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Dibromido(2,2′-dimethyl-4,4′-bi-1,3-thiazole-κ^2N,N')mercury(II)

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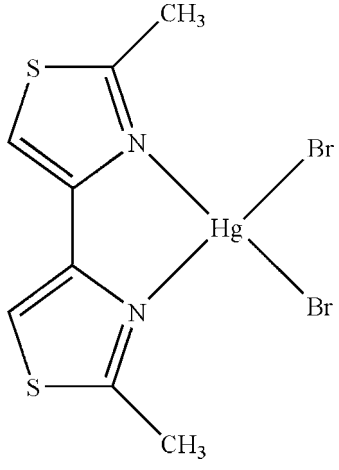
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.007 Å; R factor = 0.026; wR factor = 0.062; data-to-parameter ratio = 25.1.

The asymmetric unit of the title compound, [$HgBr_2$-($C_8H_8N_2S_2$)], contains two crystallographically independent molecules. The Hg^{II} atoms are four-coordinated in a distorted tetrahedral geometry by two N atoms from a 2,2′-dimethyl-4,4′-bi-1,3-thiazole ligand and two Br atoms. In the crystal structure, intermolecular C—H···Br hydrogen bonds and π–π contacts between the thiazole rings [centroid–centroid distances = 3.670 (3) and 3.614 (2) Å] stabilize the structure.

Related literature

For metal complexes with 2,2′-dimethyl-4,4′-bithiazole ligands, see: Abedi & Yahyazade Bali (2010); Al-Hashemi *et al.* (2009, 2010); Khavasi *et al.* (2008); Notash *et al.* (2008, 2009). For related structures, see: Kalateh *et al.* (2008); Safari *et al.* (2009).



Experimental

Crystal data

[$HgBr_2(C_8H_8N_2S_2)$]
M_r = 556.69
Triclinic, $P\overline{1}$
a = 10.2799 (6) Å
b = 11.1595 (7) Å
c = 11.6821 (7) Å
α = 88.4456 (11)°
β = 85.3290 (11)°
γ = 77.1162 (11)°
V = 1302.02 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 18.25 mm^{-1}
T = 100 K
0.14 × 0.12 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.070, T_{max} = 0.240
20881 measured reflections
6912 independent reflections
5865 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.062
S = 0.94
6912 reflections
275 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.28 e Å^{-3}
$\Delta\rho_{min}$ = −1.68 e Å^{-3}

Table 1
Selected bond lengths (Å).

Hg1—N1	2.379 (4)	Hg2—N3	2.357 (4)
Hg1—N2	2.383 (4)	Hg2—N4	2.410 (4)
Hg1—Br1	2.4970 (5)	Hg2—Br3	2.4999 (5)
Hg1—Br2	2.5206 (5)	Hg2—Br4	2.4957 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···Br4^{i}	0.98	2.92	3.826 (5)	155
C10—H10A···Br4^{i}	0.95	2.92	3.760 (5)	148
C16—H16B···Br3^{ii}	0.98	2.87	3.772 (5)	154
C16—H16C···Br2^{iii}	0.98	2.88	3.837 (5)	165

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

Data collection: *APEX2* (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: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2386).

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supporting information

Acta Cryst. (2011). E**67**, m76–m77 [https://doi.org/10.1107/S1600536810051494]

Dibromido(2,2′-dimethyl-4,4′-bi-1,3-thiazole-κ^2N,N')mercury(II)

Anita Abedi

S1. Comment

Recently, we reported the synthesis and crystal structure of [HgI_2(dm4bt)] (dm4bt is 2,2′-dimethyl-4,4′-bithiazole) (Abedi & Yahyazade Bali, 2010). Dm4bt is a good bidentate ligand, and numerous complexes with dm4bt have been prepared, such as that of zinc (Khavasi *et al.*, 2008), thallium (Notash *et al.*, 2008), cadmium (Notash *et al.*, 2009) and copper (Al-Hashemi *et al.*, 2009, 2010). For further investigation of dm4bt, we synthesis the title complex and report herein its crystal structure.

