

Bis(2-amino-3-methylpyridine- κN^1)-dichloridomercury(II)

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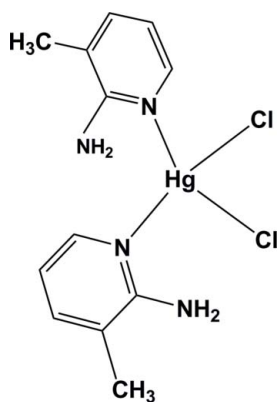
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.013$ Å; R factor = 0.047; wR factor = 0.116; data-to-parameter ratio = 15.5.

In the title compound, $[HgCl_2(C_6H_8N_2)_2]$, the two independent Hg^{II} cations are each located on a twofold rotation axis and coordinated by two pyridine N atoms from two 2-amino-3-methylpyridine ligands and two Cl^- anions in a distorted tetrahedral geometry. An intramolecular $N-H\cdots Cl$ hydrogen bond occurs in each independent complex molecule. Intermolecular $N-H\cdots Cl$ hydrogen bonds occur in the crystal structure.

Related literature

For coordination modes of 2-amino-3-methylpyridine (ampy), see: Arab Ahmadi *et al.* (2011); Tadjarodi *et al.* (2010); Amani Komaei *et al.* (1999); Ziegler *et al.* (2000); Castillo *et al.* (2001); Chen *et al.* (2005). For proton-transfer compounds incorporating ampy, see: Carnevale *et al.* (2010).



Experimental

Crystal data

 $[HgCl_2(C_6H_8N_2)_2]$
 $M_r = 487.78$

 Monoclinic, $P2_1/c$
 $a = 16.495$ (3) Å

 $b = 6.6320$ (13) Å
 $c = 16.273$ (3) Å
 $\beta = 119.56$ (3)°
 $V = 1548.5$ (7) Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 10.28$ mm⁻¹
 $T = 298$ K
 $0.30 \times 0.30 \times 0.27$ mm

Data collection

 Stoe IPDS 2T diffractometer
 Absorption correction: numerical
 [shape of crystal determined
 optically (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)]
 $T_{min} = 0.149$, $T_{max} = 0.168$

 5454 measured reflections
 2912 independent reflections
 2493 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.052$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.116$
 $S = 1.03$
 2912 reflections
 188 parameters
 4 restraints

 H atoms treated by a mixture of
 independent and constrained
 refinement
 $\Delta\rho_{max} = 2.40$ e Å⁻³
 $\Delta\rho_{min} = -2.67$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2A\cdots Cl1$	0.86 (2)	2.58 (4)	3.420 (9)	164 (10)
$N2-H2B\cdots Cl2^i$	0.87 (2)	2.72 (7)	3.420 (8)	139 (8)
$N4-H4A\cdots Cl1^{ii}$	0.86 (2)	2.70 (7)	3.409 (8)	140 (9)
$N4-H4B\cdots Cl2$	0.87 (2)	2.59 (4)	3.424 (9)	162 (9)

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5594).

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supporting information

Acta Cryst. (2012). E68, m1099 [https://doi.org/10.1107/S1600536812032126]

Bis(2-amino-3-methylpyridine- κN^1)dichloridomercury(II)**Azadeh Tadjarodi, Keyvan Bijanzad and Behrouz Notash****S1. Comment**

2-Amino-3-methylpyridine (ampy) is capable of coordinating to metals not only through the nitrogen atom of the pyridyl group (Arab Ahmadi *et al.*, 2011; Tadjarodi *et al.*, 2010; Amani Komaei *et al.*, 1999; Ziegler *et al.*, 2000; Castillo *et al.*, 2001) but also *via* the nitrogen atom of the amino group (Chen *et al.*, 2005). So far, different structures of proton-transfer compounds, [(ampyH)₂CoX₄] (*X* = Cl, Br) have been reported (Carnevale *et al.* (2010).

