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Synthesis and structure of the mercury chloride complex of 2,2′-(2-bromo-5-*tert*-butyl-1,3-phenylene)bis(1-methyl-1*H*-benzimidazole)

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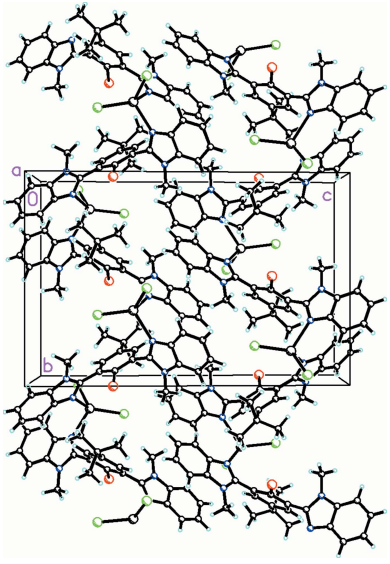
In the title mercury complex, *catena*-poly[[dichloridomercury(II)]-μ-2,2′-(2-bromo-5-*tert*-butyl-1,3-phenylene)bis(1-methyl-1*H*-benzimidazole)-κ^2N^3:$N^{3'}$], $[HgCl_2(C_{26}H_{25}BrN_4)]_n$, the Hg^{II} atom is coordinated by two Cl atoms and by two N atoms from two 2,2′-(2-bromo-5-*tert*-butyl-1,3-phenylene)bis(1-methyl-1*H*-benzimidazole) ligands. The metal cation adopts a distorted tetrahedral coordination geometry with with bond angles around mercury of 100.59 (15)° [N—Hg—N] and 126.35 (7)° [Cl—Hg—Cl]. This arrangement gives rise to a zigzag helical 1-D polymer propagating along the *b*-axis direction.

1. Chemical context

In the last one decade, 1,3-bis(benzimidazol-2-yl)benzene-based ligands have been studied extensively due to the presence of active sites for binding of metal atoms (Yang *et al.*, 2012; Tam *et al.*, 2011; Dorazco-Gonzalez, 2014). Very recently, dinuclear zinc complexes containing (benzimidazol-2-yl)benzene-based ligands have shown remarkable anticancer activities (Xie *et al.*, 2014). Helical and non-helical complexes with copper(I) have been reported by Ruettimann *et al.* (1992). Palladium complexes with bromo-functionalized benzimidazole derivatives have been utilized for Heck reactions (Reddy & Krishna, 2005).

A survey of the structural investigations of mercury halide complexes with benzimidazole derivatives have shown that they come in two main types, *viz*. polymeric, bridging either through the halide (Zhang *et al.*, 2015; Li *et al.*, 2007; Shen *et al.*, 2005) or through alternative N atoms from the benzimidazole moieties (Xiao *et al.*, 2009, 2011; Huang *et al.*, 2006; Li *et al.*, 2007, 2012*a*,*b*; Dey *et al.*, 2013; Du *et al.*, 2011; Chen *et al.*, 2013; Su *et al.*, 2003; Xu *et al.*, 2011), or discrete molecules, *i.e.* non-polymeric (Xiao *et al.*, 2011; Wu *et al.*, 2009; Zhao *et al.*, 2012; Lou *et al.*, 2012; Zhu *et al.*, 2009; Carballo *et al.*, 1993; Yan *et al.*, 2012; Hu *et al.*, 2012, 2015; Ding *et al.*, 2012; Matthews *et al.*, 1998; Manjunatha *et al.*, 2011; Wang *et al.*, 2007, 2009, 2012, 2015; Chen *et al.*, 2014; Su *et al.*, 2003; Quiroz-Castro *et al.*, 2000; Yang & Luo, 2012; He *et al.*, 2012; Bouchouit *et al.*, 2015).

In the present case, during the attempted synthesis of the C-2 mercurated derivative **3** from 2,2′-(2-bromo-5-*tert*-butyl-1,3-phenylene)bis(1-methyl-1*H*-benzimidazole), **1**, using *n*-BuLi and mercuric chloride, the mercury complex **2** was isolated unexpectedly (Fig. 1).