The asymmetric unit of the title compound (Fig. 1) contains two crystallographically independent molecules. The Hg^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from a dm4bt ligand and two Br atoms. The Hg—N and Hg—Br bond lengths (Table 1) and angles are within normal range found in [$Hg(SCN)_2$(dm4bt)] (Safari *et al.*, 2009) and {$HgBr_2$[$NH(py)_2$]} [$NH(py)_2$ is di-2-pyridylamine] (Kalateh *et al.*, 2008).

In the crystal structure, intermolecular C—H···Br hydrogen bonds (Table 2) and π–π contacts (Fig. 2) between the thiazole rings, *Cg*1···*Cg*2^{i} and *Cg*3···*Cg*4^{ii} [symmetry codes: (i) 2-x, 1-y, -z; (ii) 1-x, 2-y, 1-z. *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the rings S1/C1/N1/C3/C2, S2/C4/N2/C6/C5, S3/C9/N3/C11/C10 and S4/C12/N4/C14/C13, respectively] stabilize the structure, with centroid–centroid distances of 3.670 (3) and 3.614 (2) Å.

S2. Experimental

For the preparation of the title compound, a solution of dm4bt (0.26 g, 1.3 mmol) in methanol (15 ml) was added to a solution of $HgBr_2$ (0.47 g, 1.3 mmol) in methanol (15 ml) at room temperature. Crystals suitable for X-ray diffraction experiment were obtained by methanol diffusion into a colorless solution in DMSO after one week (yield: 0.52 g, 71.8%).

S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.95 (CH) and 0.98 (CH_3) Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C). The highest residual electron density was found at 0.85 Å from Hg2 atom and the deepest hole at 0.70 Å from Hg1 atom.