We report herein the synthesis and molecular structure of the title compound, [Hg(ampy)₂Cl₂]. The asymmetric unit of the title compound consists of two half of one mercury, one ampy and one chloride atom. The coordination sphere of the mononuclear complex consists of two chloride ions and two pyridyl nitrogen atoms from two ampy ligands in a distorted tetrahedral geometry (Fig. 1). In the crystal structure of [Hg(ampy)₂Cl₂], there are several intermolecular N–H···Cl hydrogen bond interactions which stabilized crystal structure (Fig. 2 & Table 1).

S2. Experimental

An ethanolic solution of 2-amino-3-methylpyridine (10 mmol) was added to a solution of HgCl₂ (5 mmol) in ethanol (10 ml) and stirred for 10 min at 50°C. Slow evaporation of the resulting filtrate gave the colorless crystals suitable for X-ray analysis (decomposition > 240 °C).

S3. Refinement

Hydrogen atoms attached to nitrogen atoms were found in difference Fourier map. H2A, H2B, H4A and H4B were refined with $U_{iso}(H) = 1.5 U_{eq}(N)$. H2A, H2B, H4A and H4B were refined with distance restraints of N—H 0.86 (2), 0.87 (2), 0.86 (2) and 0.87 (2), respectively. H atoms attached to C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å (CH), with C—H = 0.96 Å (CH₃), and $U_{iso}(H) = 1.2, 1.5 U_{eq}(C)$.

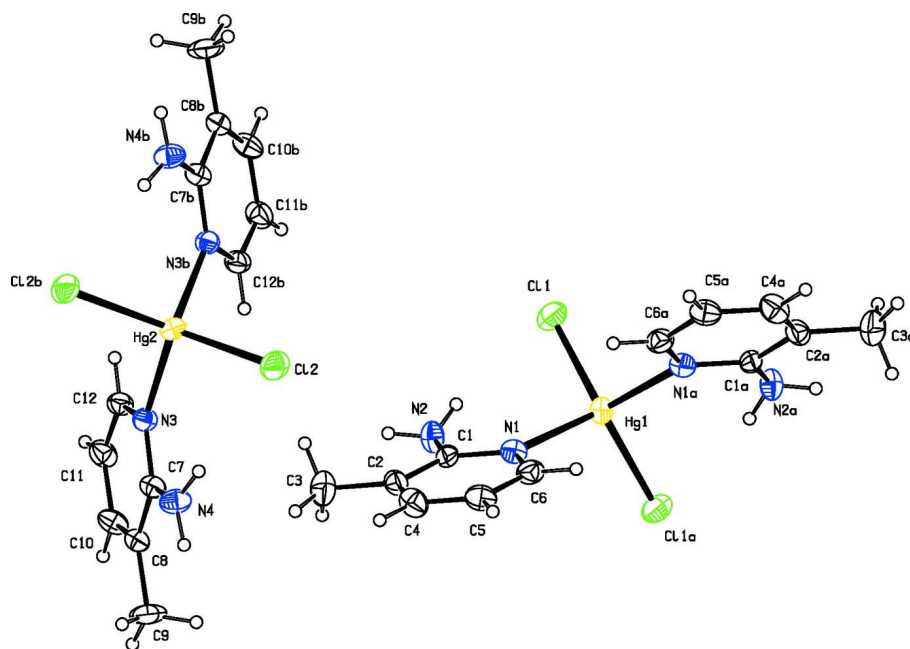


Figure 1

The molecular structure of $[\text{Hg}(\text{ampy})_2\text{Cl}_2]$ with displacement ellipsoids drawn at 30% probability level.