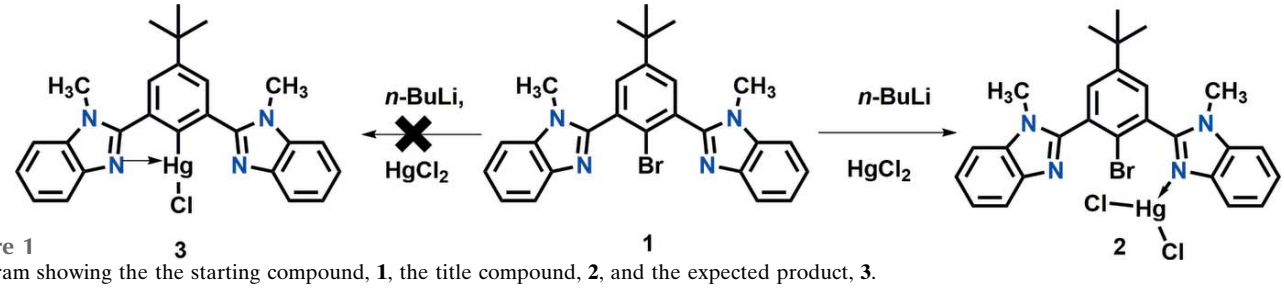
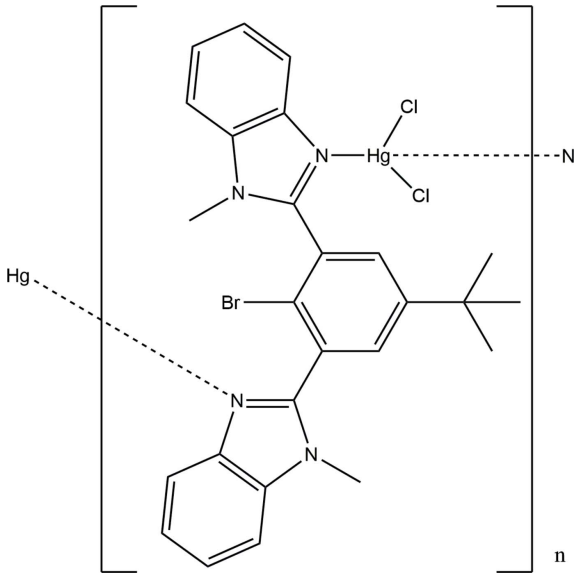


Figure 1
Diagram showing the the starting compound, **1**, the title compound, **2**, and the expected product, **3**.

2. Structural commentary

The structure of **2** with empirical formula, $C_{26}H_{25}BrCl_2HgN_4$, is reported in this paper. As a result of the presence of the Br and *t*-butyl substituents on the central ring, coordination of the Hg^{II} atom to this ring is prevented and thus a monomeric complex is formed, as has previously been observed for an $HgCl_2$ complex with a similar ligand but with a central pyridine ring rather than a phenyl ring (Liu *et al.*, 2007).

Another related structure has recently been reported of a dinuclear structure of $HgCl_2$ with a similar ligand to **1** where there is a methyl substituent on the C1 atom of the imidazole ring (Hu *et al.*, 2015). In the case of **2**, however, a zigzag polymeric structure forms in the *b*-axis direction, in which the $HgCl_2$ moiety is linked by atoms N1 from one ligand and N3 from an adjoining ligand. The coordination environment around the mercury atom is distorted tetrahedral with bond angles ranging from 100.6 (2) to 126.35 (7)° (Fig. 2). The two Hg—N bond lengths are equivalent at 2.333 (4) and 2.338 (4) Å. However, the metal–halogen bonds are not similar [Hg—Cl1 = 2.4424 (13) and Hg—Cl2 = 2.4020 (15) Å]. The ligand adopts a conformation whereby the two benzimidazole moieties are not coplanar with each other or the central phenyl ring. The dihedral angles between the benzimidazole moieties N1/N2/C1–C7 and N3/N4/C19–C24 are 60.9 (2)° while they make dihedral angles of 55.6 (2) and 84.2 (2)°, respectively, with the central ring.



3. Supramolecular features

The combination of $HgCl_2$ with 2,2′-(2-bromo-5-*tert*-butyl-1,3-phenylene)bis(1-methyl-1*H*-benzimidazole) results in a zigzag helical 1-D coordination polymer that propagates along the *b*-axis direction. This is mediated by the $HgCl_2$ moiety, which is linked by atoms N1 from one ligand and N3 from an adjoining ligand (Fig. 2). Although helices are inherently chiral in nature, the overall structure is not chiral as the individual helices are related by a center of inversion. The internal structure of this polymer is stabilized by both C—H···Cl and C—H···N interactions (Table 1). In addition, there are both C—H···π (Table 1) and π–π interactions [$Cg6\cdots Cg6(1-x,-y,-z)$ = 3.531 (2) Å, where $Cg6$ is the centroid of the benzimidazole ring system N3/N4/C19–C24 and C25]. There are no halogen bonds or C—H···Br interactions present. Apart from van der Waals interactions, there are no significant interactions between the zigzag chains of the coordination polymer (Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (Version 5.37 with updates May 2016; Groom *et al.*, 2016) reveals that there