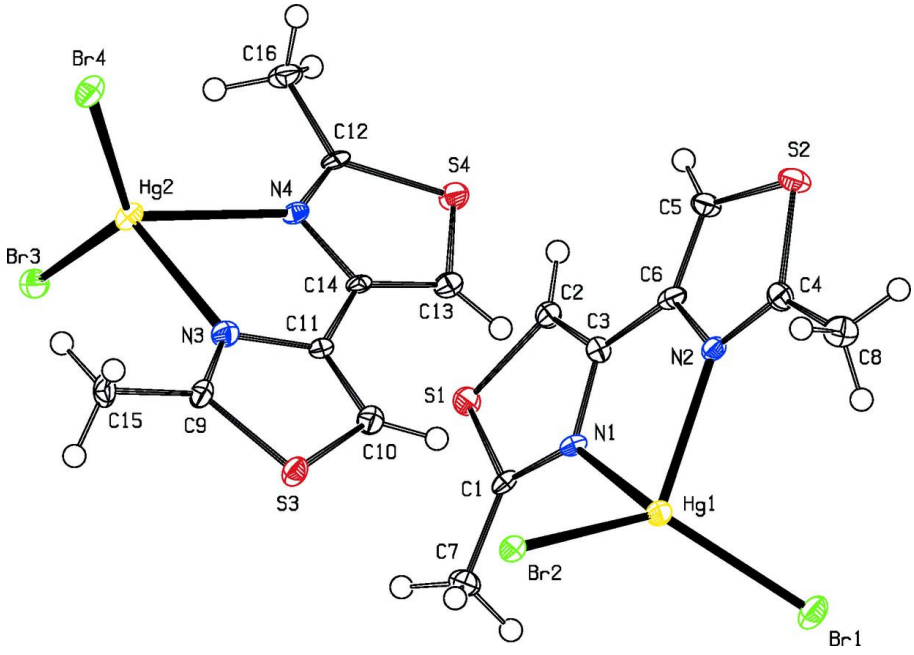

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

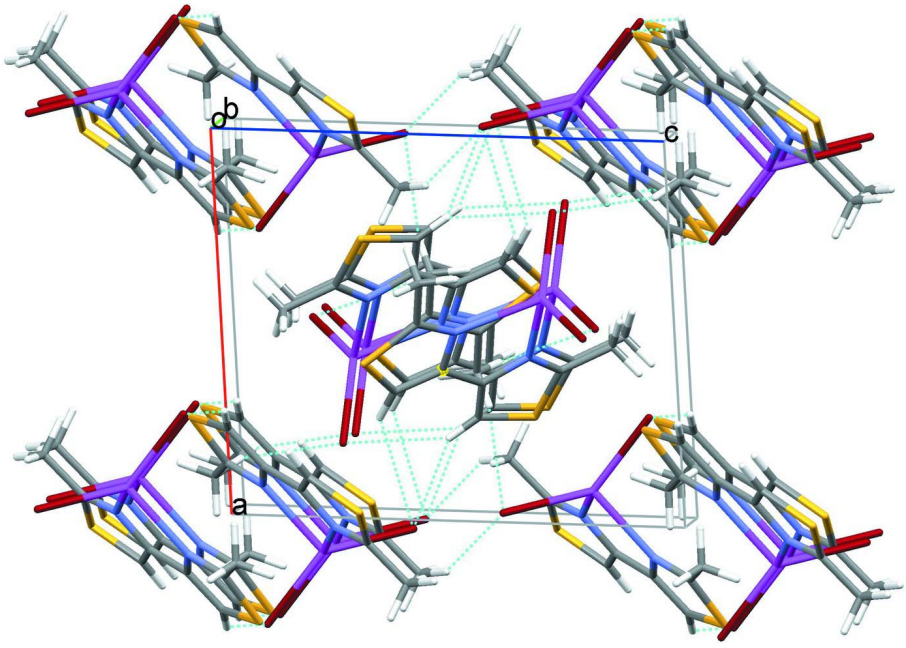

Figure 2

Crystal packing diagram for the title compound. Dashed lines denote hydrogen bonds.

Dibromido(2,2′-dimethyl-4,4′-bi-1,3-thiazole-κ^2N,N')mercury(II)

Crystal data

$[HgBr_2(C_8H_8N_2S_2)]$
$M_r = 556.69$

Triclinic, $P\overline{1}$
Hall symbol: -P 1

a = 10.2799 (6) Å
b = 11.1595 (7) Å
c = 11.6821 (7) Å
α = 88.4456 (11)°
β = 85.3290 (11)°
γ = 77.1162 (11)°
V = 1302.02 (14) Å^3
Z = 4
F(000) = 1008

D_x = 2.840 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2931 reflections
θ = 3.0–29.0°
μ = 18.25 mm^{-1}
T = 100 K
Prism, colorless
0.14 × 0.12 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.070, T_{max} = 0.240

20881 measured reflections
6912 independent reflections
5865 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 29.0°, θ_{min} = 1.8°
h = −14→14
k = −15→15
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.062
S = 0.94
6912 reflections
275 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
$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 2.0838P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.28 e Å^{-3}
$\Delta\rho_{min}$ = −1.68 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Hg1	1.080846 (18)	0.703396 (17)	0.207265 (14)	0.01438 (5)
Br1	1.27509 (5)	0.73077 (5)	0.07429 (4)	0.01974 (10)
Br2	1.01869 (5)	0.79183 (4)	0.40562 (4)	0.01472 (9)
S1	0.96732 (13)	0.30682 (11)	0.30191 (10)	0.0162 (2)
S2	0.74266 (12)	0.71656 (11)	−0.06846 (10)	0.0167 (2)
N1	1.0123 (4)	0.5145 (4)	0.2400 (3)	0.0126 (8)
N2	0.9123 (4)	0.6940 (3)	0.0815 (3)	0.0118 (7)
C1	1.0489 (4)	0.4251 (4)	0.3135 (4)	0.0117 (8)
C2	0.8814 (5)	0.3826 (4)	0.1925 (4)	0.0160 (9)
H2A	0.8189	0.3523	0.1522	0.019*
C3	0.9157 (5)	0.4932 (4)	0.1714 (4)	0.0129 (9)
C4	0.8605 (5)	0.7689 (4)	0.0020 (4)	0.0148 (9)
C5	0.7668 (5)	0.5861 (4)	0.0144 (4)	0.0150 (9)
H5A	0.7206	0.5217	0.0097	0.018*
C6	0.8618 (5)	0.5883 (4)	0.0881 (4)	0.0131 (9)
C7	1.1512 (5)	0.4226 (5)	0.3961 (4)	0.0186 (10)
H7A	1.1390	0.5043	0.4296	0.028*

