

## Mercury(II) thiolate complexes of two flexible benzimidazole-based ligands

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Received 17 March 2011

Accepted 3 June 2011

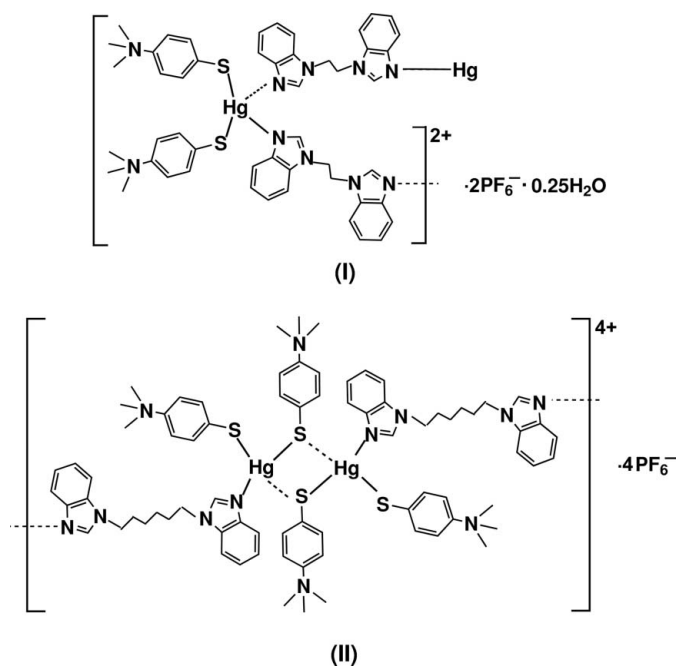
Online 23 June 2011

The structure of *catena*-poly[[[bis[4-(trimethylammonio)benzenethiolate- $\kappa$ S]mercury(II)]- $\mu$ -1,1'-(ethane-1,2-diyl)bis(1*H*-benzimidazole)- $\kappa^2$ N<sup>3</sup>:N<sup>3'</sup>] bis(hexafluoridophosphate) 0.25-hydrate],  $\{[\text{Hg}(\text{C}_{16}\text{H}_{14}\text{N}_4)(\text{C}_9\text{H}_{13}\text{NS})_2](\text{PF}_6)_2 \cdot 0.25\text{H}_2\text{O}\}_n$ , contains a one-dimensional zigzag chain. The Hg<sup>II</sup> cation is coordinated by two S atoms of two 4-(trimethylammonio)benzenethiolate (Tab) ligands and by two N atoms from two different 1,1'-(ethane-1,2-diyl)bis(1*H*-benzimidazole) ligands, forming a distorted seesaw-shaped coordination geometry. The F atoms of the hexafluoridophosphate anion interact with the H atoms of the Tab ligand, generating a two-dimensional network. Furthermore, this layer is connected to neighbouring layers *via* H $\cdots\pi$  interactions, thereby forming a three-dimensional hydrogen-bonded structure. In *catena*-poly[[[4-(trimethylammonio)benzenethiolate- $\kappa$ S]mercury(II)]bis[ $\mu$ -4-(trimethylammonio)benzenethiolate- $\kappa^2$ S:S][[4-(trimethylammonio)benzenethiolate- $\kappa$ S]mercury(II)]- $\mu$ -1,1'-(hexane-1,6-diyl)bis(1*H*-benzimidazole)- $\kappa^2$ N<sup>3</sup>:N<sup>3'</sup>] tetrakis(hexafluoridophosphate)],  $\{[\text{Hg}_2(\text{C}_{20}\text{H}_{22}\text{N}_4)(\text{C}_9\text{H}_{13}\text{NS})_4](\text{PF}_6)_4\}_n$ , each Hg<sup>II</sup> cation is coordinated by two S atoms of two Tab ligands and one N atom of the 1,1'-(hexane-1,6-diyl)bis(1*H*-benzimidazole) (hbbm) ligand, forming a distorted T-shaped coordination geometry, while longer secondary Hg $\cdots$ S bonds join two such units across a centre of inversion to give the tetravalent cation. Adjacent  $\{[\text{Hg}(\text{Tab})_2(\mu\text{-hbbm})]^{4+}$  cations are linked through the centrosymmetric hbbm ligands to afford a one-dimensional chain extending along the *b* axis. Several F atoms interact with the H atoms of the Tab and hbbm ligands, while the S atom interacts with an aromatic H atom of a different Tab ligand, to afford a complex intra- and intermolecular hydrogen-bonding arrangement in a three-dimensional structure.

