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

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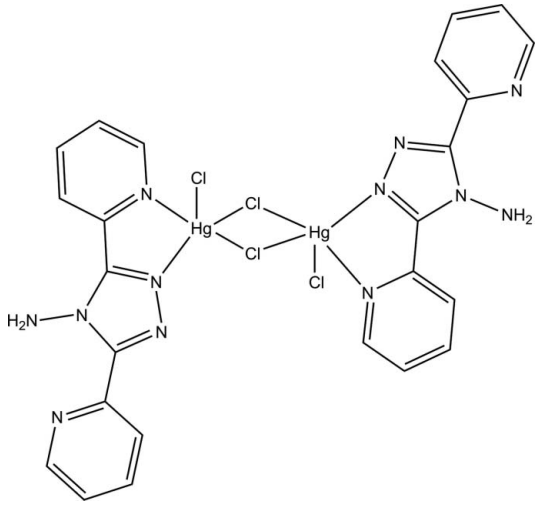
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 13.7.

In the centrosymmetric binuclear title complex, $[Hg_2Cl_4(C_{12}H_{10}N_6)_2]$, 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···N hydrogen bond. In the crystal, the binuclear units are connected by intermolecular N—H···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

$[Hg_2Cl_4(C_{12}H_{10}N_6)_2]$
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) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 10.85 mm^{-1}
T = 296 K
0.28 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.475, T_{max} = 1.000
14063 measured reflections
2596 independent reflections
2071 reflections with $I > 2\sigma(I)$
R_{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
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···Cl2^{i}	0.89	2.80	3.446 (3)	131
N5—H5A···Cl1^{ii}	0.89	2.77	3.512 (4)	142
N5—H5B···Cl1^{iii}	0.89	2.62	3.452 (4)	155
N5—H5B···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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supporting information

Acta Cryst. (2011). E**67**, m1180 [doi:10.1107/S1600536811029886]

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

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S1. 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 $HgCl_2$ 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 Hg_2Cl_2 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).

S2. Experimental

A mixture of 2-bpt (23.8 mg, 0.1 mmol), $HgCl_2$ (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 $C_{24}H_{20}Cl_4Hg_2N_{12}$: C, 28.27; H, 1.98; N, 16.49%. Found: C, 28.30; H, 1.94; N, 16.47%.

S3. 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_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(N).

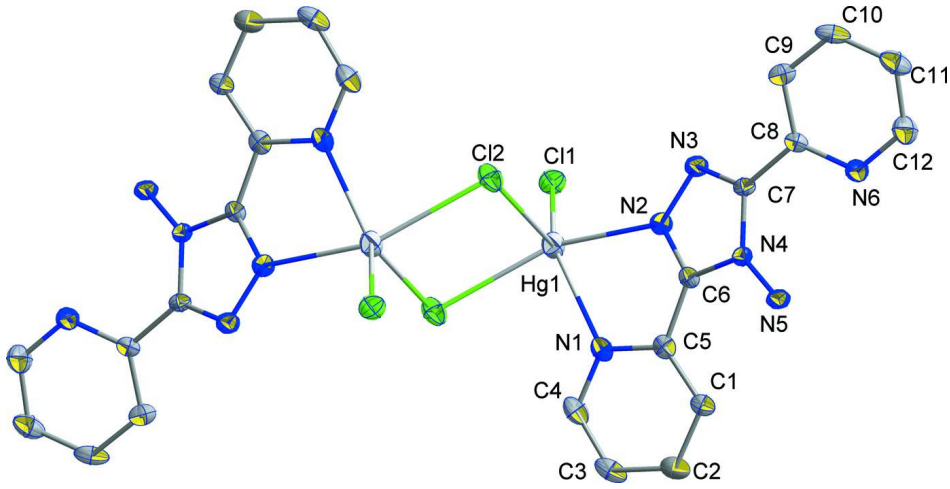

Figure 1

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

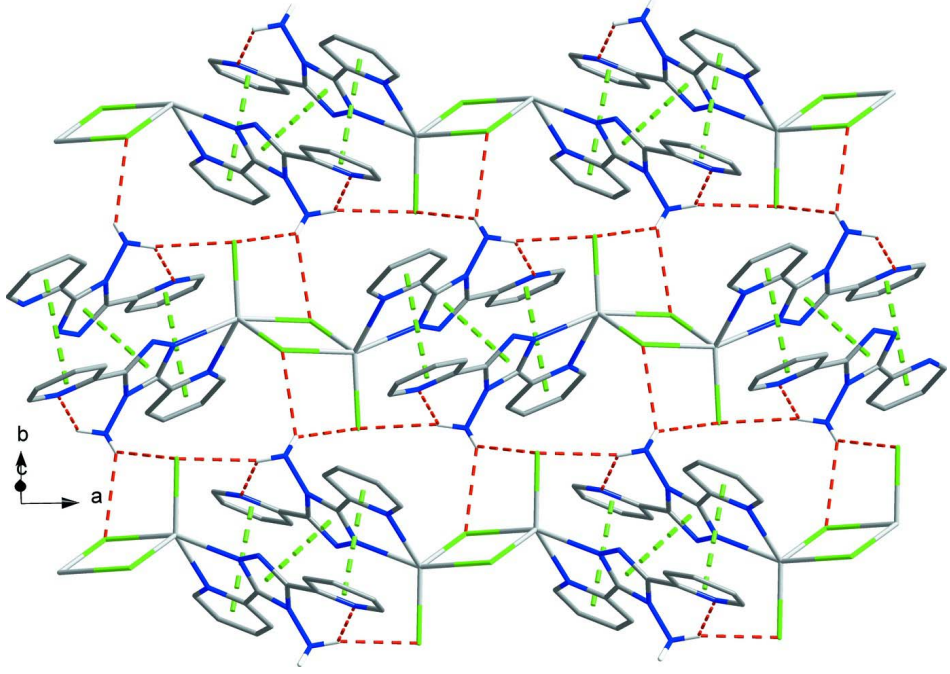

Figure 2

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

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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) Å^3
Z = 4
F(000) = 1904
D_x = 2.306 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 5032 reflections
θ = 2.5–28.1°
μ = 10.85 mm^{-1}
T = 296 K
Block, colourless
0.28 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.475, T_{max} = 1.000

14063 measured reflections
2596 independent reflections
2071 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −8→13
k = −16→17
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.058
S = 1.08
2596 reflections
190 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 2.8778P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{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*
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 (Å²)

	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)
Cl1	0.0512 (7)	0.0409 (6)	0.0458 (6)	−0.0077 (5)	0.0005 (5)	−0.0119 (5)
Cl2	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 (Å, º)

Hg1—N2	2.385 (3)	C1—C2	1.383 (6)
Hg1—N1	2.388 (3)	C1—C5	1.384 (6)
Hg1—Cl1	2.4111 (10)	C1—H1	0.9300
Hg1—Cl2	2.5998 (11)	C2—C3	1.368 (7)
Hg1—Cl2^{i}	2.7061 (11)	C2—H2	0.9300
Cl2—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—Cl1	106.24 (9)	C2—C3—H3	120.4
N1—Hg1—Cl1	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)
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 code: (i) −*x*+1, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5*A*···Cl2^{ii}	0.89	2.80	3.446 (3)	131
N5—H5*A*···Cl1^{iii}	0.89	2.77	3.512 (4)	142
N5—H5*B*···Cl1^{iv}	0.89	2.62	3.452 (4)	155
N5—H5*B*···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.