H7B	1.2407	0.3995	0.3561	0.028*
H7C	1.1418	0.3625	0.4571	0.028*
C8	0.8973 (5)	0.8888 (4)	−0.0288 (4)	0.0189 (10)
H8A	0.9945	0.8786	−0.0294	0.028*
H8B	0.8531	0.9507	0.0280	0.028*
H8C	0.8684	0.9155	−0.1050	0.028*
Hg2	0.411665 (18)	0.785100 (16)	0.717555 (15)	0.01467 (5)
Br3	0.50713 (5)	0.58257 (4)	0.80847 (4)	0.01660 (10)
Br4	0.19137 (5)	0.93379 (4)	0.74712 (4)	0.01734 (10)
S3	0.72536 (12)	1.05628 (11)	0.68030 (10)	0.0150 (2)
S4	0.59092 (12)	0.68616 (11)	0.31954 (10)	0.0161 (2)
N3	0.5664 (4)	0.9109 (4)	0.6782 (3)	0.0142 (8)
N4	0.5044 (4)	0.7580 (3)	0.5213 (3)	0.0110 (7)
C9	0.6015 (5)	0.9912 (4)	0.7442 (4)	0.0136 (9)
C10	0.7285 (5)	0.9747 (4)	0.5581 (4)	0.0154 (9)
H10A	0.7849	0.9794	0.4904	0.018*
C11	0.6378 (4)	0.9014 (4)	0.5721 (4)	0.0114 (8)
C12	0.4840 (4)	0.6864 (4)	0.4407 (4)	0.0138 (9)
C13	0.6630 (5)	0.7909 (4)	0.3806 (4)	0.0137 (9)
H13A	0.7328	0.8249	0.3443	0.016*
C14	0.6059 (4)	0.8182 (4)	0.4879 (4)	0.0100 (8)
C15	0.5358 (5)	1.0239 (5)	0.8604 (4)	0.0176 (10)
H15A	0.4717	0.9721	0.8807	0.026*
H15B	0.4885	1.1105	0.8608	0.026*
H15C	0.6036	1.0107	0.9164	0.026*
C16	0.3766 (5)	0.6164 (5)	0.4523 (4)	0.0181 (10)
H16A	0.3632	0.5912	0.5326	0.027*
H16B	0.4023	0.5434	0.4038	0.027*
H16C	0.2932	0.6685	0.4281	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.01399 (9)	0.01808 (10)	0.01340 (8)	−0.00844 (7)	−0.00148 (6)	0.00061 (6)
Br1	0.0193 (2)	0.0236 (3)	0.0190 (2)	−0.0124 (2)	0.00513 (19)	−0.00411 (18)
Br2	0.0117 (2)	0.0184 (2)	0.0138 (2)	−0.00327 (17)	0.00036 (16)	−0.00020 (17)
S1	0.0190 (6)	0.0165 (6)	0.0161 (5)	−0.0099 (5)	−0.0037 (4)	0.0045 (4)
S2	0.0160 (6)	0.0177 (6)	0.0179 (5)	−0.0051 (5)	−0.0079 (5)	0.0019 (4)
N1	0.0086 (18)	0.015 (2)	0.0150 (18)	−0.0052 (15)	−0.0010 (15)	0.0000 (15)
N2	0.0097 (18)	0.0125 (19)	0.0134 (18)	−0.0036 (15)	0.0000 (14)	0.0017 (14)
C1	0.007 (2)	0.012 (2)	0.015 (2)	−0.0021 (16)	0.0031 (16)	−0.0011 (16)
C2	0.017 (2)	0.020 (2)	0.014 (2)	−0.011 (2)	−0.0026 (18)	0.0032 (18)
C3	0.013 (2)	0.015 (2)	0.011 (2)	−0.0035 (18)	−0.0011 (17)	0.0001 (16)
C4	0.017 (2)	0.018 (2)	0.011 (2)	−0.0052 (19)	−0.0008 (17)	−0.0031 (17)
C5	0.014 (2)	0.016 (2)	0.015 (2)	−0.0045 (18)	−0.0055 (18)	0.0006 (17)
C6	0.009 (2)	0.016 (2)	0.015 (2)	−0.0045 (18)	0.0010 (17)	−0.0052 (17)
C7	0.018 (2)	0.022 (3)	0.019 (2)	−0.008 (2)	−0.0075 (19)	0.0053 (19)
C8	0.020 (3)	0.015 (2)	0.023 (2)	−0.005 (2)	−0.004 (2)	−0.0003 (19)