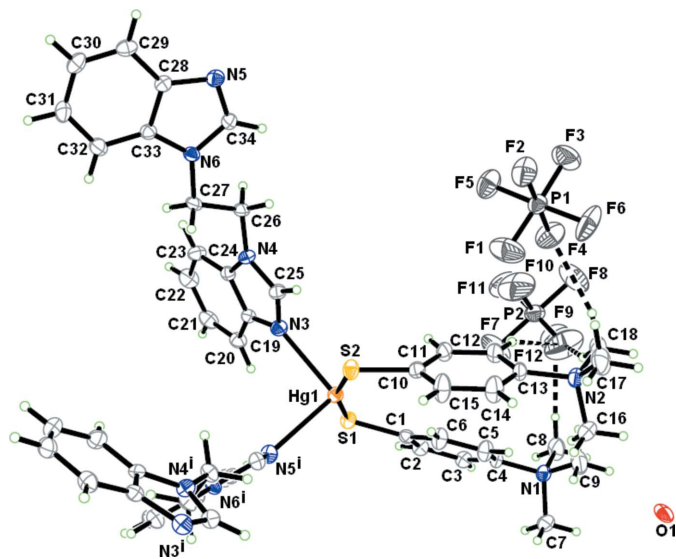
## Comment

In previous studies (Chen *et al.*, 2006), we employed  $[\text{Hg}(\text{Tab})_2](\text{PF}_6)_2$  [Tab is 4-(trimethylammonio)benzenethiolate]

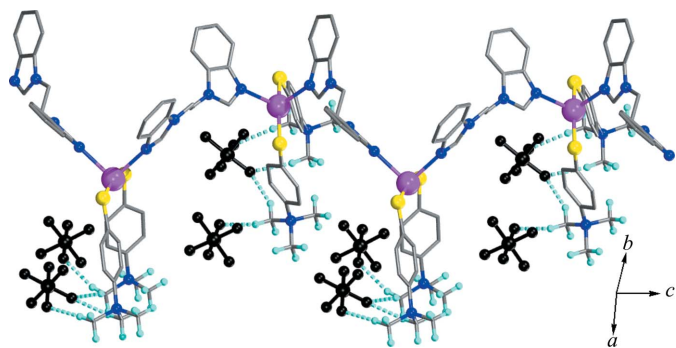
as a potential model complex for mimicking the reactivity of unsaturated HgS<sub>2</sub> sites in the detoxification of mercury by metallothioneins (MTs) (Stillman *et al.*, 1983; Cheesman *et al.*, 1988; Fleischer *et al.*, 2005; Baba *et al.*, 2008; Vig *et al.*, 2003), in DNA-binding proteins (Patra & Goldberg, 2002; Henkel & Krebs, 2004), in mercury reductase and organomercury lyase (Bharara *et al.*, 2005, 2006; Chan *et al.*, 2002; Qian *et al.*, 1998), and in metalleregulatory protein (MerR) (Moore *et al.*, 1990; Ralston & O'Halloran, 1990; Gruff & Koch, 1990; Helmann *et al.*, 1990; Govindaswamy *et al.*, 1992). The chemistry of  $[\text{Hg}(\text{Tab})_2](\text{PF}_6)_2$  was analysed with some donor ligands (*e.g.* Tab, NCS<sup>-</sup> and I<sup>-</sup>), naturally encountered inorganic anions (*e.g.* Cl<sup>-</sup>, NO<sub>2</sub><sup>-</sup> and NO<sub>3</sub><sup>-</sup>), organic amines and N-heterocyclic compounds [*e.g.* ethane-1,2-diamine, pyridine, 1,10-phenanthroline (phen) and *N*-methylimidazole] (Tang *et al.*, 2009), and various carboxylic acids and amino acids (*e.g.* acetic, salicylic and oxalic acids) (Tang *et al.*, 2011). However, most of these mercury thiolate compounds are monomeric and only a few are coordination polymers. As an extension of this work, we undertook reactions of  $[\text{Hg}(\text{Tab})_2](\text{PF}_6)_2$  with two bridging ligands, namely 1,1'-(ethane-1,2-diyl)bis(1*H*-benzimidazole) (ebbm) and 1,1'-(hexane-1,6-diyl)bis(1*H*-benzimidazole) (hbbm), and the two title Hg–Tab coordination polymers, (I) and (II), were isolated therefrom. Here, we report the crystal structures of complexes (I) and (II).