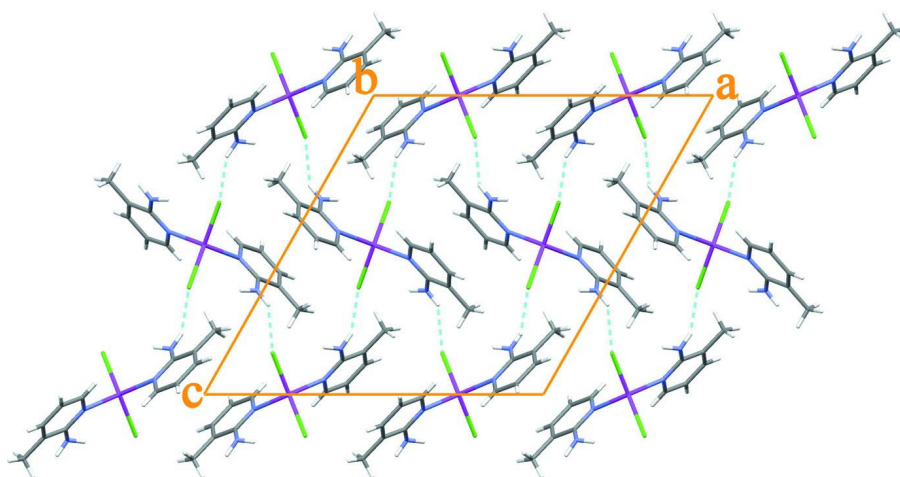


Figure 2

The packing diagram of the title compound showing hydrogen bonding as blue dashed lines.

Bis(2-amino-3-methylpyridine- κN^1)dichloridomercury(II)

Crystal data

$[\text{HgCl}_2(\text{C}_6\text{H}_8\text{N}_2)_2]$

$M_r = 487.78$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 16.495\ (3)\ \text{\AA}$

$b = 6.6320\ (13)\ \text{\AA}$

$c = 16.273\ (3)\ \text{\AA}$

$\beta = 119.56\ (3)^\circ$

$V = 1548.5\ (7)\ \text{\AA}^3$

$Z = 4$

$F(000) = 920$

$D_x = 2.092\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2912 reflections

$\theta = 2.5\text{--}26.0^\circ$

$\mu = 10.28\ \text{mm}^{-1}$

$T = 298$ K $0.30 \times 0.30 \times 0.27$ mm
 Block, colorless

Data collection

Stoe IPDS 2T diffractometer	5454 measured reflections
Radiation source: fine-focus sealed tube	2912 independent reflections
Graphite monochromator	2493 reflections with $I > 2\sigma(I)$
rotation method scans	$R_{\text{int}} = 0.052$
Absorption correction: numerical	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.5^\circ$
[shape of crystal determined optically (<i>X-SHAPE</i> and <i>X-RED32</i> ; Stoe & Cie, 2005)]	$h = -16 \rightarrow 20$
$T_{\text{min}} = 0.149$, $T_{\text{max}} = 0.168$	$k = -7 \rightarrow 8$
	$l = -19 \rightarrow 20$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0773P)^2]$
$wR(F^2) = 0.116$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2912 reflections	$\Delta\rho_{\text{max}} = 2.40 \text{ e } \text{\AA}^{-3}$
188 parameters	$\Delta\rho_{\text{min}} = -2.67 \text{ e } \text{\AA}^{-3}$
4 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0064 (5)
Secondary atom site location: difference Fourier map	

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.0000	0.19701 (7)	0.2500	0.04474 (19)
Hg2	0.5000	0.76184 (6)	0.2500	0.04007 (19)
Cl1	0.13755 (15)	0.0118 (3)	0.36667 (16)	0.0565 (6)
Cl2	0.35836 (16)	0.9352 (4)	0.22391 (16)	0.0590 (6)
N1	0.0500 (5)	0.4038 (9)	0.1715 (4)	0.0407 (15)
N2	0.1527 (6)	0.1618 (12)	0.1736 (6)	0.0497 (17)
N3	0.4556 (4)	0.5485 (9)	0.1232 (4)	0.0359 (14)
N4	0.3477 (6)	0.7778 (10)	0.0184 (5)	0.0472 (19)
C1	0.1163 (5)	0.3496 (11)	0.1495 (5)	0.0362 (16)
C2	0.1430 (6)	0.4814 (13)	0.1001 (5)	0.0441 (19)
C3	0.2151 (7)	0.4171 (18)	0.0751 (8)	0.069 (3)
H3A	0.2217	0.5192	0.0370	0.104*

