

Di- μ -chlorido-bis{[4-amino-3,5-bis(2-pyridyl)-4H-1,2,4-triazole- κ N¹]chlorido-mercury(II)}

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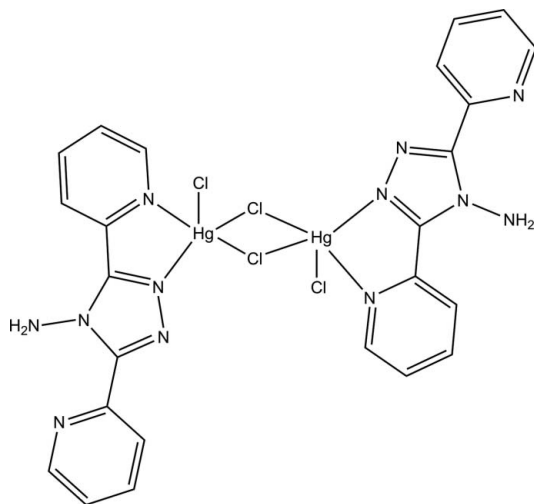
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 13.7.

In the centrosymmetric binuclear title complex, $[\text{Hg}_2\text{Cl}_4(\text{C}_{12}\text{H}_{10}\text{N}_6)_2]$, the Hg^{II} ion is five-coordinated by two N atoms and three chloride ions with a distorted square-pyramidal geometry. In the complex, there is an intramolecular N—H \cdots N hydrogen bond. In the crystal, the binuclear units are connected by intermolecular N—H \cdots Cl hydrogen bonds, as well as π – π stacking interactions [centroid–centroid distances = 3.526 (2) and 3.696 (2) Å], forming a two-dimensional layered structure parallel to (010).

Related literature

For background information on triazole derivatives, see: Klingele *et al.* (2009); Shao *et al.* (2004); Huang *et al.* (2011). For the coordination compounds synthesized with related triazole ligands, see: Du *et al.* (2007, 2008). For a description of the geometry of complexes with five-coordinate metal ions, see: Addison *et al.* (1984).



Experimental

Crystal data

$[\text{Hg}_2\text{Cl}_4(\text{C}_{12}\text{H}_{10}\text{N}_6)_2]$
 $M_r = 1019.50$
 Orthorhombic, $Pbca$
 $a = 11.3634$ (4) Å
 $b = 14.9962$ (6) Å
 $c = 17.2328$ (7) Å

$V = 2936.6$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 10.85$ mm⁻¹
 $T = 296$ K
 $0.28 \times 0.22 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.475$, $T_{\text{max}} = 1.000$

14063 measured reflections
 2596 independent reflections
 2071 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.058$
 $S = 1.08$
 2596 reflections

190 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.53$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—H5A \cdots Cl1 ⁱ	0.89	2.80	3.446 (3)	131
N5—H5A \cdots Cl1 ⁱⁱ	0.89	2.77	3.512 (4)	142
N5—H5B \cdots Cl1 ⁱⁱⁱ	0.89	2.62	3.452 (4)	155
N5—H5B \cdots N6	0.89	2.47	2.956 (5)	115

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 2$; (ii) $-x + \frac{3}{2}, y + \frac{1}{2}, z$; (iii) $-x + 2, -y + 1, -z + 2$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2294).

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supplementary materials

Acta Cryst. (2011). E67, m1180 [doi:10.1107/S1600536811029886]

Di- μ -chlorido-bis{[4-amino-3,5-bis(2-pyridyl)-4H-1,2,4-triazole- κ N¹]}chloridomercury(II)}

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Comment

1,2,4-triazole and its derivatives have been extensively used to prepare diverse coordination complexes (Klingele *et al.*, 2009; Shao *et al.*, 2004; Huang *et al.*, 2011). Recently, a series of interesting metallosupramolecular systems have been constructed using the triazole ligands 4-amino-3,5-bis(4-pyridyl)-1,2,4-triazole and 4-amino-3,5-bis(3-pyridyl)-1,2,4-triazole, using different synthetic methods (Du *et al.*, 2007, 2008). In this context, the analogous ligand, 4-amino-3,5-bis(2-pyridyl)-1,2,4-triazole (2-bpt), that may exhibit different conformations and coordination modes, has received our attention.