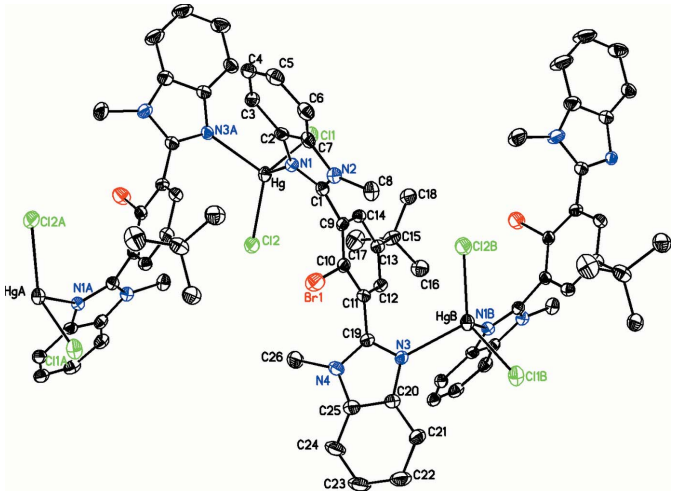


Figure 2
Diagram showing the three units which assemble to form a coordination polymer and illustrating its zigzag helical nature (with H atoms omitted for clarity). Displacement parameters are drawn at the 30% probability level. [Symmetry codes: (*A*) $1-x,\frac{1}{2}+y,z-\frac{1}{2}$; (*B*) $1-x,y-\frac{1}{2},z-\frac{1}{2}$.]

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

*Cg*1 is the centroid of the imidazole ring N1/N2/C1/C2/C7.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···N3^{i}	0.95	2.65	3.459 (7)	144
C8—H8*A*···Cl2^{ii}	0.98	2.71	3.643 (6)	160
C8—H8*B*···Cl1^{iii}	0.98	2.82	3.719 (6)	152
C21—H21*B*···Cl1^{ii}	0.95	2.77	3.616 (3)	149
C16—H16*B*···*Cg*1^{ii}	0.98	2.91	3.671 (8)	135

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

is no report in the literature for a mercury complex with 2,2′-(2-bromo-5-*tert*-butyl-1,3-phenylene)bis(1-methyl-1*H*-benzimidazole) that has been structurally characterized. A cadmium complex, bis[1,3-bis(benzimidazol-2-yl)benzene]-dichloridocadmium(II), in which the Cd is coordinated by two Cl atoms and two N atoms in a distorted tetrahedral configuration has been reported (Jiang *et al.*, 2010). In the title complex **2**, cadmium is replaced by an Hg^{II} atom along with a slight modification of the ligand.

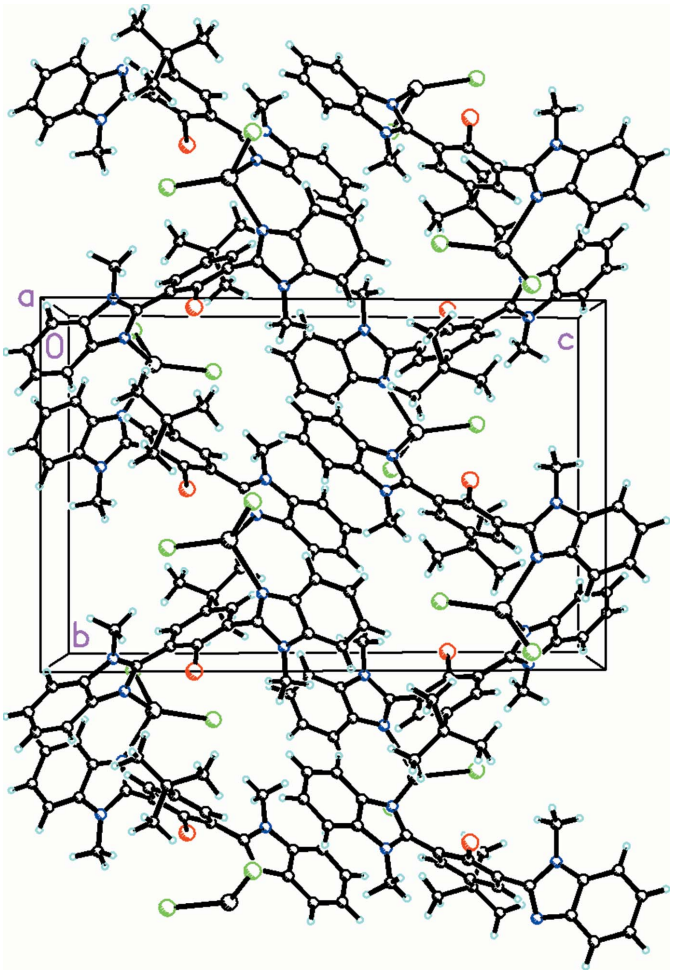


Figure 3
Packing diagram showing two units of the polymer, which repeat in the *b*-axis direction, viewed along the *a* axis.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[HgCl_2(C_{26}H_{25}BrN_4)]$
M_r	744.90
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	123
a, *b*, *c* (Å)	9.50481 (18), 13.3872 (2), 20.3322 (4)
β (°)	93.0955 (19)
V (Å^3)	2583.36 (9)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	14.57
Crystal size (mm)	0.37 × 0.09 × 0.03
Data collection	
Diffractometer	Agilent Xcalibur, Ruby, Gemini
Absorption correction	Analytical [*CrysAlis PRO* (Agilent, 2012) based on expressions derived by Clark & Reid (1995)]
T_{min}, T_{max}	0.331, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9778, 5217, 4596
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.628
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.104, 1.07
No. of reflections	5217
No. of parameters	300
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.34, −1.88

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXS2013* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *SHELXTL* (Sheldrick, 2008).

