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## Structure Reports

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Bis(2-trifluoromethyl-1*H*-benzimidazol-3-ium) tetrachloridomercurate dihydrate

Ming-Liang Liu

Ordered Matter Science Research Center, Southeast University, Nanjing 211189, People's Republic of China

Correspondence e-mail: jgsdxlm@163.com

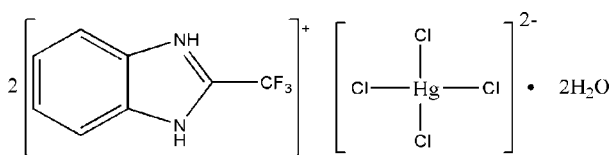
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.013$  Å; disorder in main residue;  $R$  factor = 0.053;  $wR$  factor = 0.119; data-to-parameter ratio = 17.1.

In the title compound,  $(\text{C}_8\text{H}_6\text{F}_3\text{N}_2)_2[\text{HgCl}_4] \cdot 2\text{H}_2\text{O}$ , the  $\text{Hg}^{\text{II}}$  cation is coordinated by four  $\text{Cl}^-$  anions in a distorted tetrahedral geometry. In the crystal, the 2-trifluoromethyl-1*H*-benzimidazolium cations link to the  $[\text{HgCl}_4]^{2-}$  complex anions and lattice water molecules *via*  $\text{N}-\text{H} \cdots \text{Cl}$  and  $\text{N}-\text{H} \cdots \text{O}$  hydrogen bonds, and the lattice water molecules further link to the Hg complex anion and the organic cations *via*  $\text{O}-\text{H} \cdots \text{Cl}$  and  $\text{O}-\text{H} \cdots \text{F}$  hydrogen bonding. One of the trifluoromethyl groups is disordered over two orientations in a 0.59 (4):0.41 (4) ratio.

## Related literature

For background to ferroelectric complexes, see: Fu *et al.* (2011); Ye *et al.* (2009). Zhang *et al.* (2009, 2010, 2012). For related structures, see: Liu (2011*a,b*, 2012*a,b,c*).



## Experimental

## Crystal data

 $(\text{C}_8\text{H}_6\text{F}_3\text{N}_2)_2[\text{HgCl}_4] \cdot 2\text{H}_2\text{O}$  $M_r = 752.72$ Triclinic,  $P\bar{1}$  $a = 9.2485$  (18) Å $b = 10.029$  (2) Å $c = 14.754$  (3) Å $\alpha = 79.40$  (3)° $\beta = 75.79$  (3)° $\gamma = 67.74$  (3)° $V = 1221.4$  (4) Å<sup>3</sup> $Z = 2$ Mo  $K\alpha$  radiation $\mu = 6.81$  mm<sup>-1</sup> $T = 293$  K

0.36 × 0.32 × 0.28 mm

## Data collection

Rigaku SCXmini diffractometer

Absorption correction: multi-scan

(CrystalClear; Rigaku, 2005)

 $T_{\text{min}} = 0.095$ ,  $T_{\text{max}} = 0.152$ 

12786 measured reflections

5564 independent reflections

4040 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.061$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.053$  $wR(F^2) = 0.119$  $S = 1.08$ 

5564 reflections

326 parameters

9 restraints

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.57$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -1.28$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N1}-\text{H1A} \cdots \text{Cl2}^{\text{ii}}$	0.86	2.23	3.081 (6)	170
$\text{N2}-\text{H2A} \cdots \text{O1}^{\text{ii}}$	0.86	1.80	2.656 (8)	174
$\text{N3}-\text{H3A} \cdots \text{O2}$	0.86	1.76	2.608 (9)	166
$\text{N4}-\text{H4A} \cdots \text{Cl1}$	0.86	2.21	3.069 (6)	175
$\text{O1}-\text{H1C} \cdots \text{F3}^{\text{iii}}$	0.85	2.25	2.994 (18)	146
$\text{O1}-\text{H1B} \cdots \text{Cl2}^{\text{iv}}$	0.85	2.55	3.279 (6)	144
$\text{O2}-\text{H2B} \cdots \text{F5}^{\text{v}}$	0.85	2.41	3.224 (13)	160
$\text{O2}-\text{H2D} \cdots \text{Cl3}^{\text{vi}}$	0.85	2.50	3.339 (10)	172

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The author thanks an anonymous advisor from the Ordered Matter Science Research Centre, Southeast University, for great help in the revision of this paper.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5519).