Herein, we present the title binuclear complex obtained by the reaction of 2-bpt and HgCl₂ under the hydrothermal condition. In the centrosymmetric title complex, the coordination sphere of each Hg^{II} ion can be described as a distorted square pyramid, as indicated by the τ value of 0.33 (Addison *et al.*, 1984). The Hg^{II} ion coordinates to one terminal chloride ion, two bridging chloride ions and two chelating nitrogen donors from the same 2-bpt ligand (Fig. 1). Each 2-bpt ligand adopts the anti-conformation considering its two terminal pyridyl nitrogen, with the bidentate chelating coordination to one Hg^{II} center. In addition, the two adjacent Hg^{II} centers are linked by a pair of chloride bridges to form a Hg₂Cl₂ subunit, in which the Hg...Hg separation is 3.856 (1) Å and the Hg–Cl–Hg angle is 93.22 (3)°. There is an intramolecular N5–H5B...N6 hydrogen bond in the complex (Table 1).

In the crystal the binuclear units are connected to form a two-dimensional supramolecular network *via* intermolecular N–H...Cl hydrogen bonds (Table 1 and Fig. 2). In addition, π – π stacking interactions are present and further reinforce the two-dimensional supramolecular network. The centroid-centroid distance of the involved pyridyl rings, (N1/C1—C5) and (N6/C8—C12)ⁱ, is 3.696 (2) Å, while the centroid-centroid distance involving the triazole rings, (N2—N4/C6,C7) and (N2—N4/C6,C7)ⁱ, is 3.526 (2) Å (Fig. 2; symmetry code: (i) = -x+2, -y+1, -z+2).

Experimental

A mixture of 2-bpt (23.8 mg, 0.1 mmol), HgCl₂ (27.1 mg, 0.1 mmol) in water (10 ml) was sealed in a Teflon-lined stainless steel vessel (20 ml), which was heated to 413 K over a period of 24 h. It was then gradually cooled to room temperature at a rate of 5 °C/h. Colourless block-like crystals, suitable for X-ray analysis, were obtained. Anal. Calc. for C₂₄H₂₀Cl₄Hg₂N₁₂: C, 28.27; H, 1.98; N, 16.49%. Found: C, 28.30; H, 1.94; N, 16.47%.

Refinement

All the H-atoms were initially located in a difference Fourier map. The C—H and N—H atoms were then constrained to an ideal geometry, and refined as riding atoms: C—H = 0.93 Å and N—H = 0.89 Å, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$.

Figures

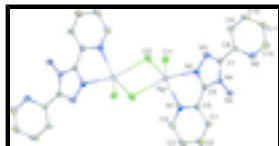


Fig. 1. The molecular structure of the title compound showing the numbering scheme and displacement ellipsoids drawn at the 30% probability level.

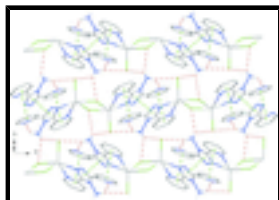


Fig. 2. A view along the *c*-axis of the two-dimensional network in the crystal of the title compound, showing the N–H···N and N–H···Cl hydrogen bonds (red dashed lines) and the π – π stacking interactions (green dashed lines) [See Table 1 and the comment section for details].