5. Synthesis and crystallization

To a solution of **1** (0.2 g, 0.42 mmol) in THF (15 ml) was added dropwise a solution of *n*-BuLi (0.3 ml, 0.47 mmol) at 195 K. The synthesis of compound **1** will be published elsewhere. The reaction mixture turned blue after immediate addition of *n*-BuLi. The reaction mixture was stirred for 30 min at 195 K followed by the addition of $HgCl_2$ (0.126 g, 0.466 mmol). The reaction mixture was warmed to room temperature and stirred for 16 h. The reaction mixture was then filtered through Whatman filter paper and the solvent was evaporated on a rotary evaporator. Colourless plate-shaped crystals were obtained by the slow evaporation of an ethyl acetate solution of the compound at room temperature.

Yield 44% (0.138 g), ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88–7.86 (*m*, 3H), 7.45–7.34 (*m*, 7H), 3.98 (*s*, 6H), 1.46 (*s*, 9H). ^{13}C NMR (100 MHz, DMSO): 152.3, 151.2, 141.6, 135.2, 131.8, 131.4, 123.3, 122.7, 121.6, 119.1, 111.0, 34.9, 31.1, 30.8. Analysis calculated for $C_{26}H_{25}N_4Cl_2BrHg$: C, 41.92; H, 3.38; N, 7.52. Found C, 42.68; H, 4.14; N, 6.29.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically and refined as riding: C—H = 0.95–0.98 Å with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms.

Acknowledgements

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supporting information

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Synthesis and structure of the mercury chloride complex of 2,2′-(2-bromo-5-*tert*-butyl-1,3-phenylene)bis(1-methyl-1*H*-benzimidazole)

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

***catena*-Poly[[dichloridomercury(II)]-μ-2,2′-(2-bromo-5-*tert*-butyl-1,3-phenylene)bis(1-methyl-1*H*-benzimidazole)-$\kappa^2N^3:N^{3'}$]**

Crystal data

$[HgCl_2(C_{26}H_{25}BrN_4)]$
$M_r = 744.90$
Monoclinic, $P2_1/c$
$a = 9.50481\ (18)$ Å
$b = 13.3872\ (2)$ Å
$c = 20.3322\ (4)$ Å
$\beta = 93.0955\ (19)°$
$V = 2583.36\ (9)$ Å^3
$Z = 4$
$F(000) = 1432$
$D_x = 1.915$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 4457 reflections
$\theta = 3.9–74.8°$
$\mu = 14.57$ mm^{-1}
$T = 123$ K
Plate, colorless
0.37 × 0.09 × 0.03 mm

Data collection

Agilent Xcalibur, Ruby, Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlis PRO (Agilent, 2012) based on expressions derived by Clark & Reid (1995)]
$T_{min} = 0.331$, $T_{max} = 1.000$
9778 measured reflections
5217 independent reflections
4596 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 75.6°$, $\theta_{min} = 4.0°$
$h = -11\rightarrow11$
$k = -10\rightarrow16$
$l = -25\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.104$
$S = 1.07$
5217 reflections
300 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.34$ e Å^{-3}
$\Delta\rho_{min} = -1.88$ 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}
Hg	0.26669 (2)	0.15196 (2)	0.17398 (2)	0.03689 (9)
Br1	0.78523 (7)	0.01223 (6)	0.26403 (4)	0.05807 (19)
Cl1	0.07681 (12)	0.04507 (10)	0.12894 (8)	0.0455 (3)
Cl2	0.3350 (3)	0.17449 (13)	0.28849 (7)	0.0680 (5)
N1	0.4632 (4)	0.0840 (3)	0.12648 (19)	0.0297 (8)
N2	0.6469 (4)	−0.0168 (3)	0.1125 (2)	0.0332 (8)
C1	0.5402 (5)	0.0084 (4)	0.1512 (2)	0.0290 (9)
C2	0.5243 (5)	0.1104 (4)	0.0687 (2)	0.0325 (10)
C3	0.4867 (6)	0.1831 (4)	0.0214 (2)	0.0380 (11)
H3A	0.407599	0.225411	0.026176	0.046*
C4	0.5690 (7)	0.1912 (5)	−0.0326 (3)	0.0443 (13)
H4A	0.546152	0.239743	−0.065535	0.053*
C5	0.6869 (7)	0.1279 (5)	−0.0392 (3)	0.0462 (13)
H5A	0.742376	0.136244	−0.076319	0.055*
C6	0.7235 (6)	0.0557 (4)	0.0054 (3)	0.0415 (12)
H6A	0.801480	0.012676	−0.000153	0.050*
C7	0.6402 (5)	0.0478 (4)	0.0599 (2)	0.0336 (10)
C8	0.7432 (5)	−0.1007 (4)	0.1193 (3)	0.0412 (11)
H8A	0.706934	−0.149329	0.150248	0.062*
H8B	0.835960	−0.077071	0.136067	0.062*
H8C	0.751825	−0.132519	0.076325	0.062*
C9	0.5103 (5)	−0.0449 (4)	0.2128 (2)	0.0295 (9)
C10	0.6114 (5)	−0.0530 (4)	0.2651 (2)	0.0328 (9)
C11	0.5801 (5)	−0.1064 (4)	0.3208 (2)	0.0347 (10)
C12	0.4486 (6)	−0.1492 (4)	0.3257 (2)	0.0340 (10)
H12A	0.429536	−0.186816	0.363769	0.041*
C13	0.3436 (5)	−0.1382 (4)	0.2757 (2)	0.0326 (10)
C14	0.3774 (5)	−0.0858 (4)	0.2192 (2)	0.0301 (9)
H14A	0.307701	−0.078004	0.184253	0.036*
C15	0.1946 (6)	−0.1774 (5)	0.2844 (3)	0.0446 (13)
C16	0.1931 (7)	−0.2560 (6)	0.3375 (3)	0.0569 (16)
H16A	0.250243	−0.313200	0.325066	0.085*
H16B	0.096006	−0.277900	0.342884	0.085*
H16C	0.232117	−0.227992	0.379161	0.085*
C17	0.1086 (9)	−0.0864 (7)	0.3074 (4)	0.069 (2)
H17A	0.014973	−0.108654	0.319073	0.103*