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## supplementary materials

*Acta Cryst.* (2012). E68, m716 [doi:10.1107/S1600536812018855]

## Bis(2-trifluoromethyl-1*H*-benzimidazol-3-ium) tetrachloridomercurate dihydrate

Ming-Liang Liu

### Comment

Recently much attention has been devoted to simple molecular-ionic compounds containing inorganic and organic ions due to the tunability of their special structural features and their potential ferroelectric property. Ferroelectric materials that exhibit reversible electric polarization in response to an external electric field have found many applications such as nonvolatile memory storage, electronics and optics. The freezing of a certain functional group at low temperature forces significant orientational motions of the guest molecules and thus induces the formation of the ferroelectric phase. (Fu *et al.*, 2011; Ye *et al.* 2009; Zhang *et al.* 2009; Zhang *et al.* 2012; Zhang *et al.* 2010). In our laboratory, the title compound has been synthesized to investigate its potential ferroelectric properties. However, it was found that the dielectric constant of the compound as a function of temperature indicates that the permittivity is basically temperature-independent ( $\epsilon = C/(T-T_0)$ ), suggesting that this compound is not ferroelectric or there may be no distinct phase transition occurring within the measured temperature (below the melting point).

The title compound,  $(C_8H_6F_3N_2)_2^+ \cdot HgCl_4^{2-} \cdot 2H_2O$ , has an asymmetric unit that consists of two 2-trifluoromethyl-1*H*-benzimidazol cations, one tetrachloridomercurate anion and two water molecules (Fig 1). The atoms of the benzimidazole ring are nearly coplanar and the trifluoromethyl group lies out of this plane. The mercury cation is coordinated by six Cl<sup>-</sup> anions in distorted tetrahedral geometry, the average Hg—Cl bond distances range from 2.364 (2) Å to 2.564 (2) Å, the Cl—Hg—Cl angles range from 102.24 (8)° to 120.36 (9)°. In the crystal structure, the 2-trifluoromethyl-1*H*-benzimidazol cations are linked to adjacent tetrachloridomercurate anions and water molecules by N—H $\cdots$ O, N—H $\cdots$ Cl and O—H $\cdots$ Cl hydrogen bonds to form one dimensional chains parallel to *ac* plane (Fig 2). One of the trifluoromethyl is disordered.

### Experimental

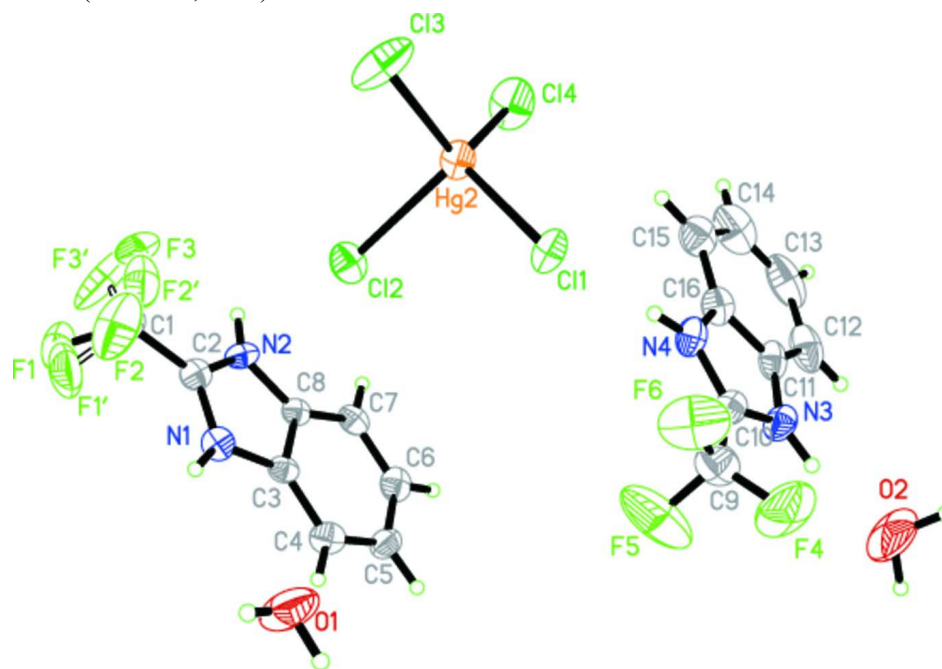
0.144 g (1 mmol) of 2-trifluoromethyl-1*H*-benzimidazol was firstly dissolved in 30 ml of ethanol which was added hydrochloric acid, to which 0.271 g (1 mmol) of mercuric chloride was added to give a solution at the ambient temperature. Single crystals suitable for X-ray structure analysis were obtained by the slow evaporation of the above solution after 5 days in air.