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Crystal data

[Hg₂Cl₄(C₁₂H₁₀N₆)₂]

$M_r = 1019.50$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 11.3634$ (4) Å

$b = 14.9962$ (6) Å

$c = 17.2328$ (7) Å

$V = 2936.6$ (2) Å³

$Z = 4$

$F(000) = 1904$

$D_x = 2.306$ Mg m⁻³

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

Cell parameters from 5032 reflections

$\theta = 2.5$ – 28.1°

$\mu = 10.85$ mm⁻¹

$T = 296$ K

Block, colourless

$0.28 \times 0.22 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

2596 independent reflections

Radiation source: fine-focus sealed tube graphite

2071 reflections with $I > 2\sigma(I)$

phi and ω scans

$R_{\text{int}} = 0.023$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

$h = -8 \rightarrow 13$

$T_{\text{min}} = 0.475$, $T_{\text{max}} = 1.000$

$k = -16 \rightarrow 17$

14063 measured reflections

$l = -20 \rightarrow 19$

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.022$

Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.058$

H-atom parameters constrained

$S = 1.08$	$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 2.8778P]$
2596 reflections	where $P = (F_o^2 + 2F_c^2)/3$
190 parameters	$(\Delta/\sigma)_{\max} = 0.001$
0 restraints	$\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -1.26 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.661120 (15)	0.459756 (11)	0.997612 (9)	0.04268 (8)
Cl1	0.66817 (10)	0.31955 (7)	0.92929 (6)	0.0460 (3)
Cl2	0.53708 (10)	0.57586 (7)	0.92105 (6)	0.0486 (3)
N1	0.7468 (3)	0.5214 (2)	1.11219 (19)	0.0384 (8)
N2	0.8392 (3)	0.5359 (2)	0.9665 (2)	0.0381 (9)
N3	0.8938 (3)	0.5633 (2)	0.89923 (19)	0.0377 (8)
N4	0.9726 (3)	0.63366 (19)	0.99779 (15)	0.0266 (7)
N5	1.0319 (3)	0.6981 (2)	1.04316 (18)	0.0356 (8)
H5A	1.0021	0.7495	1.0264	0.053*
H5B	1.1086	0.6932	1.0335	0.053*
N6	1.1599 (3)	0.6863 (2)	0.89418 (19)	0.0413 (9)
C1	0.9194 (4)	0.5833 (3)	1.1697 (2)	0.0377 (10)
H1	0.9916	0.6116	1.1636	0.045*
C2	0.8783 (5)	0.5612 (3)	1.2427 (2)	0.0489 (12)
H2	0.9231	0.5735	1.2866	0.059*
C3	0.7707 (5)	0.5210 (3)	1.2493 (3)	0.0554 (13)
H3	0.7406	0.5068	1.2980	0.066*
C4	0.7081 (4)	0.5017 (3)	1.1836 (3)	0.0504 (12)
H4	0.6354	0.4738	1.1888	0.060*
C5	0.8509 (4)	0.5626 (3)	1.1058 (2)	0.0326 (9)
C6	0.8872 (4)	0.5792 (3)	1.0255 (2)	0.0292 (8)
C7	0.9726 (3)	0.6220 (2)	0.9190 (2)	0.0286 (8)
C8	1.0551 (3)	0.6651 (2)	0.8653 (2)	0.0300 (9)
C9	1.0248 (4)	0.6771 (3)	0.7884 (2)	0.0438 (10)
H9	0.9512	0.6599	0.7702	0.053*
C10	1.1062 (5)	0.7153 (3)	0.7393 (2)	0.0506 (13)
H10	1.0883	0.7250	0.6873	0.061*