H3B	0.1962	0.2928	0.0404	0.104*
H3C	0.2737	0.3980	0.1318	0.104*
C4	0.1028 (7)	0.6659 (13)	0.0756 (6)	0.051 (2)
H4	0.1206	0.7549	0.0432	0.061*
C5	0.0361 (7)	0.7229 (12)	0.0981 (6)	0.049 (2)
H5	0.0088	0.8499	0.0813	0.059*
C6	0.0103 (6)	0.5893 (13)	0.1459 (5)	0.0454 (19)
H6	-0.0352	0.6267	0.1609	0.055*
C7	0.3884 (6)	0.5942 (11)	0.0346 (5)	0.0373 (16)
C8	0.3618 (6)	0.4525 (12)	-0.0402 (5)	0.0403 (17)
C9	0.2853 (7)	0.5040 (17)	-0.1374 (6)	0.066 (3)
H9A	0.2783	0.3968	-0.1801	0.100*
H9B	0.3005	0.6267	-0.1581	0.100*
H9C	0.2280	0.5215	-0.1364	0.100*
C10	0.4071 (8)	0.2741 (12)	-0.0193 (6)	0.050 (2)
H10	0.3904	0.1785	-0.0668	0.060*
C11	0.4775 (7)	0.2304 (13)	0.0704 (6)	0.049 (2)
H11	0.5096	0.1087	0.0833	0.058*
C12	0.4993 (6)	0.3695 (12)	0.1401 (5)	0.0405 (17)
H12	0.5458	0.3394	0.2012	0.049*
H2A	0.158 (7)	0.107 (14)	0.224 (4)	0.061*
H4A	0.301 (5)	0.788 (14)	-0.038 (4)	0.061*
H2B	0.202 (4)	0.161 (15)	0.168 (7)	0.061*
H4B	0.348 (7)	0.845 (14)	0.064 (5)	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0379 (3)	0.0561 (3)	0.0446 (3)	0.000	0.0238 (2)	0.000
Hg2	0.0326 (3)	0.0476 (3)	0.0330 (3)	0.000	0.0108 (2)	0.000
Cl1	0.0393 (11)	0.0617 (13)	0.0566 (12)	-0.0032 (9)	0.0147 (10)	0.0151 (9)
Cl2	0.0442 (11)	0.0714 (14)	0.0564 (12)	0.0166 (10)	0.0210 (10)	-0.0068 (10)
N1	0.043 (4)	0.041 (4)	0.036 (3)	0.001 (3)	0.018 (3)	0.001 (2)
N2	0.048 (4)	0.051 (4)	0.063 (5)	0.006 (3)	0.037 (4)	0.001 (3)
N3	0.036 (3)	0.036 (3)	0.034 (3)	0.007 (3)	0.016 (3)	0.001 (2)
N4	0.049 (5)	0.039 (4)	0.040 (4)	0.008 (3)	0.012 (3)	0.003 (3)
C1	0.029 (4)	0.046 (4)	0.033 (3)	-0.007 (3)	0.014 (3)	-0.009 (3)
C2	0.045 (5)	0.054 (5)	0.039 (4)	-0.015 (4)	0.025 (4)	-0.009 (3)
C3	0.055 (6)	0.085 (8)	0.081 (7)	-0.007 (5)	0.044 (6)	0.003 (5)
C4	0.065 (6)	0.043 (4)	0.052 (5)	-0.015 (4)	0.034 (4)	-0.003 (4)
C5	0.058 (6)	0.042 (5)	0.042 (4)	0.002 (4)	0.020 (4)	0.002 (3)
C6	0.040 (4)	0.049 (5)	0.039 (4)	0.009 (4)	0.014 (4)	0.001 (3)
C7	0.045 (4)	0.037 (4)	0.030 (3)	-0.006 (3)	0.018 (3)	-0.001 (3)
C8	0.042 (4)	0.049 (4)	0.031 (4)	0.002 (3)	0.019 (3)	0.002 (3)
C9	0.054 (6)	0.087 (7)	0.029 (4)	0.010 (5)	-0.002 (4)	-0.007 (4)
C10	0.066 (6)	0.050 (5)	0.036 (4)	-0.001 (4)	0.027 (4)	-0.009 (3)
C11	0.058 (6)	0.049 (5)	0.045 (5)	0.012 (4)	0.030 (5)	0.004 (3)
C12	0.042 (4)	0.044 (4)	0.032 (3)	0.005 (3)	0.016 (3)	0.004 (3)

