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A one-dimensional Hg^{II} coordination polymer based on bis(pyridin-3-ylmethyl)sulfane

Suk-Hee Moon,[a] Youngjin Kang[b]* and Ki-Min Park[c]*

[a]Department of Food and Nutrition, Kyungnam College of Information and Technology, Busan 47011, Republic of Korea, [b]Division of Science Education, Kangwon National University, Chuncheon 24341, Republic of Korea, and [c]Research institute of Natural Science, Gyeongsang National University, Jinju 52828, Republic of Korea. *Correspondence e-mail: kangy@kangwon.ac.kr, kmpark@gnu.ac.kr

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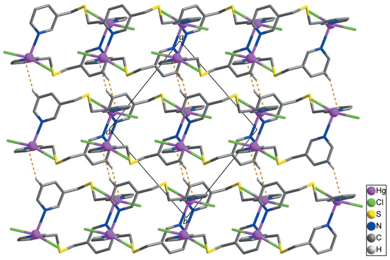
The reaction of mercury(II) chloride with bis(pyridin-3-ylmethyl)sulfane (L, $C_{12}H_{12}N_2S$) in methanol afforded the title crystalline coordination polymer *catena*-poly[[dichloridomercury(II)]-μ-bis(pyridin-3-ylmethyl)sulfane-κ^2N:N'], $[HgCl_2L]_n$. The asymmetric unit consists of one Hg^{II} cation, one L ligand and two chloride anions. Each Hg^{II} ion is coordinated by two pyridine N atoms from separate L ligands and two chloride anions. The metal adopts a highly distorted tetrahedral geometry, with bond angles about the central atom in the range 97.69 (12)–153.86 (7)°. Each L ligand bridges two Hg^{II} ions, forming an infinite $–(Hg–L)_n–$ zigzag chain along the b axis, with an Hg$\cdots$Hg separation of 10.3997 (8) Å. In the crystal, adjacent chains are connected by intermolecular C—H$\cdots$Cl hydrogen bonds, together with Hg—Cl$\cdots\pi$ interactions [chloride-to-centroid distance = 3.902 (3) Å], that form between a chloride anion and the one of the pyridine rings of L, generating a two-dimensional layer extending parallel to (101). These layers are further linked by intermolecular C—H$\cdots\pi$ hydrogen bonds, forming a three-dimensional supramolecular network.



1. Chemical context

The structural topology of coordination polymers generated from the self-assembly of transition metal ions and organic molecules functioning as spacer ligands depends mainly on the structures of the spacer ligands and the coordination geometries adopted by the metal ions. The flexibility, length and coordinating ability of the spacer ligands exert strong influences on the formation of coordination polymers and their resulting diverse topologies (Zheng *et al.*, 2009; Leong & Vittal, 2011; Liu *et al.* 2011). For this reason, both rigid and flexible dipyridyl-type spacer ligands with strong coordinating ability and functional characteristics have been widely used to construct a variety of coordination polymers with interesting structures and attractive potential applications in material science (Silva *et al.*, 2015; Furukawa *et al.*, 2014; Wang *et al.*, 2012).

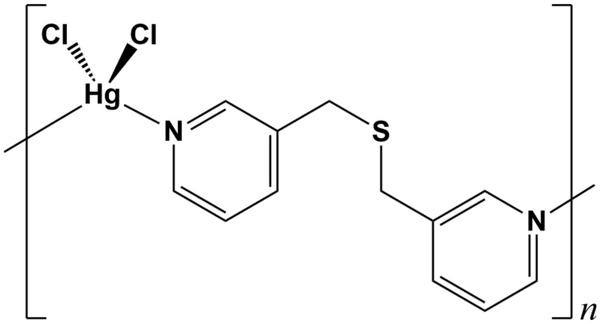


Table 1
Selected geometric parameters (Å, °).

Hg1—Cl1	2.3610 (16)	Hg1—N2^{i}	2.434 (5)
Hg1—Cl2	2.3751 (16)	Hg1—N1	2.436 (5)
Cl1—Hg1—Cl2	153.86 (7)	Cl1—Hg1—N1	97.69 (12)
Cl1—Hg1—N2^{i}	100.29 (12)	Cl2—Hg1—N1	97.91 (13)
Cl2—Hg1—N2^{i}	98.03 (12)	N2^{i}—Hg1—N1	98.39 (16)

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

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*2 is the centroid of the N2/C8–C12 ring.