### Refinement

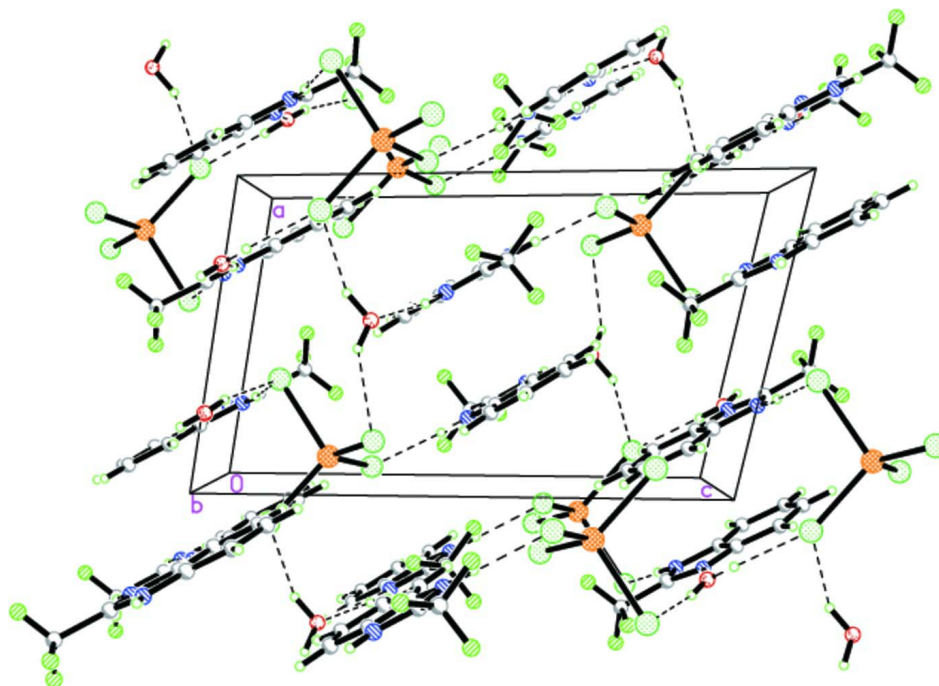
H atoms were placed in calculated positions (O—H = 0.85 Å; N—H = 0.89 Å; C—H = 0.93 Å for *Csp*<sup>2</sup> atoms and C—H = 0.96 Å and 0.97 Å for *Csp*<sup>3</sup> atoms), assigned fixed  $U_{iso}$  values [ $U_{iso} = 1.2U_{eq}(Csp^2)$  and  $1.5U_{eq}(Csp^3, N, O)$ ] and allowed to ride. The trifluoromethyl group is disordered over two sites. The site occupancies were refined and restraints were applied to the thermal parameters.

**Computing details**

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

**Figure 1**

The molecular structure of the title compound, showing the atomic numbering scheme with 30% probability displacement ellipsoids.


**Figure 2**

The packing of the title compound with view along the *b* axis. For the sake of clarity only the major component of the disordered trifluoromethyl group is shown.