Geometric parameters (Å, °)

Hg1—N1	2.287 (7)	C2—C3	1.497 (14)
Hg1—N1 ⁱ	2.287 (7)	C3—H3A	0.9600
Hg1—C11 ⁱ	2.452 (2)	C3—H3B	0.9600
Hg1—C11	2.452 (2)	C3—H3C	0.9600
Hg2—N3	2.303 (6)	C4—C5	1.373 (15)
Hg2—N3 ⁱⁱ	2.303 (6)	C4—H4	0.9300
Hg2—C12 ⁱⁱ	2.446 (2)	C5—C6	1.378 (13)
Hg2—C12	2.446 (2)	C5—H5	0.9300
N1—C1	1.356 (11)	C6—H6	0.9300
N1—C6	1.360 (10)	C7—C8	1.425 (10)
N2—C1	1.354 (11)	C8—C10	1.351 (12)
N2—H2A	0.86 (2)	C8—C9	1.498 (11)
N2—H2B	0.87 (2)	C9—H9A	0.9600
N3—C12	1.345 (10)	C9—H9B	0.9600
N3—C7	1.350 (9)	C9—H9C	0.9600
N4—C7	1.352 (10)	C10—C11	1.375 (13)
N4—H4A	0.86 (2)	C10—H10	0.9300
N4—H4B	0.87 (2)	C11—C12	1.365 (12)
C1—C2	1.397 (11)	C11—H11	0.9300
C2—C4	1.355 (13)	C12—H12	0.9300
N1—Hg1—N1 ⁱ	106.3 (3)	C2—C3—H3C	109.5
N1—Hg1—C11 ⁱ	108.60 (16)	H3A—C3—H3C	109.5
N1 ⁱ —Hg1—C11 ⁱ	106.35 (17)	H3B—C3—H3C	109.5
N1—Hg1—C11	106.35 (17)	C2—C4—C5	120.7 (8)
N1 ⁱ —Hg1—C11	108.60 (16)	C2—C4—H4	119.6
C11 ⁱ —Hg1—C11	119.88 (11)	C5—C4—H4	119.6
N3—Hg2—N3 ⁱⁱ	104.2 (3)	C4—C5—C6	119.0 (8)
N3—Hg2—C12 ⁱⁱ	107.38 (18)	C4—C5—H5	120.5
N3 ⁱⁱ —Hg2—C12 ⁱⁱ	106.20 (16)	C6—C5—H5	120.5
N3—Hg2—C12	106.20 (16)	N1—C6—C5	121.3 (9)
N3 ⁱⁱ —Hg2—C12	107.38 (18)	N1—C6—H6	119.4
C12 ⁱⁱ —Hg2—C12	123.91 (13)	C5—C6—H6	119.4
C1—N1—C6	119.2 (7)	N3—C7—N4	118.5 (6)
C1—N1—Hg1	123.3 (5)	N3—C7—C8	120.6 (7)
C6—N1—Hg1	117.5 (6)	N4—C7—C8	120.9 (7)
C1—N2—H2A	119 (7)	C10—C8—C7	117.7 (7)
C1—N2—H2B	106 (7)	C10—C8—C9	122.6 (8)
H2A—N2—H2B	116 (10)	C7—C8—C9	119.7 (7)
C12—N3—C7	119.4 (6)	C8—C9—H9A	109.5
C12—N3—Hg2	117.3 (5)	C8—C9—H9B	109.5
C7—N3—Hg2	123.3 (5)	H9A—C9—H9B	109.5
C7—N4—H4A	112 (7)	C8—C9—H9C	109.5
C7—N4—H4B	120 (7)	H9A—C9—H9C	109.5
H4A—N4—H4B	120 (10)	H9B—C9—H9C	109.5
N2—C1—N1	117.8 (7)	C8—C10—C11	121.6 (8)