Hg2	0.01185 (9)	0.01587 (9)	0.01664 (9)	−0.00476 (7)	0.00171 (7)	−0.00051 (6)
Br3	0.0161 (2)	0.0170 (2)	0.0169 (2)	−0.00399 (18)	−0.00171 (17)	0.00080 (17)
Br4	0.0137 (2)	0.0168 (2)	0.0201 (2)	−0.00250 (18)	0.00373 (18)	0.00131 (17)
S3	0.0160 (6)	0.0169 (6)	0.0139 (5)	−0.0084 (5)	0.0024 (4)	−0.0025 (4)
S4	0.0136 (5)	0.0197 (6)	0.0151 (5)	−0.0042 (5)	0.0012 (4)	−0.0057 (4)
N3	0.0134 (19)	0.015 (2)	0.0149 (18)	−0.0048 (16)	−0.0012 (15)	−0.0004 (15)
N4	0.0065 (17)	0.0114 (18)	0.0140 (17)	0.0002 (14)	0.0005 (14)	−0.0018 (14)
C9	0.012 (2)	0.015 (2)	0.013 (2)	−0.0031 (17)	0.0027 (17)	0.0006 (17)
C10	0.015 (2)	0.017 (2)	0.014 (2)	−0.0043 (18)	0.0002 (18)	−0.0004 (17)
C11	0.007 (2)	0.015 (2)	0.012 (2)	−0.0022 (17)	−0.0010 (16)	0.0004 (16)
C12	0.0029 (19)	0.020 (2)	0.017 (2)	0.0006 (17)	0.0003 (16)	−0.0006 (18)
C13	0.011 (2)	0.013 (2)	0.017 (2)	−0.0019 (17)	−0.0004 (17)	−0.0004 (17)
C14	0.0051 (19)	0.009 (2)	0.015 (2)	−0.0003 (16)	−0.0022 (16)	0.0033 (16)
C15	0.022 (3)	0.023 (3)	0.009 (2)	−0.009 (2)	0.0028 (18)	−0.0022 (18)
C16	0.012 (2)	0.023 (3)	0.021 (2)	−0.0072 (19)	−0.0017 (19)	−0.006 (2)

Geometric parameters (Å, º)

Hg1—N1	2.379 (4)	Hg2—N3	2.357 (4)
Hg1—N2	2.383 (4)	Hg2—N4	2.410 (4)
Hg1—Br1	2.4970 (5)	Hg2—Br3	2.4999 (5)
Hg1—Br2	2.5206 (5)	Hg2—Br4	2.4957 (5)
S1—C2	1.709 (5)	S3—C10	1.708 (5)
S1—C1	1.727 (4)	S3—C9	1.713 (5)
S2—C5	1.708 (5)	S4—C13	1.715 (5)
S2—C4	1.729 (5)	S4—C12	1.720 (5)
N1—C1	1.309 (6)	N3—C9	1.324 (6)
N1—C3	1.389 (6)	N3—C11	1.383 (6)
N2—C4	1.298 (6)	N4—C12	1.310 (6)
N2—C6	1.388 (6)	N4—C14	1.387 (5)
C1—C7	1.480 (6)	C9—C15	1.483 (6)
C2—C3	1.368 (6)	C10—C11	1.368 (6)
C2—H2A	0.9500	C10—H10A	0.9500
C3—C6	1.467 (7)	C11—C14	1.475 (6)
C4—C8	1.496 (7)	C12—C16	1.483 (6)
C5—C6	1.358 (6)	C13—C14	1.353 (6)
C5—H5A	0.9500	C13—H13A	0.9500
C7—H7A	0.9800	C15—H15A	0.9800
C7—H7B	0.9800	C15—H15B	0.9800
C7—H7C	0.9800	C15—H15C	0.9800
C8—H8A	0.9800	C16—H16A	0.9800
C8—H8B	0.9800	C16—H16B	0.9800
C8—H8C	0.9800	C16—H16C	0.9800
N1—Hg1—N2	71.23 (13)	N3—Hg2—N4	70.25 (13)
N1—Hg1—Br1	124.79 (9)	N3—Hg2—Br4	104.07 (10)
N2—Hg1—Br1	103.63 (9)	N4—Hg2—Br4	115.64 (9)
N1—Hg1—Br2	98.36 (9)	N3—Hg2—Br3	114.30 (10)

