



# Crystal structure of *cyclo*-tris( $\mu$ -3,4,5,6-tetrafluoro-*o*-phenylene- $\kappa^2$ C<sup>1</sup>:C<sup>2</sup>)trimercury–tetracyanoethylene (1/1)

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**Keywords:** crystal structure; trimeric perfluoro-*o*-phenylene mercury; tetracyanoethylene; complexation; X-ray diffraction; TGA

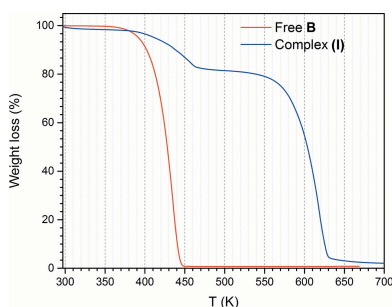
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The title compound, [Hg<sub>3</sub>(C<sub>6</sub>F<sub>4</sub>)<sub>3</sub>] $\cdot$ C<sub>6</sub>N<sub>4</sub>, contains one molecule of tetracyanoethylene **B** per one molecule of mercury macrocycle **A**, *i.e.*, **A** $\cdot$ **B**, and crystallizes in the monoclinic space group *C2/c*. Macrocycle **A** and molecule **B** both occupy special positions on a twofold rotation axis and the inversion centre, respectively. The supramolecular unit [**A** $\cdot$ **B**] is built by the simultaneous coordination of one of the nitrile N atoms of **B** to the three mercury atoms of the macrocycle **A**. The Hg $\cdot$  $\cdot$  $\cdot$ N distances range from 2.990 (4) to 3.030 (4) Å and are very close to those observed in the related adducts of the macrocycle **A** with other nitrile derivatives. The molecule of **B** is almost perpendicular to the mean plane of the macrocycle **A** at the dihedral angle of 88.20 (5)°. The donor–acceptor Hg $\cdot$  $\cdot$  $\cdot$ N interactions do not affect the C $\equiv$ N bond lengths [1.136 (6) and 1.140 (6) Å]. The *trans* nitrile group of **B** coordinates to another macrocycle **A**, forming an infinite mixed-stack [**A** $\cdot$ **B**] $_{\infty}$  architecture toward [101]. The remaining N atoms of two nitrile groups of **B** are not engaged in any donor–acceptor interactions. In the crystal, the mixed stacks are held together by intermolecular C–F $\cdot$  $\cdot$  $\cdot$ C $\equiv$ N secondary interactions [2.846 (5)–2.925 (5) Å].

## 1. Chemical context

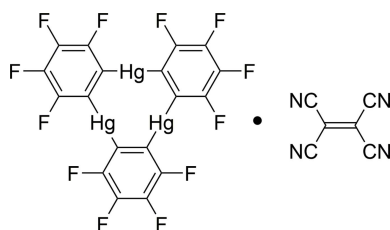
Trimeric perfluoro-*o*-phenylene mercury (**A**) is a versatile Lewis acid that is applied for complexation with different substrates, in particular, for the obtaining of charge-transfer complexes based on donor–acceptor intermolecular interactions (Hasegawa *et al.*, 2004). Importantly, some physical properties of the guest substrates can change upon complexation. For example, unusual optical properties of the organic molecules in supramolecular complexes with macrocycle **A** have previously been observed (Haneline *et al.*, 2002; Elbjairami *et al.*, 2007; Filatov *et al.*, 2009, 2011). Moreover, using complexation with **A**, the stabilization of different organic (diphenylpolyyenes; Taylor & Gabbai, 2006; Taylor *et al.*, 2008) and metal-organic (nickelocene; Haneline & Gabbai, 2004a) molecules was achieved under ambient conditions. In this paper, a complex of **A** with tetracyanoethylene (**B**) – an unstable dienophilic ( $\sigma$ -electron donor and  $\pi$ -electron acceptor) compound – [Hg<sub>3</sub>(C<sub>6</sub>F<sub>4</sub>)<sub>3</sub>] $\cdot$ C<sub>6</sub>N<sub>4</sub>, (**I**), was prepared and studied by X-ray diffraction analysis to get a deeper understanding of the complexation process.