N2—C1—C2	121.4 (7)	C8—C10—H10	119.2
N1—C1—C2	120.7 (7)	C11—C10—H10	119.2
C4—C2—C1	119.1 (8)	C12—C11—C10	118.6 (8)
C4—C2—C3	121.1 (8)	C12—C11—H11	120.7
C1—C2—C3	119.8 (8)	C10—C11—H11	120.7
C2—C3—H3A	109.5	N3—C12—C11	122.1 (7)
C2—C3—H3B	109.5	N3—C12—H12	118.9
H3A—C3—H3B	109.5	C11—C12—H12	118.9
N1 ⁱ —Hg1—N1—C1	152.6 (6)	C1—C2—C4—C5	-0.5 (12)
C11 ⁱ —Hg1—N1—C1	-93.3 (5)	C3—C2—C4—C5	179.4 (8)
C11—Hg1—N1—C1	37.0 (6)	C2—C4—C5—C6	-0.2 (13)
N1 ⁱ —Hg1—N1—C6	-27.8 (5)	C1—N1—C6—C5	-0.1 (11)
C11 ⁱ —Hg1—N1—C6	86.3 (5)	Hg1—N1—C6—C5	-179.8 (6)
C11—Hg1—N1—C6	-143.4 (5)	C4—C5—C6—N1	0.5 (13)
N3 ⁱⁱ —Hg2—N3—C12	-31.0 (5)	C12—N3—C7—N4	-177.6 (8)
C12 ⁱⁱ —Hg2—N3—C12	81.4 (6)	Hg2—N3—C7—N4	2.9 (10)
C12—Hg2—N3—C12	-144.2 (6)	C12—N3—C7—C8	1.8 (12)
N3 ⁱⁱ —Hg2—N3—C7	148.5 (7)	Hg2—N3—C7—C8	-177.7 (6)
C12 ⁱⁱ —Hg2—N3—C7	-99.1 (6)	N3—C7—C8—C10	-1.2 (13)
C12—Hg2—N3—C7	35.3 (6)	N4—C7—C8—C10	178.3 (9)
C6—N1—C1—N2	-178.2 (7)	N3—C7—C8—C9	178.3 (8)
Hg1—N1—C1—N2	1.4 (9)	N4—C7—C8—C9	-2.3 (13)
C6—N1—C1—C2	-0.6 (10)	C7—C8—C10—C11	-0.9 (15)
Hg1—N1—C1—C2	179.0 (5)	C9—C8—C10—C11	179.7 (10)
N2—C1—C2—C4	178.4 (8)	C8—C10—C11—C12	2.1 (16)
N1—C1—C2—C4	0.9 (11)	C7—N3—C12—C11	-0.5 (13)
N2—C1—C2—C3	-1.5 (11)	Hg2—N3—C12—C11	179.0 (7)
N1—C1—C2—C3	-179.0 (7)	C10—C11—C12—N3	-1.5 (15)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A \cdots C11	0.86 (2)	2.58 (4)	3.420 (9)	164 (10)
N2—H2B \cdots C12 ⁱⁱⁱ	0.87 (2)	2.72 (7)	3.420 (8)	139 (8)
N4—H4A \cdots C11 ^{iv}	0.86 (2)	2.70 (7)	3.409 (8)	140 (9)
N4—H4B \cdots C12	0.87 (2)	2.59 (4)	3.424 (9)	162 (9)

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