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C10—H10$\cdots$Cl1^{ii}	0.93	2.80	3.526 (6)	136
C2—H2$\cdots$*Cg*2^{iii}	0.93	2.89	3.689 (7)	145

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

Our group has also synthesized the flexible dipyridyl-type ligand bis(pyridine-3-ylmethyl)sulfane (*L*), and has reported its Ag^{I} and Co^{II} coordination polymers (Moon *et al.*, 2017*a*,*b*). Our continuing interest in the development of coordination polymers based on this ligand led us to investigate a coordination polymer with an Hg^{II} cation. The reaction of mercury(II) chloride with *L* (synthesized according to a previously reported procedure: Park *et al.*, 2010; Lee *et al.*, 2012) afforded the title compound. Herein, we describe its structure, which involves a one-dimensional zigzag-chain.

2. Structural commentary

Fig. 1 shows the molecular structure of the title compound, [Hg*L*Cl$_2$]$_n$, *L* = bis(pyridine-3-ylmethyl)sulfane, $C_{12}H_{12}N_2S$. The asymmetric unit comprises one Hg^{II} cation, one *L* ligand and two chloride anions. The Hg^{II} ion is four-coordinated, binding to two Cl anions and two pyridine N atoms from two separate symmetry-related *L* ligands, forming a highly distorted tetrahedral geometry (Fig. 1), with the tetrahedral angles falling in the range of 97.69 (12)–153.86 (7)° (Table 1). The S atoms of the *L* ligands are surprisingly not bound to the soft Hg^{II} cations. Each *L* ligand bridges two Hg^{II} cations, resulting in an infinite zigzag chain propagating along the *b*-axis direction (Fig. 2). The separation between the Hg^{II} ions in the chain is 10.3997 (8) Å. In the *L* ligand, the dihedral angle between the two terminal pyridine rings is 78.52 (18)°, and the flexible thioether moiety [C4–C6–S1–C7–C8] shows a bent arrangement with a *gauche*--*anti* configuration [C4—C6—S1—C7 = 71.9 (5)°; C6—S1—C7—C8 = 172.1 (5)°]. The conformation of the *L* ligand, along with its N$_{py}$—Hg—N$_{py}$ coordination angle [98.39 (16)°], may induce the zigzag topology of the chain.

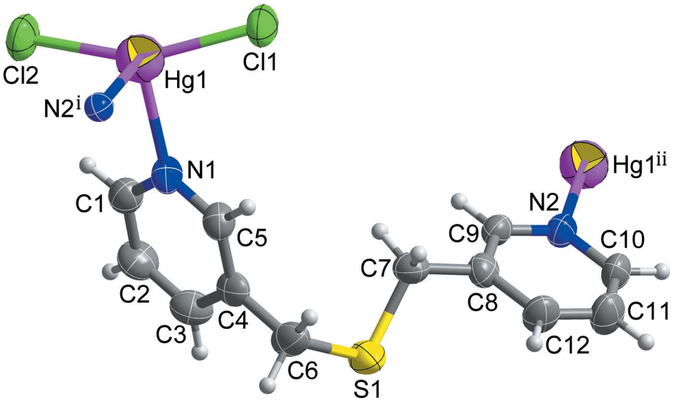


Figure 1
View of the molecular structure of the title compound, showing the atom-numbering scheme [symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$]. Displacement ellipsoids are drawn at the 50% probability level.

3. Supramolecular features

In the crystal structure, adjacent zigzag chains are connected by C10—H10$\cdots$Cl1 hydrogen bonds (Fig. 3, Table 2) and Hg—Cl$\cdots\pi$ interactions (Chifotides & Dunbar, 2013; Matter *et al.*, 2009) between the chloride anions and the pyridine rings of *L* with Cl2$\cdots$*Cg*1^{iv} = 3.902 (3) Å and Hg1—Cl2$\cdots$*Cg*1^{iv} = 77.21 (6)° [Fig. 3; *Cg*1 is the centroid of the N1/C1–C5 ring; symmetry code: (iv) $-x+1, -y+1, -z+1$], generating layers extending parallel to (101). Neighboring layers are linked by C2—H2$\cdots$*Cg*2 hydrogen bonds (Table 2; Fig. 4), resulting in the formation of a three-dimensional supramolecular network.