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C11	1.2143 (5)	0.7389 (3)	0.7688 (3)	0.0536 (13)
H11	1.2710	0.7650	0.7371	0.064*
C12	1.2368 (4)	0.7232 (3)	0.8453 (3)	0.0515 (12)
H12	1.3102	0.7392	0.8646	0.062*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.04114 (12)	0.03899 (12)	0.04791 (13)	-0.00931 (7)	0.00559 (8)	-0.00763 (7)
C11	0.0512 (7)	0.0409 (6)	0.0458 (6)	-0.0077 (5)	0.0005 (5)	-0.0119 (5)
C12	0.0474 (7)	0.0458 (6)	0.0524 (7)	0.0020 (5)	0.0129 (5)	0.0116 (5)
N1	0.038 (2)	0.0356 (19)	0.0413 (19)	-0.0031 (16)	0.0071 (16)	0.0029 (15)
N2	0.039 (2)	0.039 (2)	0.0355 (19)	-0.0087 (17)	0.0010 (16)	-0.0032 (16)
N3	0.041 (2)	0.040 (2)	0.0321 (18)	-0.0088 (17)	0.0007 (16)	-0.0049 (15)
N4	0.0283 (17)	0.0246 (16)	0.0271 (16)	-0.0013 (13)	-0.0005 (14)	-0.0011 (13)
N5	0.042 (2)	0.0365 (19)	0.0283 (17)	-0.0086 (16)	-0.0004 (16)	-0.0082 (14)
N6	0.042 (2)	0.048 (2)	0.0347 (18)	-0.0137 (17)	0.0009 (16)	0.0035 (16)
C1	0.043 (3)	0.037 (2)	0.033 (2)	0.0008 (19)	0.0031 (19)	0.0026 (18)
C2	0.063 (3)	0.049 (3)	0.035 (2)	0.005 (3)	0.004 (2)	0.004 (2)
C3	0.073 (4)	0.053 (3)	0.040 (3)	0.002 (3)	0.021 (3)	0.008 (2)
C4	0.051 (3)	0.047 (3)	0.054 (3)	-0.007 (2)	0.017 (2)	0.009 (2)
C5	0.036 (2)	0.024 (2)	0.038 (2)	0.0060 (18)	0.0041 (18)	0.0025 (17)
C6	0.030 (2)	0.025 (2)	0.0319 (19)	0.0008 (17)	0.0031 (17)	-0.0020 (16)
C7	0.033 (2)	0.0270 (19)	0.0261 (18)	0.0032 (17)	-0.0026 (17)	-0.0008 (15)
C8	0.037 (2)	0.028 (2)	0.0251 (19)	0.0000 (18)	0.0040 (17)	-0.0004 (15)
C9	0.052 (3)	0.047 (3)	0.032 (2)	-0.002 (2)	-0.007 (2)	-0.0006 (18)
C10	0.085 (4)	0.041 (2)	0.026 (2)	0.003 (3)	0.007 (2)	0.0065 (18)
C11	0.072 (4)	0.045 (3)	0.044 (3)	-0.011 (3)	0.017 (3)	0.004 (2)
C12	0.050 (3)	0.051 (3)	0.054 (3)	-0.018 (2)	0.005 (2)	0.002 (2)

Geometric parameters (\AA , $^\circ$)

Hg1—N2	2.385 (3)	C1—C2	1.383 (6)
Hg1—N1	2.388 (3)	C1—C5	1.384 (6)
Hg1—C11	2.4111 (10)	C1—H1	0.9300
Hg1—C12	2.5998 (11)	C2—C3	1.368 (7)
Hg1—C12 ⁱ	2.7061 (11)	C2—H2	0.9300
C12—Hg1 ⁱ	2.7061 (11)	C3—C4	1.368 (7)
N1—C5	1.339 (5)	C3—H3	0.9300
N1—C4	1.340 (5)	C4—H4	0.9300
N2—C6	1.324 (5)	C5—C6	1.465 (5)
N2—N3	1.378 (5)	C7—C8	1.468 (5)
N3—C7	1.301 (5)	C8—C9	1.380 (5)
N4—C6	1.355 (5)	C9—C10	1.378 (6)
N4—C7	1.368 (4)	C9—H9	0.9300
N4—N5	1.414 (4)	C10—C11	1.376 (8)
N5—H5A	0.8901	C10—H10	0.9300
N5—H5B	0.8900	C11—C12	1.365 (6)