The asymmetric unit of (I) contains an  $[\text{Hg}(\text{Tab})_2(\text{ebbm})]^{2+}$  cation (Fig. 1), two  $\text{PF}_6^-$  anions and a partial-occupancy (0.25) solvent water molecule. The Hg<sup>II</sup> centre in this cation is coordinated by two S atoms from the Tab ligands and by two N atoms from two different ebbm ligands, displaying a seesaw-shaped coordination geometry. Each  $[\text{Hg}(\text{Tab})_2]$  unit is linked by a pair of ebbm ligands to form a one-dimensional zigzag chain extending along the *c*-axis direction (Fig. 2). Relative to the *trans* configuration of  $[\text{Hg}(\text{Tab})_2](\text{PF}_6)_2$ , the two Tab



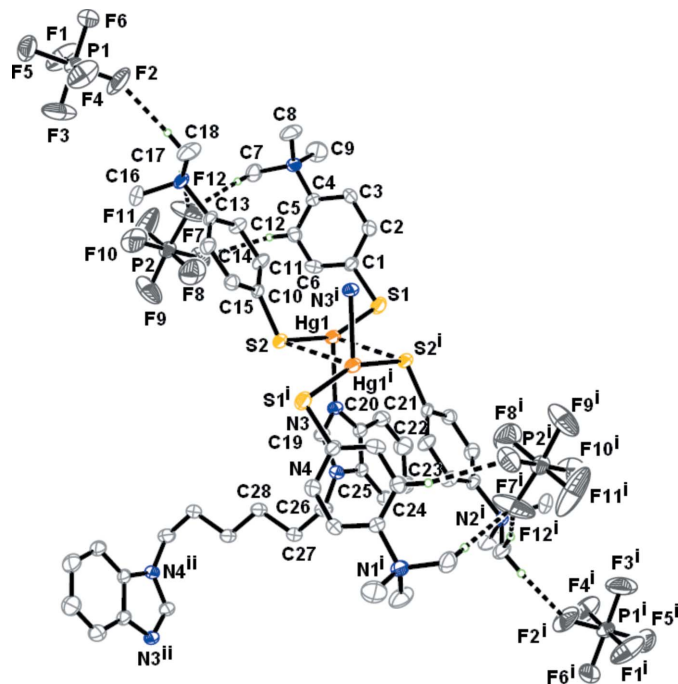
**Figure 1**  
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i)  $x, -y + \frac{3}{2}, z + \frac{1}{2}$ .]



**Figure 2**  
A view of a section of the one-dimensional chain of (I), extending along the  $c$ -axis direction. Dashed lines indicate C—H $\cdots$ F hydrogen bonds.

ligands in (I) are oriented in the same direction, with a dihedral angle between the phenyl groups of  $37.9(3)^\circ$ . The mean Hg—S bond length [2.3761 (17) Å; Table 1] is comparable with that in [Hg(Tab)<sub>2</sub>(Ac)](PF<sub>6</sub>) $\cdot$ 0.5H<sub>2</sub>O [Ac is acetyl; 2.3752 (19) Å; Tang *et al.*, 2011], but slightly longer than those in [Hg(Tab)<sub>2</sub>](PF<sub>6</sub>)<sub>2</sub> and [Hg(Tab)<sub>2</sub>(phen)](PF<sub>6</sub>)<sub>2</sub> [2.331 (3) and 2.344 (3) Å, respectively; Tang *et al.*, 2009]. The average Hg—N bond length [2.543 (6) Å] is longer than those observed in [Hg(L)(SCN)<sub>2</sub>] [2.421 (2) Å; *L* is 1,4-bis(4-pyridyl)-2,3-diaza-1,3-butadiene; Mahmoudi *et al.*, 2007] and [HgI<sub>2</sub>(L) $\cdot$ 1.5MeOH]<sub>*n*</sub> [2.418 (7) Å; *L* is *N,N'*-bis(4-pyridyl)-1,4-benzenedicarboxamide; Li *et al.*, 2005]. The S—Hg—S angle in (I) [160.72 (6) $^\circ$ ] deviates significantly from the linear S—Hg—S angle in [Hg(Tab)<sub>2</sub>](PF<sub>6</sub>)<sub>2</sub>. The N—Hg—N angle of 94.61 (17) $^\circ$  is comparable with that in [Hg(L)(SCN)<sub>2</sub>]<sub>*n*</sub> [93.76 (10) $^\circ$ ; *L* is 1,4-bis(3-pyridyl)-2,3-diaza-1,3-butadiene; Mahmoudi *et al.*, 2007].