4. Database survey

A search of the Cambridge Structural Database (Version 5.38, update May 2017; Groom *et al.*, 2016) for the title ligand (*L*) gave three hits. Two (REJCAL, RENHOI; Hanton *et al.*, 2006) are copper(I) iodide coordination polymers adopting staircase- and loop-type structures, respectively. The other (EXEZOW; Seo *et al.*, 2003) is a cyclic dimer-type silver(I) BF$_4$ complex. Recently, our group has also reported the crystal structures of silver(I) (Moon *et al.*, 2017*a*) and cobalt(II) (Moon *et al.*, 2017*b*) NO$_3$ coordination polymers that display twisted ribbon- and loop-type topologies, respectively. In these complexes, the flexible thioether moiety (C$_{py}$–C–S–C–C$_{py}$) of

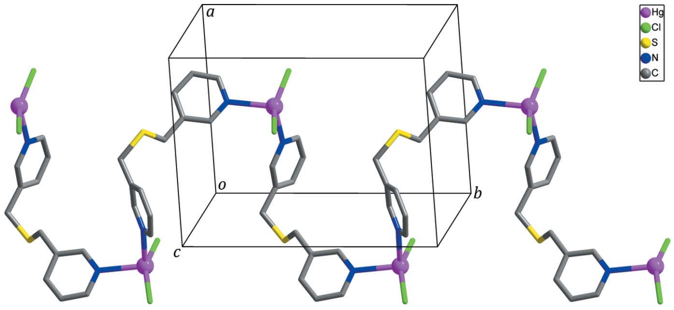


Figure 2
The polymeric zigzag chain propagating along the *b*-axis direction. H atoms are omitted for clarity.

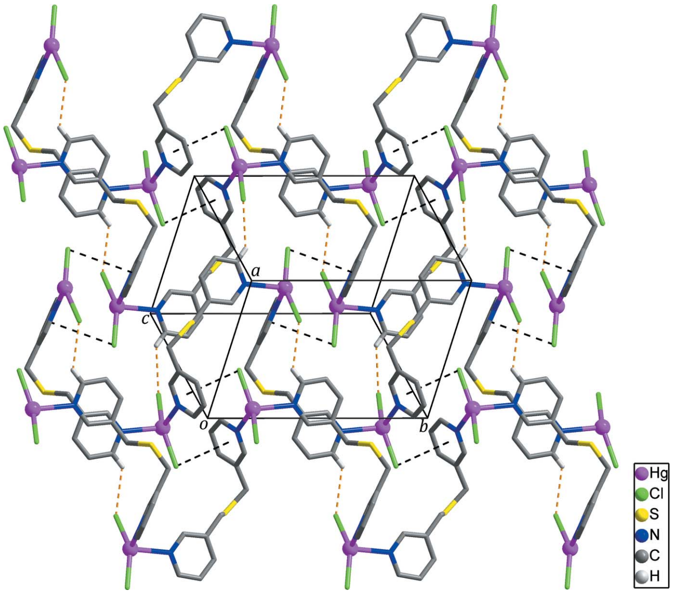


Figure 3
The layer formed through intermolecular C–H···Cl hydrogen bonds (yellow dashed lines) and Hg—Cl···π interactions (black dashed lines) between the zigzag chains. H atoms not involved in intermolecular interactions are omitted for clarity.

the *L* ligand adopts a bent arrangement that is similar to that of the Hg^{II} polymer described here. However, the title compound displays a zigzag topology and is the first example of an Hg^{II} coordination polymer with the ligand *L*.

5. Synthesis and crystallization

The *L* ligand was synthesized according to a literature method (Park *et al.*, 2010; Lee *et al.*, 2012). Crystals of the title compound were obtained by slow evaporation of a methanol solution of *L* with $HgCl_2$ in a 1:1 molar ratio.

