—C1	0.6 (9)	N2—C10—C11—C7	-1.4 (11)
C5—N3—C6—C7	-70.9 (7)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

*Cg*1 is the centroid of the N1/C1—C5 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>
N3—H3...C12 ⁱⁱⁱ	0.86	2.78	3.467 (5)	138
C8—H8...C11 ^{iv}	0.93	2.80	3.654 (6)	153
C6—H6 <i>B</i> ... <i>Cg</i> 1 ⁱⁱⁱ	0.97	2.71	3.465 (7)	135

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