H17B	0.098912	−0.037282	0.271679	0.103*
H17C	0.157701	−0.055702	0.345930	0.103*
C18	0.1272 (7)	−0.2131 (5)	0.2188 (3)	0.0504 (14)
H18A	0.189918	−0.261007	0.198742	0.076*
H18B	0.111504	−0.155783	0.189316	0.076*
H18C	0.036859	−0.245312	0.226242	0.076*
N3	0.7624 (4)	−0.2007 (3)	0.3870 (2)	0.0334 (8)
N4	0.7052 (7)	−0.0512 (4)	0.4249 (3)	0.0574 (15)
C19	0.6851 (6)	−0.1200 (4)	0.3764 (3)	0.0389 (11)
C20	0.8389 (4)	−0.1846 (3)	0.44605 (14)	0.0393 (11)
C21	0.9323 (4)	−0.2448 (2)	0.48302 (18)	0.0436 (12)
H21B	0.958442	−0.308251	0.466606	0.052*
C22	0.9875 (5)	−0.2123 (3)	0.54401 (18)	0.0604 (18)
H22B	1.051354	−0.253523	0.569280	0.073*
C23	0.9493 (6)	−0.1196 (4)	0.56803 (19)	0.085 (3)
H23B	0.987023	−0.097343	0.609714	0.102*
C24	0.8559 (6)	−0.0593 (3)	0.5311 (2)	0.092 (4)
H24B	0.829779	0.004111	0.547474	0.111*
C25	0.8007 (5)	−0.0918 (3)	0.4701 (2)	0.0562 (17)
C26	0.6419 (11)	0.0482 (6)	0.4279 (4)	0.080 (3)
H26D	0.560680	0.052189	0.396154	0.121*
H26E	0.711628	0.098707	0.417059	0.121*
H26F	0.610913	0.060333	0.472366	0.121*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg	0.03625 (13)	0.03134 (14)	0.04333 (13)	0.00299 (7)	0.00463 (8)	0.00013 (8)
Br1	0.0463 (3)	0.0589 (4)	0.0671 (4)	−0.0147 (3)	−0.0146 (3)	0.0142 (3)
Cl1	0.0290 (5)	0.0381 (7)	0.0696 (8)	−0.0006 (5)	0.0036 (5)	0.0048 (6)
Cl2	0.1242 (16)	0.0414 (8)	0.0383 (6)	0.0101 (9)	0.0035 (8)	−0.0041 (6)
N1	0.0269 (18)	0.030 (2)	0.0319 (17)	−0.0004 (15)	0.0016 (14)	0.0021 (15)
N2	0.0281 (18)	0.034 (2)	0.0383 (19)	−0.0019 (16)	0.0042 (15)	−0.0003 (17)
C1	0.0243 (19)	0.030 (2)	0.033 (2)	−0.0040 (17)	0.0014 (16)	−0.0013 (18)
C2	0.034 (2)	0.034 (3)	0.0289 (19)	−0.0077 (19)	−0.0034 (17)	−0.0009 (19)
C3	0.044 (3)	0.034 (3)	0.035 (2)	−0.010 (2)	−0.002 (2)	0.005 (2)
C4	0.061 (3)	0.039 (3)	0.033 (2)	−0.018 (3)	−0.001 (2)	0.003 (2)
C5	0.051 (3)	0.053 (3)	0.035 (2)	−0.023 (3)	0.009 (2)	−0.006 (2)
C6	0.041 (3)	0.042 (3)	0.042 (2)	−0.011 (2)	0.010 (2)	−0.008 (2)
C7	0.032 (2)	0.032 (2)	0.037 (2)	−0.0111 (19)	0.0068 (18)	−0.0054 (19)
C8	0.030 (2)	0.037 (3)	0.057 (3)	0.002 (2)	0.008 (2)	−0.003 (2)
C9	0.030 (2)	0.026 (2)	0.032 (2)	0.0013 (17)	−0.0007 (17)	0.0030 (17)
C10	0.029 (2)	0.026 (2)	0.042 (2)	−0.0050 (18)	−0.0071 (18)	0.0024 (19)
C11	0.039 (2)	0.032 (3)	0.032 (2)	0.001 (2)	−0.0086 (18)	−0.0024 (19)
C12	0.039 (3)	0.032 (3)	0.030 (2)	0.0009 (19)	0.0011 (19)	0.0045 (18)
C13	0.031 (2)	0.036 (3)	0.032 (2)	0.0023 (19)	0.0047 (18)	−0.0002 (18)
C14	0.027 (2)	0.033 (2)	0.0302 (19)	0.0032 (18)	0.0007 (16)	−0.0002 (17)
C15	0.032 (3)	0.060 (4)	0.042 (3)	−0.003 (2)	0.006 (2)	0.015 (3)