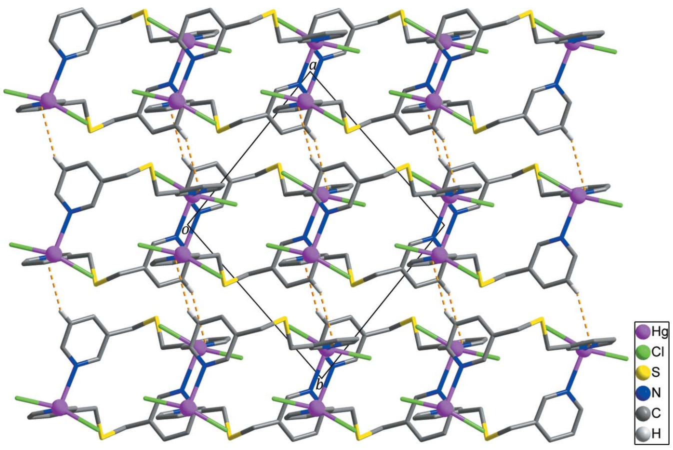


Figure 4
The three-dimensional supramolecular network generated by intermolecular C—H···π interactions (yellow dashed lines) between the layers of polymer chains. H atoms not involved in intermolecular interactions are omitted for clarity.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[HgCl_2(C_{12}H_{12}N_2S)]$
M_r	487.79
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	298
a, b, c (Å)	10.4724 (11), 13.1128 (14), 10.8914 (12)
β (°)	100.1171 (18)
V (Å^3)	1472.4 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	10.94
Crystal size (mm)	0.45 × 0.40 × 0.30
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.447, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8706, 3197, 2413
R_{int}	0.047
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.076, 1.03
No. of reflections	3197
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.62, −1.62

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

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and refined as riding: C—H = 0.93 Å for Csp^2—H and 0.97 Å for methylene C—H with $U_{iso}(H) = 1.2U_{eq}(C)$.

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A one-dimensional Hg^{II} coordination polymer based on bis(pyridin-3-ylmethyl)sulfane

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

Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (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) and *publCIF* (Westrip, 2010).

catena-Poly[[dichloridomercury(II)]-μ-bis(pyridin-3-ylmethyl)sulfane-κ^2N:N']

Crystal data

$[HgCl_2(C_{12}H_{12}N_2S)]$
$M_r = 487.79$
Monoclinic, $P2_1/n$
$a = 10.4724$ (11) Å
$b = 13.1128$ (14) Å
$c = 10.8914$ (12) Å
$\beta = 100.1171$ (18)°
$V = 1472.4$ (3) Å^3
$Z = 4$
$F(000) = 912$
$D_x = 2.200$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9216 reflections
$\theta = 2.5$–28.2°
$\mu = 10.94$ mm^{-1}
$T = 298$ K
Plate, colorless
0.45 × 0.40 × 0.30 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min} = 0.447$, $T_{max} = 0.746$
8706 measured reflections
3197 independent reflections
2413 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.5°$
$h = -13 \rightarrow 11$
$k = -16 \rightarrow 10$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.076$
$S = 1.03$
3197 reflections
163 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -1.62$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Hg1	0.62237 (2)	0.33807 (2)	0.42736 (2)	0.04266 (10)
Cl1	0.54910 (16)	0.36205 (14)	0.21164 (15)	0.0559 (4)
Cl2	0.75516 (17)	0.37587 (15)	0.62207 (16)	0.0633 (5)
S1	−0.06074 (16)	0.35443 (14)	0.33023 (18)	0.0598 (5)
N1	0.4127 (5)	0.3509 (4)	0.4938 (4)	0.0416 (12)
N2	−0.1449 (4)	0.6533 (4)	0.0651 (4)	0.0408 (12)
C1	0.4063 (6)	0.3940 (5)	0.6036 (6)	0.0467 (15)
H1	0.4823	0.4178	0.6525	0.056*
C2	0.2918 (7)	0.4044 (5)	0.6469 (6)	0.0551 (17)
H2	0.2897	0.4384	0.7215	0.066*
C3	0.1800 (7)	0.3642 (5)	0.5789 (7)	0.0537 (17)
H3	0.1018	0.3697	0.6079	0.064*
C4	0.1849 (6)	0.3153 (4)	0.4666 (6)	0.0414 (14)
C5	0.3037 (6)	0.3121 (4)	0.4282 (6)	0.0425 (14)
H5	0.3081	0.2812	0.3523	0.051*
C6	0.0678 (6)	0.2659 (5)	0.3898 (7)	0.0545 (17)
H6A	0.0341	0.2151	0.4405	0.065*
H6B	0.0944	0.2307	0.3201	0.065*
C7	0.0153 (6)	0.4169 (5)	0.2132 (6)	0.0462 (15)
H7A	0.0896	0.4559	0.2536	0.055*
H7B	0.0457	0.3660	0.1605	0.055*
C8	−0.0790 (5)	0.4860 (5)	0.1354 (5)	0.0403 (13)
C9	−0.0627 (5)	0.5903 (4)	0.1356 (5)	0.0379 (13)
H9	0.0090	0.6181	0.1873	0.045*
C10	−0.2482 (6)	0.6139 (5)	−0.0097 (6)	0.0464 (15)
H10	−0.3048	0.6575	−0.0601	0.056*
C11	−0.2726 (6)	0.5132 (5)	−0.0141 (6)	0.0574 (17)
H11	−0.3457	0.4882	−0.0663	0.069*
C12	−0.1897 (6)	0.4473 (5)	0.0583 (6)	0.0503 (16)
H12	−0.2068	0.3776	0.0563	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.03985 (13)	0.04678 (16)	0.03812 (15)	0.00356 (11)	−0.00208 (9)	−0.00140 (12)
Cl1	0.0515 (9)	0.0733 (12)	0.0385 (9)	0.0022 (8)	−0.0039 (7)	−0.0006 (8)
Cl2	0.0602 (10)	0.0726 (12)	0.0482 (10)	−0.0080 (9)	−0.0154 (8)	−0.0059 (9)
S1	0.0373 (8)	0.0776 (13)	0.0666 (12)	0.0107 (8)	0.0149 (8)	0.0249 (10)
N1	0.041 (3)	0.048 (3)	0.035 (3)	0.011 (2)	0.006 (2)	−0.002 (2)