In (I), the F atoms of the PF<sub>6</sub><sup>−</sup> anions in one chain interact with the methyl H atoms of the Tab ligands in the same and in neighbouring chains and afford a two-dimensional network

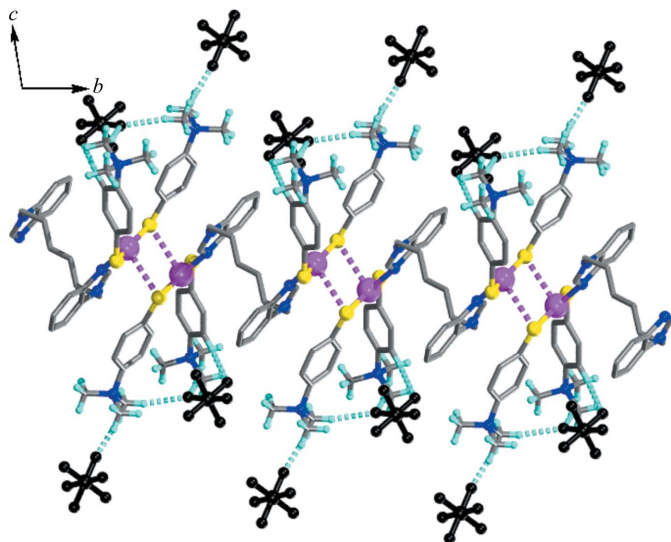


**Figure 3**  
The molecular structure of (II), with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i)  $-x + 2, -y + 1, -z + 2$ ; (ii)  $-x + 3, -y + 2, -z + 2$ .]

(Table 2). Furthermore, this layer is connected to neighbouring layers *via* H $\cdots$  $\pi$  interactions [H2A $\cdots$ Cg( $-x + 1, -y + 2, -z + 2$ ) = 2.63 Å, where Cg is the centroid of the N5/C28/C33/N6/C34 ring], thereby completing a three-dimensional hydrogen-bonded network (Table 2).

The asymmetric unit of (II) comprises half a {[Hg(Tab)<sub>2</sub>]<sub>2</sub>( $\mu$ -hbbm)}<sup>4+</sup> cation and two PF<sub>6</sub><sup>−</sup> anions. Each Hg<sup>II</sup> cation is coordinated by two S atoms of two Tab ligands and one N atom of the 1,1'-(hexane-1,6-diyl)bis(1H-benzimidazole) (hbbm) ligand, forming a distorted T-shaped coordination geometry, while longer secondary Hg $\cdots$ S bonds join two such units across a centre of inversion to give the tetravalent cation. Adjacent {[Hg(Tab)<sub>2</sub>]<sub>2</sub>( $\mu$ -hbbm)}<sup>4+</sup> units are linked through the centrosymmetric hbbm ligands to afford a one-dimensional chain extending along the  $b$  axis (Fig. 4). Therefore, each Hg<sup>II</sup> centre in (II) may be viewed as having a pseudo-four-coordinated pinwheel-shaped geometry. Similar to (I), the two Tab ligands of (II) are also in a *cis* configuration, with a dihedral angle between the two Tab-ligand phenyl groups of  $77.4(3)^\circ$ . The mean Hg—S bond length in (II) [2.3813 (16) Å] is slightly longer than that in (I), while the Hg—N bond length [2.362 (4) Å] is much shorter than that observed in (I). The secondary Hg $\cdots$ S separation [3.1325 (16) Å] is intermediate between that observed in [Hg(Tab)<sub>2</sub>(N<sup>*i*</sup>Prim)](PF<sub>6</sub>)<sub>2</sub> [2.805 (5) Å; N<sup>*i*</sup>Prim is *N*-isopropylimidazole; Tang *et al.*, 2009] and that in [Hg(SCH<sub>2</sub>COOH)<sub>2</sub>] [3.379 (3) Å; Bramlett *et al.*, 2004]. The S—Hg—S angle in (II) [156.38 (6) $^\circ$ ] is smaller than that in (I).