N6—C8	1.329 (5)	C11—H11	0.9300
N6—C12	1.333 (5)	C12—H12	0.9300
N2—Hg1—N1	69.78 (12)	C2—C3—C4	119.3 (4)
N2—Hg1—C11	106.24 (9)	C2—C3—H3	120.4
N1—Hg1—C11	136.70 (9)	C4—C3—H3	120.4
N2—Hg1—Cl2	91.45 (9)	N1—C4—C3	122.9 (5)
N1—Hg1—Cl2	112.43 (8)	N1—C4—H4	118.6
Cl1—Hg1—Cl2	110.74 (4)	C3—C4—H4	118.6
N2—Hg1—Cl2 ⁱ	156.52 (9)	N1—C5—C1	122.3 (4)
N1—Hg1—Cl2 ⁱ	89.27 (8)	N1—C5—C6	113.9 (4)
Cl1—Hg1—Cl2 ⁱ	96.23 (4)	C1—C5—C6	123.7 (4)
Cl2—Hg1—Cl2 ⁱ	86.78 (3)	N2—C6—N4	108.6 (3)
Hg1—Cl2—Hg1 ⁱ	93.22 (3)	N2—C6—C5	121.7 (4)
C5—N1—C4	117.9 (4)	N4—C6—C5	129.6 (4)
C5—N1—Hg1	118.1 (3)	N3—C7—N4	110.3 (3)
C4—N1—Hg1	122.7 (3)	N3—C7—C8	124.9 (3)
C6—N2—N3	108.4 (3)	N4—C7—C8	124.8 (3)
C6—N2—Hg1	114.3 (3)	N6—C8—C9	123.5 (4)
N3—N2—Hg1	135.5 (3)	N6—C8—C7	116.2 (3)
C7—N3—N2	106.9 (3)	C9—C8—C7	120.2 (4)
C6—N4—C7	105.9 (3)	C10—C9—C8	118.4 (4)
C6—N4—N5	123.9 (3)	C10—C9—H9	120.8
C7—N4—N5	129.4 (3)	C8—C9—H9	120.8
N4—N5—H5A	103.4	C11—C10—C9	118.7 (4)
N4—N5—H5B	107.9	C11—C10—H10	120.6
H5A—N5—H5B	112.5	C9—C10—H10	120.6
C8—N6—C12	116.7 (4)	C12—C11—C10	118.6 (4)
C2—C1—C5	118.7 (4)	C12—C11—H11	120.7
C2—C1—H1	120.6	C10—C11—H11	120.7
C5—C1—H1	120.6	N6—C12—C11	124.1 (5)
C3—C2—C1	118.9 (4)	N6—C12—H12	118.0
C3—C2—H2	120.6	C11—C12—H12	118.0
C1—C2—H2	120.6		
N2—Hg1—Cl2—Hg1 ⁱ	-156.57 (9)	C2—C1—C5—C6	-177.3 (4)
N1—Hg1—Cl2—Hg1 ⁱ	-87.88 (9)	N3—N2—C6—N4	-0.5 (4)
Cl1—Hg1—Cl2—Hg1 ⁱ	95.44 (4)	Hg1—N2—C6—N4	-167.7 (2)
Cl2 ⁱ —Hg1—Cl2—Hg1 ⁱ	0.0	N3—N2—C6—C5	-177.9 (4)
N2—Hg1—N1—C5	-3.4 (3)	Hg1—N2—C6—C5	14.9 (5)
Cl1—Hg1—N1—C5	89.1 (3)	C7—N4—C6—N2	0.9 (4)
Cl2—Hg1—N1—C5	-86.3 (3)	N5—N4—C6—N2	171.6 (3)
Cl2 ⁱ —Hg1—N1—C5	-172.6 (3)	C7—N4—C6—C5	178.0 (4)
N2—Hg1—N1—C4	-169.9 (4)	N5—N4—C6—C5	-11.2 (6)
Cl1—Hg1—N1—C4	-77.4 (4)	N1—C5—C6—N2	-17.9 (5)
Cl2—Hg1—N1—C4	107.1 (3)	C1—C5—C6—N2	159.1 (4)
Cl2 ⁱ —Hg1—N1—C4	20.9 (3)	N1—C5—C6—N4	165.3 (4)
N1—Hg1—N2—C6	-5.9 (3)	C1—C5—C6—N4	-17.8 (7)