**Bis(2-trifluoromethyl-1*H*-benzimidazol-3-ium) tetrachloridomercurate dihydrate**
*Crystal data*
 $(C_8H_6F_3N_2)[HgCl_4] \cdot 2H_2O$ 
 $M_r = 752.72$ 

 Triclinic,  $P\bar{1}$ 

 Hall symbol:  $-P\ 1$ 
 $a = 9.2485\ (18)\ \text{\AA}$ 
 $b = 10.029\ (2)\ \text{\AA}$ 
 $c = 14.754\ (3)\ \text{\AA}$ 
 $\alpha = 79.40\ (3)^\circ$ 
 $\beta = 75.79\ (3)^\circ$ 
 $\gamma = 67.74\ (3)^\circ$ 
 $V = 1221.4\ (4)\ \text{\AA}^3$ 
 $Z = 2$ 
 $F(000) = 716$ 
 $D_x = 2.047\ \text{Mg m}^{-3}$ 

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

Cell parameters from 4366 reflections

 $\theta = 3.0\text{--}26.0^\circ$ 
 $\mu = 6.81\ \text{mm}^{-1}$ 
 $T = 293\ \text{K}$ 

Block, colourless

 $0.36 \times 0.32 \times 0.28\ \text{mm}$ 
*Data collection*

Rigaku SCXmini

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

CCD\_Profile\_fitting scans

Absorption correction: multi-scan

 (*CrystalClear*; Rigaku, 2005)

 $T_{\min} = 0.095$ ,  $T_{\max} = 0.152$ 

12786 measured reflections

5564 independent reflections

 4040 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.061$ 
 $\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.1^\circ$ 
 $h = -12 \rightarrow 12$ 
 $k = -13 \rightarrow 12$ 
 $l = -19 \rightarrow 19$

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 1.355P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
5564 reflections	$(\Delta/\sigma)_{\max} = 0.022$
326 parameters	$\Delta\rho_{\max} = 0.57 \text{ e } \text{\AA}^{-3}$
9 restraints	$\Delta\rho_{\min} = -1.28 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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.

**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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
F1	0.7017 (13)	0.721 (2)	0.7840 (6)	0.093 (6)	0.59 (4)
F2	0.499 (3)	0.677 (2)	0.8538 (16)	0.123 (10)	0.59 (4)
F3	0.535 (3)	0.8571 (9)	0.8821 (10)	0.112 (9)	0.59 (4)
F1'	0.656 (4)	0.652 (3)	0.7911 (14)	0.137 (16)	0.41 (4)
F3'	0.639 (4)	0.841 (2)	0.843 (3)	0.16 (2)	0.41 (4)
F2'	0.4537 (9)	0.751 (3)	0.8841 (12)	0.102 (11)	0.41 (4)
N1	0.7197 (6)	0.4910 (6)	0.9609 (4)	0.0463 (14)	
H1A	0.6964	0.4371	0.9319	0.056*	
N2	0.7409 (6)	0.6807 (6)	0.9988 (4)	0.0446 (13)	
H2A	0.7328	0.7692	0.9978	0.053*	
C1	0.6080 (8)	0.7210 (7)	0.8664 (5)	0.064 (2)	
C2	0.6894 (8)	0.6313 (8)	0.9408 (5)	0.0446 (16)	
C3	0.7956 (7)	0.4460 (7)	1.0370 (5)	0.0392 (15)	
C4	0.8554 (9)	0.3110 (8)	1.0833 (5)	0.0522 (18)	
H4	0.8479	0.2294	1.0662	0.063*	
C5	0.9278 (9)	0.3035 (8)	1.1571 (5)	0.0532 (18)	
H5	0.9701	0.2150	1.1913	0.064*	
C6	0.9371 (8)	0.4285 (9)	1.1801 (5)	0.0535 (18)	
H6	0.9860	0.4200	1.2300	0.064*	
C7	0.8793 (8)	0.5611 (8)	1.1340 (5)	0.0456 (16)	
H7	0.8871	0.6425	1.1511	0.055*	
C8	0.8083 (7)	0.5692 (7)	1.0604 (5)	0.0376 (14)	
F4	0.2353 (11)	0.1121 (7)	0.5538 (6)	0.146 (3)	
F5	0.3648 (10)	0.1573 (10)	0.4248 (7)	0.167 (4)	
F6	0.1251 (8)	0.2625 (7)	0.4538 (6)	0.124 (2)	
N3	0.3498 (7)	0.3080 (7)	0.5958 (4)	0.0579 (16)	