In (II), because the PF<sub>6</sub><sup>−</sup> anions are located between the chains (Fig. 4), several F atoms interact with the H atoms of



**Figure 4**  
A view of a section of the one-dimensional chain in (II), extending along the *b*-axis direction, formed by secondary Hg...S interactions. Dashed lines indicate C—H...F hydrogen bonds and the secondary Hg—S bonds.

the Tab and hbbm ligands and the S atom of the Tab ligand interacts with a H atom of a neighbouring Tab ligand. These interactions generate a three-dimensional network overall (Table 3).

## Experimental

To a solution of [Hg(Tab)<sub>2</sub>](PF<sub>6</sub>)<sub>2</sub> (0.082 g, 0.1 mmol) in MeCN (5 ml) was added a solution of ebbm (0.013 g, 0.05 mmol) in MeOH (2 ml). The resulting mixture was stirred for 1 h to form a colourless solution and was then filtered. Diethyl ether (20 ml) was layered onto the filtrate and colourless prisms of [Hg(Tab)<sub>2</sub>(ebbm)](PF<sub>6</sub>)<sub>2</sub>·0.25H<sub>2</sub>O, (I), formed after several days. These were collected by filtration, washed with Et<sub>2</sub>O and dried *in vacuo* (yield 0.092 g, 85.0% based on Hg). Analysis found: C 37.32, H 3.70, N 7.58%; calculated for C<sub>34</sub>H<sub>40.5</sub>F<sub>12</sub>HgN<sub>6</sub>O<sub>0.25</sub>P<sub>2</sub>S<sub>2</sub>: C 37.40, H 3.75, N 7.70%. IR (KBr,  $\nu$ , cm<sup>-1</sup>): 1615 (*w*), 1492 (*m*), 956 (*m*), 840 (*s*).

To a solution of [Hg(Tab)<sub>2</sub>](PF<sub>6</sub>)<sub>2</sub> (0.082 g, 0.1 mmol) in MeCN (5 ml) was added a solution of hbbm (0.016 g, 0.05 mmol) in MeOH (2 ml). The resulting mixture was stirred for 1 h to form a colourless solution and was then filtered. Diethyl ether (20 ml) was layered onto the filtrate and colourless prisms of {[Hg(Tab)<sub>2</sub>]<sub>2</sub>( $\mu$ -hbbm)}(PF<sub>6</sub>)<sub>4</sub>, (II), formed after several days. These were collected by filtration, washed with Et<sub>2</sub>O and dried *in vacuo* (yield 0.044 g, 89.0% based on Hg). Analysis found: C 34.45, H 3.72, N 5.43%; calculated for C<sub>28</sub>H<sub>37</sub>F<sub>12</sub>HgN<sub>4</sub>P<sub>2</sub>S<sub>2</sub>: C 34.17, H 3.80, N 5.69%. IR (KBr,  $\nu$ , cm<sup>-1</sup>): 1614 (*w*), 1490 (*m*), 958 (*m*), 837 (*s*).

## Compound (I)

### Crystal data

[Hg(C <sub>16</sub> H <sub>14</sub> N <sub>4</sub> )(C <sub>9</sub> H <sub>13</sub> NS) <sub>2</sub> ](PF <sub>6</sub> ) <sub>2</sub> ·0.25H <sub>2</sub> O	$\beta = 97.14 (3)^\circ$
$M_r = 1091.87$	$V = 4034.9 (14) \text{ \AA}^3$
Monoclinic, $P2_1/c$	$Z = 4$
$a = 19.589 (4) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 12.808 (3) \text{ \AA}$	$\mu = 4.09 \text{ mm}^{-1}$
$c = 16.207 (3) \text{ \AA}$	$T = 223 \text{ K}$
	$0.30 \times 0.15 \times 0.10 \text{ mm}$

**Table 1**  
Selected bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) for (I) and (II).

	(I)	(II)
Hg1—S1	2.3698 (16)	2.3617 (16)
Hg1—S2	2.3816 (16)	2.4010 (16)
Hg1—N3	2.533 (5)	2.362 (4)
Hg1—N5 <sup>i</sup>	2.554 (6)	
S1—Hg1—S2	160.72 (6)	156.38 (6)
S1—Hg1—N3	98.10 (13)	110.36 (12)
S2—Hg1—N3	95.32 (13)	93.26 (12)