supplementary materials

Cl1—Hg1—N2—C6	-140.4 (3)	N2—N3—C7—N4	0.6 (4)
Cl2—Hg1—N2—C6	107.5 (3)	N2—N3—C7—C8	176.7 (3)
Cl2 ⁱ —Hg1—N2—C6	22.2 (4)	C6—N4—C7—N3	-0.9 (4)
N1—Hg1—N2—N3	-168.5 (4)	N5—N4—C7—N3	-171.0 (4)
Cl1—Hg1—N2—N3	57.0 (4)	C6—N4—C7—C8	-177.0 (3)
Cl2—Hg1—N2—N3	-55.1 (4)	N5—N4—C7—C8	12.9 (6)
Cl2 ⁱ —Hg1—N2—N3	-140.3 (3)	C12—N6—C8—C9	1.8 (6)
C6—N2—N3—C7	-0.1 (4)	C12—N6—C8—C7	178.2 (4)
Hg1—N2—N3—C7	163.2 (3)	N3—C7—C8—N6	-148.0 (4)
C5—C1—C2—C3	-1.0 (6)	N4—C7—C8—N6	27.6 (5)
C1—C2—C3—C4	1.6 (7)	N3—C7—C8—C9	28.6 (6)
C5—N1—C4—C3	-0.9 (7)	N4—C7—C8—C9	-155.9 (4)
Hg1—N1—C4—C3	165.7 (4)	N6—C8—C9—C10	-1.8 (6)
C2—C3—C4—N1	-0.6 (7)	C7—C8—C9—C10	-178.1 (4)
C4—N1—C5—C1	1.5 (6)	C8—C9—C10—C11	0.7 (7)
Hg1—N1—C5—C1	-165.7 (3)	C9—C10—C11—C12	0.2 (7)
C4—N1—C5—C6	178.5 (4)	C8—N6—C12—C11	-0.8 (7)
Hg1—N1—C5—C6	11.3 (4)	C10—C11—C12—N6	-0.2 (7)
C2—C1—C5—N1	-0.5 (6)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—H5A \cdots Cl2 ⁱⁱ	0.89	2.80	3.446 (3)	131
N5—H5A \cdots Cl1 ⁱⁱⁱ	0.89	2.77	3.512 (4)	142
N5—H5B \cdots Cl1 ^{iv}	0.89	2.62	3.452 (4)	155
N5—H5B \cdots N6	0.89	2.47	2.956 (5)	115

Symmetry codes: (ii) $x+1/2, -y+3/2, -z+2$; (iii) $-x+3/2, y+1/2, z$; (iv) $-x+2, -y+1, -z+2$.

Fig. 1

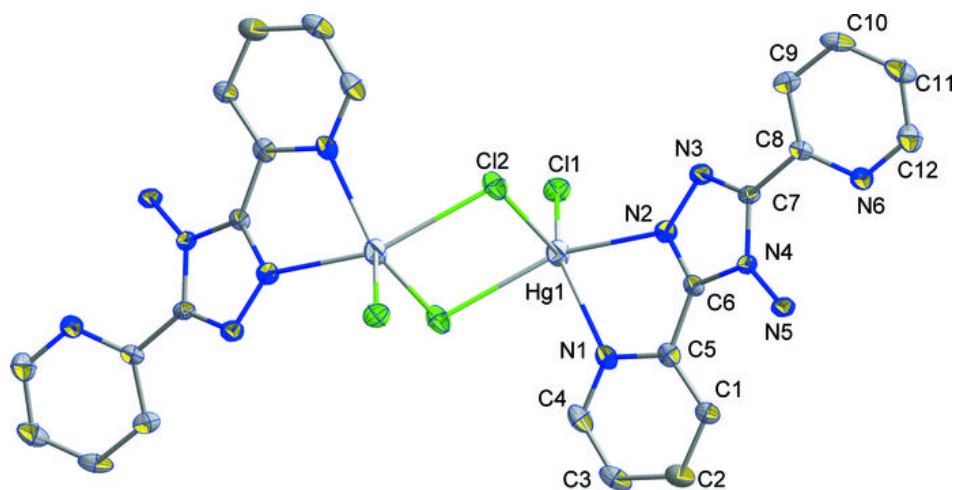


Fig. 2