C16	0.057 (4)	0.061 (4)	0.053 (3)	−0.016 (3)	0.005 (3)	0.009 (3)
C17	0.060 (4)	0.073 (5)	0.075 (5)	0.013 (4)	0.027 (3)	0.007 (4)
C18	0.047 (3)	0.050 (4)	0.054 (3)	−0.020 (3)	−0.004 (2)	0.011 (3)
N3	0.0333 (19)	0.027 (2)	0.0393 (19)	−0.0024 (16)	−0.0082 (16)	0.0031 (16)
N4	0.074 (4)	0.044 (3)	0.051 (3)	0.019 (3)	−0.027 (3)	−0.016 (2)
C19	0.045 (3)	0.034 (3)	0.037 (2)	−0.001 (2)	−0.011 (2)	0.003 (2)
C20	0.043 (3)	0.039 (3)	0.035 (2)	−0.001 (2)	−0.004 (2)	0.002 (2)
C21	0.042 (3)	0.042 (3)	0.045 (3)	0.004 (2)	−0.006 (2)	0.007 (2)
C22	0.055 (4)	0.077 (5)	0.048 (3)	0.012 (3)	−0.018 (3)	0.002 (3)
C23	0.106 (7)	0.090 (6)	0.055 (4)	0.031 (5)	−0.043 (5)	−0.027 (4)
C24	0.124 (8)	0.075 (6)	0.070 (5)	0.039 (5)	−0.057 (5)	−0.037 (4)
C25	0.070 (4)	0.049 (4)	0.048 (3)	0.013 (3)	−0.021 (3)	−0.005 (3)
C26	0.110 (7)	0.047 (4)	0.079 (5)	0.035 (4)	−0.042 (5)	−0.021 (4)

Geometric parameters (Å, º)

Hg—N1	2.333 (4)	C13—C15	1.530 (7)
Hg—N3^{i}	2.338 (4)	C14—H14A	0.9500
Hg—Cl2	2.4020 (15)	C15—C16	1.508 (8)
Hg—Cl1	2.4424 (13)	C15—C18	1.525 (8)
Br1—C10	1.870 (5)	C15—C17	1.553 (10)
N1—C1	1.331 (6)	C16—H16A	0.9800
N1—C2	1.383 (6)	C16—H16B	0.9800
N2—C1	1.359 (6)	C16—H16C	0.9800
N2—C7	1.374 (7)	C17—H17A	0.9800
N2—C8	1.452 (7)	C17—H17B	0.9800
C1—C9	1.483 (6)	C17—H17C	0.9800
C2—C3	1.401 (7)	C18—H18A	0.9800
C2—C7	1.404 (7)	C18—H18B	0.9800
C3—C4	1.387 (8)	C18—H18C	0.9800
C3—H3A	0.9500	N3—C19	1.318 (7)
C4—C5	1.417 (10)	N3—C20	1.387 (4)
C4—H4A	0.9500	N4—C19	1.355 (7)
C5—C6	1.358 (9)	N4—C25	1.369 (6)
C5—H5A	0.9500	N4—C26	1.463 (9)
C6—C7	1.401 (7)	C20—C21	1.3900
C6—H6A	0.9500	C20—C25	1.3900
C8—H8A	0.9800	C21—C22	1.3900
C8—H8B	0.9800	C21—H21B	0.9500
C8—H8C	0.9800	C22—C23	1.3900
C9—C14	1.389 (7)	C22—H22B	0.9500
C9—C10	1.398 (6)	C23—C24	1.3900
C10—C11	1.387 (7)	C23—H23B	0.9500
C11—C12	1.383 (8)	C24—C25	1.3900
C11—C19	1.478 (6)	C24—H24B	0.9500
C12—C13	1.392 (7)	C26—H26D	0.9800
C12—H12A	0.9500	C26—H26E	0.9800
C13—C14	1.399 (7)	C26—H26F	0.9800