N2—Hg1—Br2	120.67 (9)	N4—Hg2—Br3	102.77 (9)
Br1—Hg1—Br2	126.492 (16)	Br4—Hg2—Br3	132.848 (17)
C2—S1—C1	90.8 (2)	C10—S3—C9	90.6 (2)
C5—S2—C4	90.4 (2)	C13—S4—C12	90.4 (2)
C1—N1—C3	112.7 (4)	C9—N3—C11	111.5 (4)
C1—N1—Hg1	131.2 (3)	C9—N3—Hg2	130.2 (3)
C3—N1—Hg1	116.2 (3)	C11—N3—Hg2	118.3 (3)
C4—N2—C6	111.8 (4)	C12—N4—C14	112.3 (4)
C4—N2—Hg1	131.6 (3)	C12—N4—Hg2	130.9 (3)
C6—N2—Hg1	116.5 (3)	C14—N4—Hg2	116.6 (3)
N1—C1—C7	124.3 (4)	N3—C9—C15	122.7 (4)
N1—C1—S1	112.7 (3)	N3—C9—S3	113.5 (3)
C7—C1—S1	123.0 (4)	C15—C9—S3	123.8 (4)
C3—C2—S1	110.1 (3)	C11—C10—S3	110.1 (3)
C3—C2—H2A	125.0	C11—C10—H10A	125.0
S1—C2—H2A	125.0	S3—C10—H10A	125.0
C2—C3—N1	113.8 (4)	C10—C11—N3	114.4 (4)
C2—C3—C6	127.8 (4)	C10—C11—C14	128.1 (4)
N1—C3—C6	118.4 (4)	N3—C11—C14	117.5 (4)
N2—C4—C8	124.7 (4)	N4—C12—C16	123.1 (4)
N2—C4—S2	113.3 (3)	N4—C12—S4	112.9 (3)
C8—C4—S2	122.0 (4)	C16—C12—S4	124.0 (4)
C6—C5—S2	109.8 (4)	C14—C13—S4	110.1 (3)
C6—C5—H5A	125.1	C14—C13—H13A	124.9
S2—C5—H5A	125.1	S4—C13—H13A	124.9
C5—C6—N2	114.7 (4)	C13—C14—N4	114.2 (4)
C5—C6—C3	127.7 (4)	C13—C14—C11	128.8 (4)
N2—C6—C3	117.7 (4)	N4—C14—C11	117.0 (4)
C1—C7—H7A	109.5	C9—C15—H15A	109.5
C1—C7—H7B	109.5	C9—C15—H15B	109.5
H7A—C7—H7B	109.5	H15A—C15—H15B	109.5
C1—C7—H7C	109.5	C9—C15—H15C	109.5
H7A—C7—H7C	109.5	H15A—C15—H15C	109.5
H7B—C7—H7C	109.5	H15B—C15—H15C	109.5
C4—C8—H8A	109.5	C12—C16—H16A	109.5
C4—C8—H8B	109.5	C12—C16—H16B	109.5
H8A—C8—H8B	109.5	H16A—C16—H16B	109.5
C4—C8—H8C	109.5	C12—C16—H16C	109.5
H8A—C8—H8C	109.5	H16A—C16—H16C	109.5
H8B—C8—H8C	109.5	H16B—C16—H16C	109.5

N2—Hg1—N1—C1	−178.0 (4)	N4—Hg2—N3—C9	177.3 (5)
Br1—Hg1—N1—C1	88.2 (4)	Br4—Hg2—N3—C9	64.7 (4)
Br2—Hg1—N1—C1	−58.3 (4)	Br3—Hg2—N3—C9	−87.2 (4)
N2—Hg1—N1—C3	1.3 (3)	N4—Hg2—N3—C11	−4.7 (3)
Br1—Hg1—N1—C3	−92.5 (3)	Br4—Hg2—N3—C11	−117.3 (3)
Br2—Hg1—N1—C3	121.0 (3)	Br3—Hg2—N3—C11	90.8 (3)
N1—Hg1—N2—C4	−177.5 (4)	N3—Hg2—N4—C12	178.4 (4)