N2	0.039 (3)	0.042 (3)	0.039 (3)	−0.004 (2)	0.000 (2)	0.002 (2)
C1	0.047 (3)	0.046 (4)	0.046 (4)	−0.003 (3)	0.004 (3)	0.001 (3)
C2	0.063 (4)	0.061 (5)	0.045 (4)	0.004 (3)	0.021 (3)	−0.009 (3)
C3	0.056 (4)	0.053 (4)	0.057 (4)	−0.001 (3)	0.024 (3)	−0.002 (3)
C4	0.043 (3)	0.033 (3)	0.049 (4)	0.011 (2)	0.009 (3)	0.012 (3)
C5	0.044 (3)	0.047 (4)	0.037 (3)	0.010 (3)	0.007 (3)	−0.003 (3)
C6	0.044 (4)	0.047 (4)	0.071 (5)	−0.001 (3)	0.008 (3)	0.017 (3)
C7	0.039 (3)	0.051 (4)	0.051 (4)	0.000 (3)	0.013 (3)	0.006 (3)
C8	0.043 (3)	0.047 (4)	0.031 (3)	0.001 (3)	0.006 (2)	−0.003 (3)
C9	0.032 (3)	0.045 (4)	0.036 (3)	−0.005 (2)	0.003 (2)	−0.002 (3)
C10	0.040 (3)	0.055 (4)	0.039 (4)	−0.005 (3)	−0.006 (3)	0.001 (3)
C11	0.056 (4)	0.055 (4)	0.053 (4)	−0.013 (3)	−0.011 (3)	−0.004 (3)
C12	0.051 (4)	0.040 (4)	0.056 (4)	−0.014 (3)	−0.002 (3)	−0.003 (3)

Geometric parameters (Å, º)

Hg1—Cl1	2.3610 (16)	C4—C5	1.381 (8)
Hg1—Cl2	2.3751 (16)	C4—C6	1.504 (9)
Hg1—N2$^{\mathrm{i}}$	2.434 (5)	C5—H5	0.9300
Hg1—N1	2.436 (5)	C6—H6A	0.9700
S1—C6	1.810 (6)	C6—H6B	0.9700
S1—C7	1.813 (6)	C7—C8	1.490 (8)
N1—C5	1.335 (8)	C7—H7A	0.9700
N1—C1	1.336 (7)	C7—H7B	0.9700
N2—C9	1.334 (7)	C8—C9	1.378 (8)
N2—C10	1.339 (7)	C8—C12	1.402 (8)
N2—Hg1$^{\mathrm{ii}}$	2.434 (5)	C9—H9	0.9300
C1—C2	1.370 (8)	C10—C11	1.345 (9)
C1—H1	0.9300	C10—H10	0.9300
C2—C3	1.376 (10)	C11—C12	1.372 (9)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.390 (9)	C12—H12	0.9300
C3—H3	0.9300		