N1—Hg—N3^{i}	100.59 (15)	C16—C15—C18	112.8 (6)
N1—Hg—Cl2	105.64 (11)	C16—C15—C13	111.5 (5)
N3^{i}—Hg—Cl2	115.22 (11)	C18—C15—C13	110.7 (5)
N1—Hg—Cl1	102.02 (10)	C16—C15—C17	107.9 (6)
N3^{i}—Hg—Cl1	103.38 (10)	C18—C15—C17	107.8 (6)
Cl2—Hg—Cl1	126.35 (7)	C13—C15—C17	105.7 (6)
C1—N1—C2	105.5 (4)	C15—C16—H16A	109.5
C1—N1—Hg	125.2 (3)	C15—C16—H16B	109.5
C2—N1—Hg	129.3 (3)	H16A—C16—H16B	109.5
C1—N2—C7	106.8 (4)	C15—C16—H16C	109.5
C1—N2—C8	128.6 (4)	H16A—C16—H16C	109.5
C7—N2—C8	124.4 (4)	H16B—C16—H16C	109.5
N1—C1—N2	112.5 (4)	C15—C17—H17A	109.5
N1—C1—C9	123.9 (4)	C15—C17—H17B	109.5
N2—C1—C9	123.5 (4)	H17A—C17—H17B	109.5
N1—C2—C3	131.1 (5)	C15—C17—H17C	109.5
N1—C2—C7	108.9 (4)	H17A—C17—H17C	109.5
C3—C2—C7	120.0 (5)	H17B—C17—H17C	109.5
C4—C3—C2	117.6 (6)	C15—C18—H18A	109.5
C4—C3—H3A	121.2	C15—C18—H18B	109.5
C2—C3—H3A	121.2	H18A—C18—H18B	109.5
C3—C4—C5	120.8 (5)	C15—C18—H18C	109.5
C3—C4—H4A	119.6	H18A—C18—H18C	109.5
C5—C4—H4A	119.6	H18B—C18—H18C	109.5
C6—C5—C4	122.5 (5)	C19—N3—C20	106.0 (4)
C6—C5—H5A	118.7	C19—N3—Hg^{ii}	123.8 (3)
C4—C5—H5A	118.7	C20—N3—Hg^{ii}	129.2 (3)
C5—C6—C7	116.5 (6)	C19—N4—C25	106.3 (5)
C5—C6—H6A	121.7	C19—N4—C26	127.3 (5)
C7—C6—H6A	121.7	C25—N4—C26	126.4 (5)
N2—C7—C6	131.2 (5)	N3—C19—N4	112.5 (4)
N2—C7—C2	106.3 (4)	N3—C19—C11	125.0 (5)
C6—C7—C2	122.5 (5)	N4—C19—C11	122.4 (5)
N2—C8—H8A	109.5	N3—C20—C21	131.9 (3)
N2—C8—H8B	109.5	N3—C20—C25	108.0 (3)
H8A—C8—H8B	109.5	C21—C20—C25	120.0
N2—C8—H8C	109.5	C20—C21—C22	120.0
H8A—C8—H8C	109.5	C20—C21—H21B	120.0
H8B—C8—H8C	109.5	C22—C21—H21B	120.0
C14—C9—C10	119.3 (4)	C23—C22—C21	120.0
C14—C9—C1	119.0 (4)	C23—C22—H22B	120.0
C10—C9—C1	121.6 (4)	C21—C22—H22B	120.0
C11—C10—C9	119.5 (4)	C22—C23—C24	120.0
C11—C10—Br1	118.6 (3)	C22—C23—H23B	120.0
C9—C10—Br1	121.8 (4)	C24—C23—H23B	120.0
C12—C11—C10	120.4 (4)	C23—C24—C25	120.0
C12—C11—C19	118.0 (5)	C23—C24—H24B	120.0

C10—C11—C19	121.6 (5)	C25—C24—H24B	120.0
C11—C12—C13	121.3 (5)	N4—C25—C24	132.8 (3)
C11—C12—H12A	119.4	N4—C25—C20	107.2 (3)
C13—C12—H12A	119.4	C24—C25—C20	120.0
C12—C13—C14	117.7 (5)	N4—C26—H26D	109.5
C12—C13—C15	120.7 (5)	N4—C26—H26E	109.5
C14—C13—C15	121.5 (4)	H26D—C26—H26E	109.5
C9—C14—C13	121.6 (4)	N4—C26—H26F	109.5
C9—C14—H14A	119.2	H26D—C26—H26F	109.5
C13—C14—H14A	119.2	H26E—C26—H26F	109.5