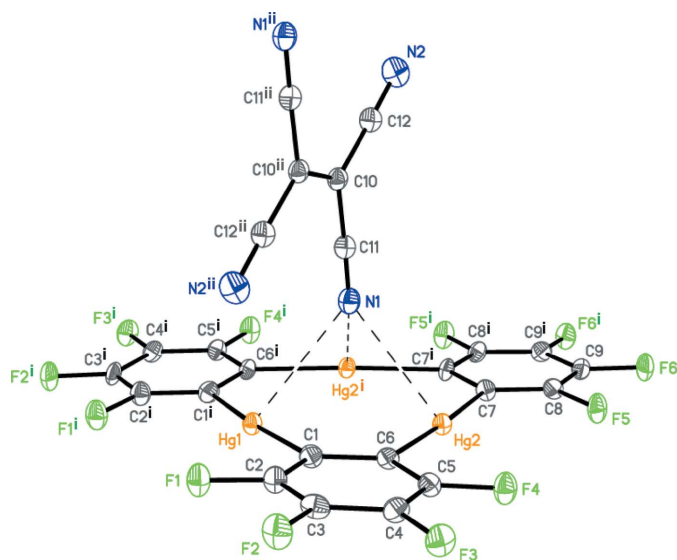
## 2. Structural commentary

Complex (**I**) contains one molecule of tetracyanoethylene **B** per one molecule of the mercury macrocycle **A**, *i.e.*, C<sub>18</sub>F<sub>12</sub>Hg<sub>3</sub> $\cdot$ C<sub>6</sub>N<sub>4</sub> (**A** $\cdot$ **B**), and crystallizes in the monoclinic

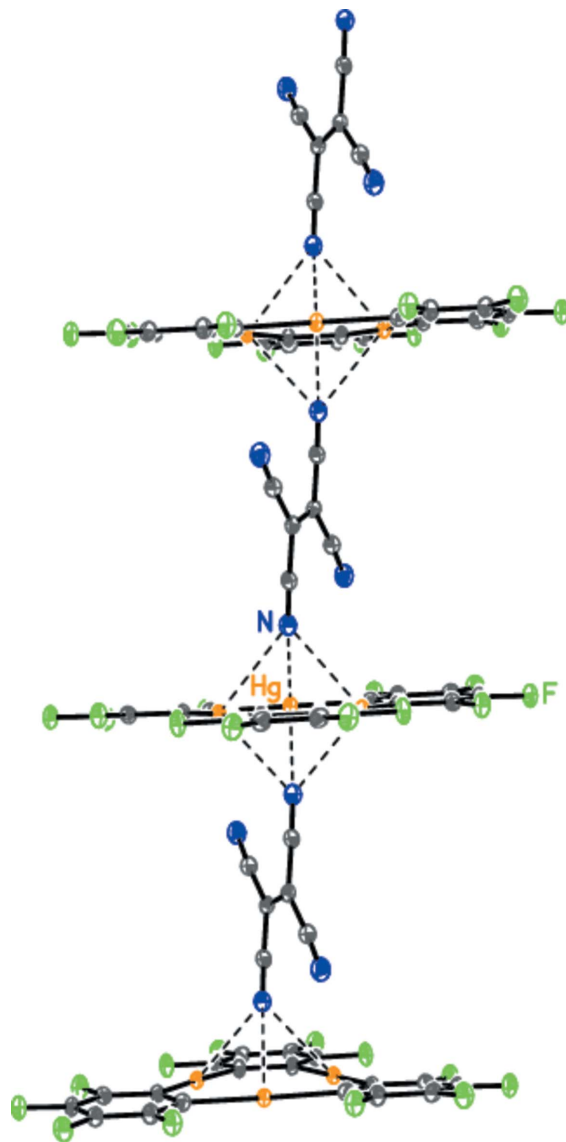
space group  $C2/c$ . Both macrocycle **A** and the molecule of **B** occupy special positions on a twofold rotation axis and inversion centre, respectively. The supramolecular unit of (**I**) is built by the simultaneous coordination of the nitrile N1 nitrogen atom of **B** to the three mercury atoms of the macrocycle **A** (Fig. 1). The Hg $\cdots$ N distances range from 2.990 (4) to 3.030 (4) Å and are very close to those observed in related adducts of macrocycle **A** with other nitrile derivatives: acetonitrile [2.93 (1)–2.99 (1) Å], acrylonitrile [2.87 (1)–2.96 (1) Å] and benzonitrile [2.97 (1)–3.13 (1) Å] (Tikhonova *et al.*, 2000) and 7,7,8,8-tetracyanoquinodimethane (**II**) [3.102 (11)–3.134 (11) Å] (Haneline & Gabbai, 2004*b*). Thus, the N1 nitrogen atom is essentially equidistant to the three Lewis acidic sites of the macrocycle **A**. The molecule of **B** is almost perpendicular to the mean plane of macrocycle **A**, making a dihedral angle of 88.20 (5)°. It is very important to point out that the donor–acceptor Hg $\cdots$ N interactions do not affect the C $\equiv$ N bond lengths [1.136 (6) and 1.140 (6) Å].