Br1—Hg1—N2—C4	−55.0 (4)	Br4—Hg2—N4—C12	−85.0 (4)
Br2—Hg1—N2—C4	93.8 (4)	Br3—Hg2—N4—C12	66.9 (4)
N1—Hg1—N2—C6	−0.9 (3)	N3—Hg2—N4—C14	5.4 (3)
Br1—Hg1—N2—C6	121.7 (3)	Br4—Hg2—N4—C14	101.9 (3)
Br2—Hg1—N2—C6	−89.5 (3)	Br3—Hg2—N4—C14	−106.2 (3)
C3—N1—C1—C7	179.2 (4)	C11—N3—C9—C15	176.8 (4)
Hg1—N1—C1—C7	−1.5 (7)	Hg2—N3—C9—C15	−5.0 (7)
C3—N1—C1—S1	0.6 (5)	C11—N3—C9—S3	−1.2 (5)
Hg1—N1—C1—S1	179.9 (2)	Hg2—N3—C9—S3	177.0 (2)
C2—S1—C1—N1	0.3 (4)	C10—S3—C9—N3	1.2 (4)
C2—S1—C1—C7	−178.3 (4)	C10—S3—C9—C15	−176.8 (5)
C1—S1—C2—C3	−1.2 (4)	C9—S3—C10—C11	−0.9 (4)
S1—C2—C3—N1	1.7 (5)	S3—C10—C11—N3	0.4 (5)
S1—C2—C3—C6	−177.4 (4)	S3—C10—C11—C14	178.7 (4)
C1—N1—C3—C2	−1.5 (6)	C9—N3—C11—C10	0.5 (6)
Hg1—N1—C3—C2	179.0 (3)	Hg2—N3—C11—C10	−177.9 (3)
C1—N1—C3—C6	177.7 (4)	C9—N3—C11—C14	−178.0 (4)
Hg1—N1—C3—C6	−1.7 (5)	Hg2—N3—C11—C14	3.6 (5)
C6—N2—C4—C8	−178.1 (4)	C14—N4—C12—C16	−176.9 (4)
Hg1—N2—C4—C8	−1.3 (7)	Hg2—N4—C12—C16	9.8 (7)
C6—N2—C4—S2	1.5 (5)	C14—N4—C12—S4	1.2 (5)
Hg1—N2—C4—S2	178.2 (2)	Hg2—N4—C12—S4	−172.1 (2)
C5—S2—C4—N2	−0.4 (4)	C13—S4—C12—N4	−1.5 (4)
C5—S2—C4—C8	179.2 (4)	C13—S4—C12—C16	176.6 (4)
C4—S2—C5—C6	−0.8 (4)	C12—S4—C13—C14	1.3 (4)
S2—C5—C6—N2	1.9 (5)	S4—C13—C14—N4	−0.9 (5)
S2—C5—C6—C3	−177.9 (4)	S4—C13—C14—C11	178.8 (4)
C4—N2—C6—C5	−2.2 (6)	C12—N4—C14—C13	−0.2 (6)
Hg1—N2—C6—C5	−179.5 (3)	Hg2—N4—C14—C13	174.1 (3)
C4—N2—C6—C3	177.6 (4)	C12—N4—C14—C11	−179.9 (4)
Hg1—N2—C6—C3	0.3 (5)	Hg2—N4—C14—C11	−5.6 (5)
C2—C3—C6—C5	−0.1 (8)	C10—C11—C14—C13	3.5 (8)
N1—C3—C6—C5	−179.3 (4)	N3—C11—C14—C13	−178.2 (5)
C2—C3—C6—N2	−179.9 (4)	C10—C11—C14—N4	−176.8 (5)
N1—C3—C6—N2	1.0 (6)	N3—C11—C14—N4	1.5 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···Br4^{i}	0.98	2.92	3.826 (5)	155
C10—H10*A*···Br4^{i}	0.95	2.92	3.760 (5)	148
C16—H16*B*···Br3^{ii}	0.98	2.87	3.772 (5)	154
C16—H16*C*···Br2^{iii}	0.98	2.88	3.837 (5)	165

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*.