C2—N1—C1—N2	−0.7 (5)	C11—C12—C13—C15	−174.2 (5)
Hg—N1—C1—N2	178.9 (3)	C10—C9—C14—C13	−2.4 (8)
C2—N1—C1—C9	−178.7 (4)	C1—C9—C14—C13	179.1 (5)
Hg—N1—C1—C9	0.8 (6)	C12—C13—C14—C9	−0.7 (8)
C7—N2—C1—N1	1.1 (5)	C15—C13—C14—C9	176.1 (5)
C8—N2—C1—N1	−173.1 (5)	C12—C13—C15—C16	−20.5 (8)
C7—N2—C1—C9	179.1 (4)	C14—C13—C15—C16	162.8 (5)
C8—N2—C1—C9	4.9 (8)	C12—C13—C15—C18	−147.0 (5)
C1—N1—C2—C3	178.3 (5)	C14—C13—C15—C18	36.3 (8)
Hg—N1—C2—C3	−1.2 (8)	C12—C13—C15—C17	96.5 (6)
C1—N1—C2—C7	0.0 (5)	C14—C13—C15—C17	−80.2 (7)
Hg—N1—C2—C7	−179.5 (3)	C20—N3—C19—N4	−0.1 (7)
N1—C2—C3—C4	−179.2 (5)	Hg^{ii}—N3—C19—N4	169.2 (4)
C7—C2—C3—C4	−1.1 (7)	C20—N3—C19—C11	−176.2 (5)
C2—C3—C4—C5	−0.1 (8)	Hg^{ii}—N3—C19—C11	−6.9 (8)
C3—C4—C5—C6	1.4 (8)	C25—N4—C19—N3	−1.0 (8)
C4—C5—C6—C7	−1.4 (8)	C26—N4—C19—N3	177.1 (8)
C1—N2—C7—C6	−179.8 (5)	C25—N4—C19—C11	175.2 (6)
C8—N2—C7—C6	−5.3 (8)	C26—N4—C19—C11	−6.6 (12)
C1—N2—C7—C2	−1.0 (5)	C12—C11—C19—N3	80.3 (8)
C8—N2—C7—C2	173.5 (4)	C10—C11—C19—N3	−99.4 (7)
C5—C6—C7—N2	178.9 (5)	C12—C11—C19—N4	−95.5 (7)
C5—C6—C7—C2	0.2 (7)	C10—C11—C19—N4	84.8 (8)
N1—C2—C7—N2	0.6 (5)	C19—N3—C20—C21	176.7 (4)
C3—C2—C7—N2	−177.9 (4)	Hg^{ii}—N3—C20—C21	8.2 (7)
N1—C2—C7—C6	179.5 (4)	C19—N3—C20—C25	1.1 (5)
C3—C2—C7—C6	1.0 (7)	Hg^{ii}—N3—C20—C25	−167.4 (3)
N1—C1—C9—C14	54.6 (7)	N3—C20—C21—C22	−175.2 (5)
N2—C1—C9—C14	−123.2 (5)	C25—C20—C21—C22	0.0
N1—C1—C9—C10	−123.9 (5)	C20—C21—C22—C23	0.0
N2—C1—C9—C10	58.3 (7)	C21—C22—C23—C24	0.0
C14—C9—C10—C11	3.6 (8)	C22—C23—C24—C25	0.0
C1—C9—C10—C11	−177.8 (5)	C19—N4—C25—C24	−175.9 (4)
C14—C9—C10—Br1	−173.0 (4)	C26—N4—C25—C24	5.9 (12)
C1—C9—C10—Br1	5.5 (7)	C19—N4—C25—C20	1.7 (7)
C9—C10—C11—C12	−1.8 (8)	C26—N4—C25—C20	−176.5 (8)
Br1—C10—C11—C12	175.0 (4)	C23—C24—C25—N4	177.4 (7)

C9—C10—C11—C19	177.9 (5)	C23—C24—C25—C20	0.0
Br1—C10—C11—C19	−5.4 (7)	N3—C20—C25—N4	−1.8 (5)
C10—C11—C12—C13	−1.4 (8)	C21—C20—C25—N4	−178.0 (5)
C19—C11—C12—C13	178.9 (5)	N3—C20—C25—C24	176.2 (4)
C11—C12—C13—C14	2.6 (8)	C21—C20—C25—C24	0.0

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

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the imidazole ring N1/N2/C1/C2/C7.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···N3^{i}	0.95	2.65	3.459 (7)	144
C8—H8*A*···Cl2^{ii}	0.98	2.71	3.643 (6)	160
C8—H8*B*···Cl1^{iii}	0.98	2.82	3.719 (6)	152
C21—H21*B*···Cl1^{ii}	0.95	2.77	3.616 (3)	149
C16—H16*B*···*Cg*1^{ii}	0.98	2.91	3.671 (8)	135

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