Taking into account the intrinsic  $C_i$  symmetry of **B**, the *trans* nitrile group of this molecule coordinates to another macrocycle **A**, forming an infinite mixed-stack  $[\mathbf{A}\bullet\mathbf{B}]_\infty$  architecture (Fig. 2). The remaining nitrogen atoms of the two nitrile groups of **B** are not engaged in any donor–acceptor interactions.



**Figure 1**  
The supramolecular unit of complex (**I**) ( $\mathbf{A}\bullet\mathbf{B}$ ). Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate the intermolecular secondary Hg $\cdots$ N interactions. [Symmetry codes: (i)  $1 - x, y, \frac{1}{2} - z$ ; (ii)  $\frac{3}{2} - x, \frac{3}{2} - y, 1 - z$ .]



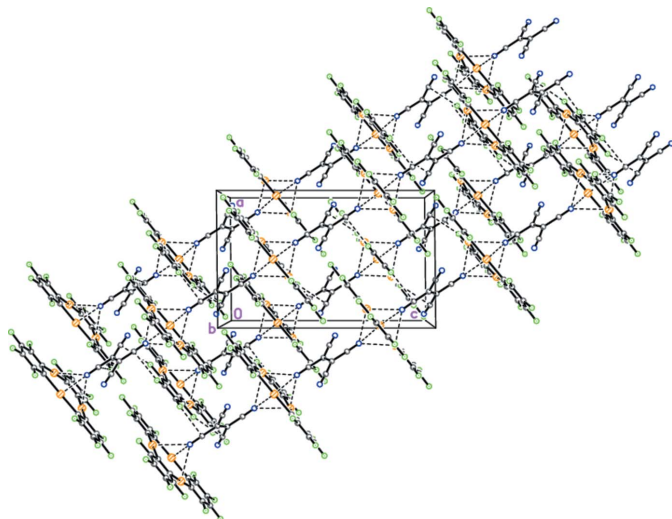
**Figure 2**  
The infinite mixed-stack  $[\mathbf{A}\bullet\mathbf{B}]_\infty$  architecture of (**I**). Dashed lines indicate the intermolecular secondary Hg $\cdots$ N interactions.

### 3. Supramolecular features

In the crystal, the mixed stacks toward [101] are held together by intermolecular C–F $\cdots$ C $\equiv$ N secondary interactions [F2 $\cdots$ C11<sup>iii</sup> 2.864 (5), F5 $\cdots$ C12<sup>iv</sup> 2.846 (5) and F6 $\cdots$ C11<sup>v</sup> 2.925 (5) Å; symmetry codes: (iii)  $-\frac{1}{2} + x, \frac{1}{2} + y, z$ ; (iv)  $1 - x, 1 - y, 1 - z$ ; (v)  $-\frac{1}{2} + x, -\frac{1}{2} + y, z$ ] (Fig. 3).