H3A	0.3878	0.2271	0.6286	0.070*
N4	0.2323 (7)	0.4628 (7)	0.4921 (4)	0.0526 (15)
H4A	0.1822	0.4993	0.4462	0.063*
C9	0.2500 (13)	0.2136 (11)	0.4902 (7)	0.076 (3)
C10	0.2768 (8)	0.3277 (8)	0.5263 (5)	0.0503 (17)
C11	0.3561 (8)	0.4384 (9)	0.6076 (5)	0.0516 (18)
C12	0.4205 (10)	0.4786 (14)	0.6680 (6)	0.079 (3)
H12	0.4753	0.4119	0.7117	0.095*
C13	0.3997 (13)	0.6218 (17)	0.6601 (8)	0.097 (4)
H13	0.4396	0.6534	0.7008	0.116*
C14	0.3236 (14)	0.7196 (14)	0.5960 (9)	0.098 (4)
H14	0.3153	0.8155	0.5935	0.117*
C15	0.2581 (11)	0.6842 (10)	0.5344 (7)	0.072 (2)
H15	0.2037	0.7525	0.4912	0.086*
C16	0.2792 (9)	0.5380 (9)	0.5415 (5)	0.0524 (18)
Hg2	0.11556 (4)	0.82505 (3)	0.24321 (2)	0.05631 (13)
Cl1	0.0685 (3)	0.6016 (2)	0.32320 (13)	0.0606 (5)
Cl2	0.3673 (3)	0.7252 (2)	0.11954 (14)	0.0653 (5)
Cl3	-0.1015 (4)	0.9354 (3)	0.1548 (2)	0.1100 (11)
Cl4	0.1746 (4)	0.9720 (3)	0.32658 (19)	0.1004 (9)
O1	0.2620 (9)	0.0518 (6)	1.0084 (5)	0.099 (2)
H1C	0.3067	0.0060	0.9601	0.148*
H1B	0.2751	-0.0072	1.0576	0.148*
O2	0.4458 (11)	0.0872 (10)	0.7187 (7)	0.166 (4)
H2B	0.5002	0.0086	0.6939	0.249*
H2D	0.3630	0.0783	0.7558	0.249*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F1	0.066 (7)	0.132 (15)	0.054 (7)	-0.020 (8)	-0.006 (5)	0.016 (7)
F2	0.085 (14)	0.187 (19)	0.124 (17)	-0.076 (13)	-0.071 (14)	0.047 (14)
F3	0.130 (16)	0.066 (9)	0.099 (9)	0.029 (8)	-0.054 (10)	0.000 (7)
F1'	0.11 (3)	0.20 (3)	0.055 (12)	0.015 (19)	-0.030 (13)	-0.034 (13)
F3'	0.15 (3)	0.16 (3)	0.21 (4)	-0.10 (2)	-0.13 (3)	0.13 (3)
F2'	0.041 (8)	0.17 (3)	0.056 (9)	-0.001 (11)	-0.007 (7)	0.001 (12)
N1	0.040 (3)	0.054 (4)	0.053 (3)	-0.023 (3)	-0.011 (3)	-0.007 (3)
N2	0.037 (3)	0.032 (3)	0.061 (4)	-0.011 (2)	-0.009 (3)	0.001 (3)
C1	0.060 (6)	0.069 (6)	0.057 (5)	-0.020 (5)	-0.013 (4)	0.007 (5)
C2	0.031 (4)	0.050 (4)	0.050 (4)	-0.016 (3)	-0.002 (3)	-0.002 (3)
C3	0.031 (3)	0.037 (4)	0.047 (4)	-0.011 (3)	-0.001 (3)	-0.009 (3)
C4	0.046 (4)	0.048 (4)	0.067 (5)	-0.024 (4)	-0.005 (4)	-0.007 (4)
C5	0.053 (5)	0.047 (4)	0.054 (4)	-0.017 (4)	-0.008 (4)	0.004 (4)
C6	0.037 (4)	0.069 (5)	0.054 (4)	-0.022 (4)	-0.002 (3)	-0.005 (4)
C7	0.039 (4)	0.051 (4)	0.050 (4)	-0.019 (3)	-0.002 (3)	-0.016 (3)
C8	0.028 (3)	0.039 (3)	0.045 (4)	-0.014 (3)	0.002 (3)	-0.006 (3)
F4	0.238 (10)	0.076 (4)	0.153 (6)	-0.092 (5)	-0.050 (6)	0.011 (4)
F5	0.130 (6)	0.189 (8)	0.213 (9)	-0.090 (6)	0.056 (6)	-0.144 (7)
F6	0.119 (5)	0.108 (5)	0.188 (7)	-0.048 (4)	-0.078 (5)	-0.035 (5)
N3	0.041 (4)	0.063 (4)	0.059 (4)	-0.012 (3)	-0.014 (3)	0.013 (3)