Cl1—Hg1—Cl2	153.86 (7)	C4—C6—S1	113.9 (4)
Cl1—Hg1—N2$^{\mathrm{i}}$	100.29 (12)	C4—C6—H6A	108.8
Cl2—Hg1—N2$^{\mathrm{i}}$	98.03 (12)	S1—C6—H6A	108.8
Cl1—Hg1—N1	97.69 (12)	C4—C6—H6B	108.8
Cl2—Hg1—N1	97.91 (13)	S1—C6—H6B	108.8
N2$^{\mathrm{i}}$—Hg1—N1	98.39 (16)	H6A—C6—H6B	107.7
C6—S1—C7	98.7 (3)	C8—C7—S1	110.2 (4)
C5—N1—C1	117.9 (5)	C8—C7—H7A	109.6
C5—N1—Hg1	123.0 (4)	S1—C7—H7A	109.6
C1—N1—Hg1	119.0 (4)	C8—C7—H7B	109.6
C9—N2—C10	118.8 (5)	S1—C7—H7B	109.6
C9—N2—Hg1$^{\mathrm{ii}}$	123.3 (4)	H7A—C7—H7B	108.1
C10—N2—Hg1$^{\mathrm{ii}}$	117.9 (4)	C9—C8—C12	116.7 (6)
N1—C1—C2	122.3 (6)	C9—C8—C7	122.2 (5)

N1—C1—H1	118.8	C12—C8—C7	121.0 (6)
C2—C1—H1	118.8	N2—C9—C8	123.1 (5)
C1—C2—C3	119.3 (6)	N2—C9—H9	118.4
C1—C2—H2	120.3	C8—C9—H9	118.4
C3—C2—H2	120.3	N2—C10—C11	121.9 (6)
C2—C3—C4	119.4 (6)	N2—C10—H10	119.0
C2—C3—H3	120.3	C11—C10—H10	119.0
C4—C3—H3	120.3	C10—C11—C12	120.1 (6)
C5—C4—C3	117.0 (6)	C10—C11—H11	120.0
C5—C4—C6	120.6 (6)	C12—C11—H11	120.0
C3—C4—C6	122.4 (6)	C11—C12—C8	119.3 (6)
N1—C5—C4	123.9 (6)	C11—C12—H12	120.4
N1—C5—H5	118.1	C8—C12—H12	120.4
C4—C5—H5	118.1		

C5—N1—C1—C2	−3.7 (9)	C6—S1—C7—C8	172.1 (5)
Hg1—N1—C1—C2	179.6 (5)	S1—C7—C8—C9	114.8 (5)
N1—C1—C2—C3	3.8 (10)	S1—C7—C8—C12	−65.0 (7)
C1—C2—C3—C4	−1.1 (10)	C10—N2—C9—C8	−0.1 (8)
C2—C3—C4—C5	−1.4 (9)	$\mathrm{Hg1}^{\mathrm{ii}}$—N2—C9—C8	176.9 (4)
C2—C3—C4—C6	177.5 (6)	C12—C8—C9—N2	−1.4 (9)
C1—N1—C5—C4	0.9 (9)	C7—C8—C9—N2	178.9 (5)
Hg1—N1—C5—C4	177.5 (4)	C9—N2—C10—C11	1.2 (9)
C3—C4—C5—N1	1.6 (9)	$\mathrm{Hg1}^{\mathrm{ii}}$—N2—C10—C11	−175.9 (5)
C6—C4—C5—N1	−177.4 (5)	N2—C10—C11—C12	−0.7 (10)
C5—C4—C6—S1	−117.0 (5)	C10—C11—C12—C8	−0.8 (10)
C3—C4—C6—S1	64.1 (7)	C9—C8—C12—C11	1.8 (9)
C7—S1—C6—C4	71.9 (5)	C7—C8—C12—C11	−178.5 (6)

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 (Å, º)

*Cg*2 is the centroid of the N2/C8–C12 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···$\mathrm{Cl1}^{\mathrm{iii}}$	0.93	2.80	3.526 (6)	136
C2—H2···$Cg2^{\mathrm{iv}}$	0.93	2.89	3.689 (7)	145

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