### 4. Comparison with compound (**II**)

It is interesting to note that the crystal structures of (**I**) and (**II**) are very similar. In both complexes, the guest molecules of tetracyanoethylene **B** and tetracyanoquinodimethane **C** are arranged perpendicularly to macrocycle **A**, with the same coordination mode of the *trans* nitrile groups to the three mercury atoms (Fig. 4). However, the supramolecular unit in

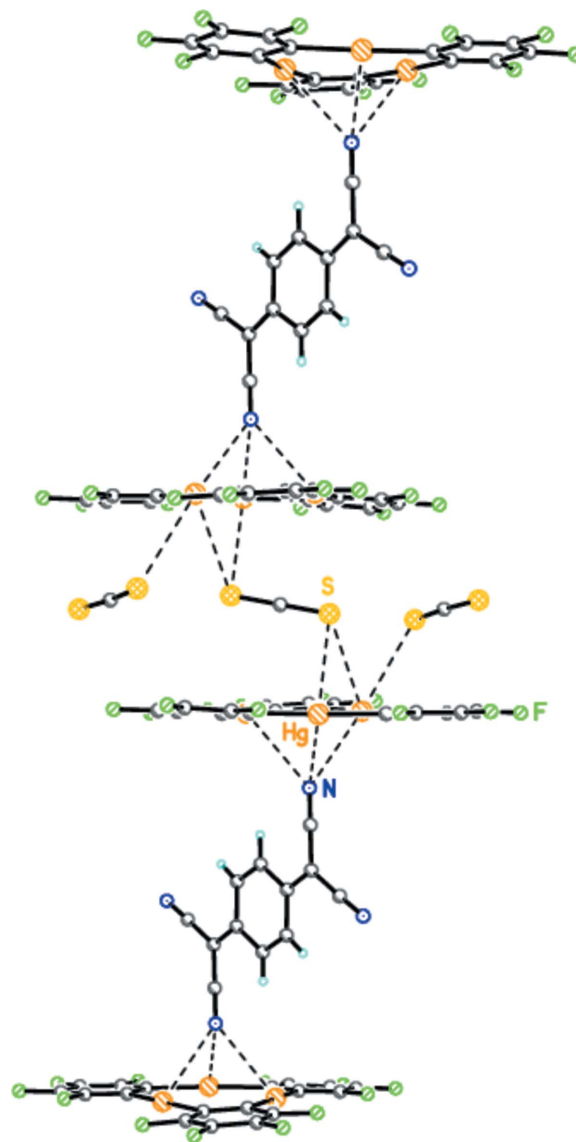


**Figure 3**  
Crystal packing of complex **(I)** along the *b* axis, showing the infinite mixed stacks toward [101]. Dashed lines indicate the intermolecular secondary Hg...N and F...C interactions.

**(I)** is **A•B** (a 1:1 ratio), whereas that in **(II)** is **A•C•A** (a 2:1 ratio) (Fig. 4). Beside the molecules of **C**, complex **(II)** includes the additional solvate CS<sub>2</sub> (**D**) molecules. The molecules of **D** participate in the construction of the supramolecular architecture of **(II)**, resulting in infinite mixed stacks [A•C•A•1.5D]<sub>∞</sub> (Fig. 4). Remarkably, the total number of donor–acceptor intermolecular interactions within the infinite mixed stacks of **(I)** and **(II)** is equal ([12 Hg...N]<sub>∞</sub> and [6 Hg...N + 6 Hg...S]<sub>∞</sub>, respectively).