N4	0.057 (4)	0.065 (4)	0.044 (3)	-0.031 (3)	-0.017 (3)	0.005 (3)
C9	0.078 (7)	0.074 (6)	0.085 (7)	-0.035 (5)	-0.005 (6)	-0.022 (6)
C10	0.037 (4)	0.054 (4)	0.055 (4)	-0.014 (3)	-0.010 (3)	0.003 (4)
C11	0.038 (4)	0.080 (5)	0.040 (4)	-0.027 (4)	-0.006 (3)	0.002 (4)
C12	0.047 (5)	0.137 (10)	0.056 (5)	-0.038 (6)	0.000 (4)	-0.015 (6)
C13	0.080 (8)	0.163 (13)	0.074 (7)	-0.069 (8)	0.011 (6)	-0.055 (8)
C14	0.100 (9)	0.119 (9)	0.101 (8)	-0.078 (8)	0.019 (7)	-0.040 (8)
C15	0.065 (6)	0.079 (6)	0.075 (6)	-0.037 (5)	-0.003 (5)	-0.008 (5)
C16	0.044 (4)	0.067 (5)	0.054 (4)	-0.032 (4)	-0.004 (4)	-0.007 (4)
Hg2	0.0667 (2)	0.0587 (2)	0.05325 (19)	-0.03158 (16)	-0.01580 (15)	-0.00235 (14)
Cl1	0.0810 (14)	0.0633 (12)	0.0535 (11)	-0.0420 (11)	-0.0290 (10)	0.0135 (9)
Cl2	0.0645 (13)	0.0756 (13)	0.0635 (12)	-0.0374 (11)	0.0002 (10)	-0.0144 (11)
Cl3	0.133 (3)	0.0746 (16)	0.155 (3)	-0.0507 (17)	-0.103 (2)	0.0420 (17)
Cl4	0.158 (3)	0.0916 (18)	0.0906 (17)	-0.0746 (19)	-0.0426 (18)	-0.0120 (15)
O1	0.142 (7)	0.050 (3)	0.112 (5)	-0.033 (4)	-0.048 (5)	0.006 (4)
O2	0.122 (7)	0.135 (7)	0.152 (8)	0.018 (6)	-0.038 (6)	0.076 (7)