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

### Data collection

Rigaku Mercury CCD area-detector diffractometer	22845 measured reflections
Absorption correction: multi-scan (REQAB; Jacobson, 1998)	9195 independent reflections
$T_{\min} = 0.373, T_{\max} = 0.685$	7542 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.045$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$	523 parameters
$wR(F^2) = 0.119$	H-atom parameters constrained
$S = 1.07$	$\Delta\rho_{\max} = 1.65 \text{ e \AA}^{-3}$
9195 reflections	$\Delta\rho_{\min} = -1.18 \text{ e \AA}^{-3}$

## Compound (II)

### Crystal data

[Hg <sub>2</sub> (C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> )(C <sub>9</sub> H <sub>13</sub> NS) <sub>4</sub> ](PF <sub>6</sub> ) <sub>4</sub>	$\gamma = 94.05 (3)^\circ$
$M_r = 1968.58$	$V = 1804.7 (6) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 1$
$a = 9.871 (2) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.364 (2) \text{ \AA}$	$\mu = 4.56 \text{ mm}^{-1}$
$c = 18.078 (4) \text{ \AA}$	$T = 223 \text{ K}$
$\alpha = 98.39 (3)^\circ$	$0.45 \times 0.20 \times 0.15 \text{ mm}$
$\beta = 97.85 (3)^\circ$	

### Data collection

Rigaku Mercury CCD area-detector diffractometer	15125 measured reflections
Absorption correction: multi-scan (REQAB; Jacobson, 1998)	6337 independent reflections
$T_{\min} = 0.234, T_{\max} = 0.548$	5615 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.045$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$	442 parameters
$wR(F^2) = 0.092$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{\max} = 1.04 \text{ e \AA}^{-3}$
6337 reflections	$\Delta\rho_{\min} = -0.85 \text{ e \AA}^{-3}$

For (I), the occupancy factor of the partial-occupancy solvent water molecule was fixed at 0.25. The two H atoms of this water molecule were not located. All other H atoms were placed in geometrically idealized positions, with C—H = 0.98  $\text{\AA}$  for methyl groups, 0.99  $\text{\AA}$  for methylene groups and 0.95  $\text{\AA}$  for aromatic groups, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic and methylene groups or  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl groups.

For both compounds, data collection: *CrystalClear* (Rigaku/MS, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97*

**Table 2**

Hydrogen-bond geometry (Å, °) for (I).

<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>
C7—H7A...F10 <sup>i</sup>	0.97	2.42	3.380 (12)	170
C9—H9C...F8 <sup>i</sup>	0.97	2.55	3.508 (12)	169
C8—H8A...F12	0.97	2.41	3.379 (12)	177
C9—H9A...F9	0.97	2.49	3.452 (12)	171
C16—H16C...F2 <sup>ii</sup>	0.97	2.53	3.462 (10)	160
C17—H17A...F9	0.97	2.39	3.286 (10)	153
C17—H17C...F4	0.97	2.43	3.363 (10)	162
C18—H18C...F12 <sup>iii</sup>	0.97	2.52	3.431 (11)	156

 Symmetry codes: (i)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (ii)  $-x + 2, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (iii)  $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$ .

(Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the NSNF of China (grant Nos. 20871088, 20901054 and 90922018), the Fund for Natural Science Key Basic Research of Jiangsu Province for Higher Education (grant No. 09KJA150002), the Specialized Research Fund for the Doctoral Programme of Higher Education of the Ministry of Education (grant No. 20093201110017), the State Key Laboratory of Coordination Chemistry of Nanjing University, the Qin-Lan and '333' Projects of Jiangsu Province, and the 'Soochow Scholar' Programme and the Programme for Innovative Research Team of Soochow University.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GG3258). Services for accessing these data are described at the back of the journal.

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**Table 3**

Hydrogen-bond geometry (Å, °) for (II).

<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>
C3—H3A...S2 <sup>i</sup>	0.94	2.83	3.564 (5)	136
C5—H5A...F7	0.94	2.49	3.387 (6)	160
C7—H7C...F12	0.97	2.35	3.296 (8)	166
C17—H17A...F12	0.97	2.39	3.341 (8)	165
C17—H17C...F2	0.97	2.31	3.260 (7)	165
C8—H8B...F11 <sup>ii</sup>	0.97	2.46	3.112 (9)	124
C17—H17B...F6 <sup>iii</sup>	0.97	2.34	3.294 (7)	167
C26—H26B...F6 <sup>iv</sup>	0.98	2.50	3.470 (7)	170

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

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