## 5. TGA analysis

Despite complexes **(I)** and **(II)** being structural analogs, they are substantially different in their chemical stability. The crystalline complex **(II)** decomposes over a few days, while complex **(I)** is stable in the solid state for several months under ambient conditions. As free **B** decomposes rapidly upon reaction with moisture to produce toxic hydrogen cyanide, the high chemical stability of complex **(I)** is surprising. Moreover, the thermal stability of complex **(I)** has been studied by thermogravimetric analysis (TGA) which revealed that, upon complexation, tetracyanoethylene is stable to higher temperatures (Fig. 5). So, the free compound **B** starts to decompose at 363 K, but, being incorporated into the supramolecular complex **(I)**, **B** is stable up to 393 K. Complex **(I)** decomposes in two different steps. The first step of a 18.3% weight loss is attributed to molecule **B** because the much lower decomposition temperature of this molecule compared to macrocycle **A**. Consequently, the second weight loss of 81.7% is attributed to decomposition of macrocycle **A**. The complete decomposition of the free **B** is complete at 445 K; however, its final decomposition temperature is equal to 467 K within the supramolecular complex **(I)**. Final decomposition of complex **(I)** occurs at 573 K, and is likely due decomposition of macrocycle **A**.



**Figure 4**  
The supramolecular structure of complex **(II)** ([A•C•A•1.5D]<sub>∞</sub>). Dashed lines indicate the intermolecular secondary Hg...N interactions.

It is known that tetracyanoethylene is used not only as a component of charge-transfer complexes for organic electronics, but also in the preparation of organic magnets (Kao *et al.*, 2012). Consequently, the increase of its thermal stability attracts special attention in the manufacturing of organic materials. The complexation method described here could help to solve this problem.

## 6. Synthesis and crystallization

Trimeric perfluoro-*o*-phenylene mercury was synthesized according to the procedure described previously (Sartori & Golloch, 1968), and purified by recrystallization in dichloromethane (Filatov *et al.*, 2009). Tetracyanoethylene was acquired from TCI America. All solvents were HPLC grade

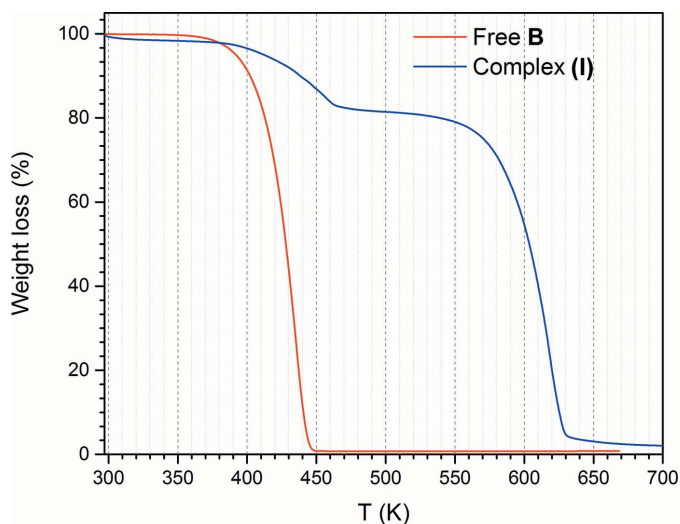


Figure 5  
TGA diagram of free **B** (in red) and complex **I** (in blue).

and used without any further purification. Thermogravimetric analysis was performed with a Hitachi STA7200 SII Nano-Technology instrument (an aluminum crucible (45 mL) was used; heating rate was 10 K min<sup>-1</sup>).

Stoichiometric amounts of trimeric perfluoro-*o*-phenylene mercury (63.8 mg, 59.6 mmol) and tetracyanoethylene (7.7 mg, 59.6 mmol) were dissolved in dichloromethane in separate tubes using ultrasonication. The contents of the tubes were mixed carefully, and then left for slow evaporation of the solvents. Complex **I** was obtained as yellow prismatic crystals, m.p. = 499–500 K.

## 7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. There is a high positive residual density of 1.19–1.78 e Å<sup>-3</sup> near the Hg1 and Hg2 atoms due to considerable absorption effects which could not be completely corrected.

## Acknowledgements

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Table 1

Experimental details.