*Geometric parameters (Å, °)*

F1—C1	1.308 (2)	N3—C10	1.308 (9)
F2—C1	1.309 (2)	N3—C11	1.375 (10)
F3—C1	1.309 (2)	N3—H3A	0.8599
F1'—C1	1.309 (2)	N4—C10	1.300 (9)
F3'—C1	1.309 (2)	N4—C16	1.376 (9)
F2'—C1	1.309 (2)	N4—H4A	0.8601
N1—C2	1.317 (9)	C9—C10	1.469 (11)
N1—C3	1.386 (8)	C11—C16	1.377 (10)
N1—H1A	0.8600	C11—C12	1.374 (12)
N2—C2	1.318 (8)	C12—C13	1.361 (15)
N2—C8	1.357 (8)	C12—H12	0.9300
N2—H2A	0.8600	C13—C14	1.347 (16)
C1—C2	1.453 (10)	C13—H13	0.9300
C3—C4	1.371 (9)	C14—C15	1.368 (14)
C3—C8	1.395 (8)	C14—H14	0.9300
C4—C5	1.390 (10)	C15—C16	1.391 (11)
C4—H4	0.9300	C15—H15	0.9300
C5—C6	1.395 (10)	Hg2—C14	2.364 (2)
C5—H5	0.9300	Hg2—C13	2.455 (3)
C6—C7	1.350 (10)	Hg2—C11	2.4734 (19)
C6—H6	0.9300	Hg2—C12	2.564 (2)
C7—C8	1.377 (9)	O1—H1C	0.8500
C7—H7	0.9300	O1—H1B	0.8500
F4—C9	1.274 (11)	O2—H2B	0.8500
F5—C9	1.274 (11)	O2—H2D	0.8500
F6—C9	1.281 (11)		
C2—N1—C3	107.7 (6)	N2—C8—C3	106.5 (6)
C2—N1—H1A	126.1	C7—C8—C3	120.8 (6)
C3—N1—H1A	126.2	C10—N3—C11	108.6 (6)
C2—N2—C8	108.9 (6)	C10—N3—H3A	125.8

C2—N2—H2A	125.6	C11—N3—H3A	125.7
C8—N2—H2A	125.5	C10—N4—C16	108.4 (6)
F1—C1—F2'	127.4 (10)	C10—N4—H4A	125.9
F1—C1—F3'	68.6 (15)	C16—N4—H4A	125.7
F2'—C1—F3'	109.5 (15)	F4—C9—F5	107.8 (10)
F1—C1—F3	106.1 (10)	F4—C9—F6	107.4 (9)
F2'—C1—F3	70.4 (12)	F5—C9—F6	105.6 (10)
F1—C1—F2	104.5 (11)	F4—C9—C10	112.6 (9)
F3'—C1—F2	135.0 (11)	F5—C9—C10	110.9 (8)
F3—C1—F2	105.9 (12)	F6—C9—C10	112.3 (8)
F2'—C1—F1'	103.1 (16)	N4—C10—N3	110.6 (7)
F3'—C1—F1'	107.4 (18)	N4—C10—C9	124.1 (8)
F3—C1—F1'	134.0 (13)	N3—C10—C9	125.2 (8)
F2—C1—F1'	68.8 (14)	N3—C11—C16	105.9 (6)
F1—C1—C2	113.7 (8)	N3—C11—C12	132.9 (9)
F2'—C1—C2	115.1 (9)	C16—C11—C12	121.2 (9)
F3'—C1—C2	111.0 (9)	C13—C12—C11	116.1 (10)
F3—C1—C2	113.6 (7)	C13—C12—H12	121.9
F2—C1—C2	112.1 (7)	C11—C12—H12	121.9
F1'—C1—C2	110.1 (9)	C14—C13—C12	122.8 (10)
N1—C2—N2	110.7 (6)	C14—C13—H13	118.6
N1—C2—C1	125.2 (6)	C12—C13—H13	118.6
N2—C2—C1	124.1 (6)	C13—C14—C15	123.0 (11)
C4—C3—N1	130.9 (6)	C13—C14—H14	118.5
C4—C3—C8	122.9 (6)	C15—C14—H14	118.5
N1—C3—C8	106.2 (6)	C14—C15—C16	114.7 (10)
C3—C4—C5	116.0 (6)	C14—C15—H15	122.6
C3—C4—H4	122.0	C16—C15—H15	122.6
C5—C4—H4	122.0	C11—C16—N4	106.5 (7)
C4—C5—C6	120.1 (7)	C11—C16—C15	122.1 (8)
C4—C5—H5	119.9	N4—C16—C15	131.4 (8)
C6—C5—H5	119.9	C14—Hg2—C13	119.35 (10)
C7—C6—C5	123.8 (7)	C14—Hg2—C11	120.36 (8)
C7—C6—H6	118.1	C13—Hg2—C11	102.26 (8)
C5—C6—H6	118.1	C14—Hg2—C12	105.49 (10)
C6—C7—C8	116.4 (6)	C13—Hg2—C12	105.13 (11)
C6—C7—H7	121.8	C11—Hg2—C12	102.10 (8)
C8—C7—H7	121.8	H1C—O1—H1B	109.5
N2—C8—C7	132.7 (6)	H2B—O2—H2D	109.5
C3—N1—C2—N2	0.2 (8)	N1—C3—C8—N2	0.0 (7)
C3—N1—C2—C1	-178.8 (6)	C4—C3—C8—C7	-1.7 (10)
C8—N2—C2—N1	-0.2 (8)	N1—C3—C8—C7	-179.9 (6)
C8—N2—C2—C1	178.9 (6)	C16—N4—C10—N3	0.3 (8)
F1—C1—C2—N1	-84.6 (15)	C16—N4—C10—C9	-178.9 (8)
F2'—C1—C2—N1	75.3 (19)	C11—N3—C10—N4	-0.9 (9)
F3'—C1—C2—N1	-160 (2)	C11—N3—C10—C9	178.3 (8)
F3—C1—C2—N1	153.8 (14)	F4—C9—C10—N4	-150.4 (9)
F2—C1—C2—N1	33.7 (19)	F5—C9—C10—N4	88.8 (12)



F1'—C1—C2—N1	-41 (3)	F6—C9—C10—N4	-29.0 (13)
F1—C1—C2—N2	96.5 (14)	F4—C9—C10—N3	30.4 (13)
F2'—C1—C2—N2	-103.6 (17)	F5—C9—C10—N3	-90.4 (12)
F3'—C1—C2—N2	22 (2)	F6—C9—C10—N3	151.8 (9)
F3—C1—C2—N2	-25.1 (14)	C10—N3—C11—C16	1.1 (8)
F2—C1—C2—N2	-145.2 (16)	C10—N3—C11—C12	-178.6 (8)
F1'—C1—C2—N2	140 (2)	N3—C11—C12—C13	-178.5 (8)
C2—N1—C3—C4	-178.1 (7)	C16—C11—C12—C13	1.8 (12)
C2—N1—C3—C8	-0.1 (7)	C11—C12—C13—C14	-1.4 (15)
N1—C3—C4—C5	178.9 (7)	C12—C13—C14—C15	1.3 (17)
C8—C3—C4—C5	1.3 (10)	C13—C14—C15—C16	-1.4 (15)
C3—C4—C5—C6	-0.3 (10)	N3—C11—C16—N4	-0.9 (8)
C4—C5—C6—C7	-0.2 (11)	C12—C11—C16—N4	178.8 (7)
C5—C6—C7—C8	-0.2 (10)	N3—C11—C16—C15	178.1 (7)
C2—N2—C8—C7	180.0 (7)	C12—C11—C16—C15	-2.2 (12)
C2—N2—C8—C3	0.1 (7)	C10—N4—C16—C11	0.4 (8)
C6—C7—C8—N2	-178.8 (7)	C10—N4—C16—C15	-178.5 (8)
C6—C7—C8—C3	1.1 (9)	C14—C15—C16—C11	1.9 (12)
C4—C3—C8—N2	178.2 (6)	C14—C15—C16—N4	-179.5 (8)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1 <i>A</i> ...C12 <sup>i</sup>	0.86	2.23	3.081 (6)	170
N2—H2 <i>A</i> ...O1 <sup>ii</sup>	0.86	1.80	2.656 (8)	174
N3—H3 <i>A</i> ...O2	0.86	1.76	2.608 (9)	166
N4—H4 <i>A</i> ...C11	0.86	2.21	3.069 (6)	175
O1—H1 <i>C</i> ...F3 <sup>iii</sup>	0.85	2.25	2.994 (18)	146
O1—H1 <i>B</i> ...C12 <sup>iv</sup>	0.85	2.55	3.279 (6)	144
O2—H2 <i>B</i> ...F5 <sup>v</sup>	0.85	2.41	3.224 (13)	160
O2—H2 <i>D</i> ...C13 <sup>vi</sup>	0.85	2.50	3.339 (10)	172

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