Crystal data	
Chemical formula	[Hg <sub>3</sub> (C <sub>6</sub> F <sub>4</sub> ) <sub>3</sub> ]-C <sub>6</sub> N <sub>4</sub>
<i>M<sub>r</sub></i>	1174.05
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.5658 (11), 13.8297 (15), 16.7166 (18)
$\beta$ (°)	90.575 (1)
<i>V</i> (Å <sup>3</sup> )	2442.5 (5)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	18.93
Crystal size (mm)	0.15 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2003)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.150, 0.250
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	13813, 3560, 3404
<i>R<sub>int</sub></i>	0.036
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.703
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.023, 0.055, 1.06
No. of reflections	3560
No. of parameters	195
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	1.78, -1.70

Computer programs: *APEX2* (Bruker, 2005), *SAINT* (Bruker, 2001), *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

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## supporting information

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## Crystal structure of *cyclo*-tris( $\mu$ -3,4,5,6-tetrafluoro-*o*-phenylene- $\kappa^2C^1:C^2$ )trimercury–tetracyanoethylene (1/1)

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### Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE* (Bruker, 2001); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

### *cyclo*-Tris( $\mu$ -3,4,5,6-tetrafluoro-*o*-phenylene- $\kappa^2C^1:C^2$ )trimercury–tetracyanoethylene (1/1)

#### Crystal data

[Hg<sub>3</sub>(C<sub>6</sub>F<sub>4</sub>)<sub>3</sub>]·C<sub>6</sub>N<sub>4</sub>

$M_r = 1174.05$

Monoclinic, *C2/c*

$a = 10.5658$  (11) Å

$b = 13.8297$  (15) Å

$c = 16.7166$  (18) Å

$\beta = 90.575$  (1)°

$V = 2442.5$  (5) Å<sup>3</sup>

$Z = 4$

$F(000) = 2080$

$D_x = 3.193$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 9624 reflections

$\theta = 4.4$ – $32.7$ °

$\mu = 18.93$  mm<sup>-1</sup>

$T = 100$  K

Prism, light-yellow

$0.15 \times 0.15 \times 0.10$  mm

#### Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2003)

$T_{\min} = 0.150$ ,  $T_{\max} = 0.250$

13813 measured reflections

3560 independent reflections

3404 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 30.0$ °,  $\theta_{\min} = 4.4$ °

$h = -14 \rightarrow 14$

$k = -19 \rightarrow 19$

$l = -23 \rightarrow 23$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.055$

$S = 1.06$

3560 reflections

195 parameters

0 restraints

Primary atom site location: difference Fourier

map

Secondary atom site location: difference Fourier

map

$w = 1/[\sigma^2(F_o^2) + (0.0191P)^2 + 19.1P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 1.78$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -1.70$  e Å<sup>-3</sup>



*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.5000	0.83281 (2)	0.2500	0.01573 (6)
Hg2	0.36631 (2)	0.60249 (2)	0.31557 (2)	0.01493 (5)
F1	0.3423 (3)	0.9966 (2)	0.33993 (17)	0.0259 (6)
F2	0.1469 (3)	0.98904 (19)	0.44275 (17)	0.0267 (6)
F3	0.0409 (3)	0.8182 (2)	0.48130 (17)	0.0253 (5)
F4	0.1388 (3)	0.65100 (19)	0.42523 (17)	0.0247 (5)
F5	0.3016 (3)	0.38265 (19)	0.35217 (16)	0.0240 (5)
F6	0.4034 (3)	0.21483 (18)	0.30301 (17)	0.0238 (5)
C1	0.3490 (4)	0.8248 (3)	0.3293 (3)	0.0186 (7)
C2	0.2968 (4)	0.9087 (3)	0.3601 (3)	0.0198 (8)
C3	0.1952 (4)	0.9069 (3)	0.4121 (3)	0.0199 (8)
C4	0.1415 (4)	0.8193 (3)	0.4332 (3)	0.0191 (8)
C5	0.1927 (4)	0.7350 (3)	0.4030 (2)	0.0177 (7)
C6	0.2958 (4)	0.7350 (3)	0.3517 (2)	0.0153 (7)
C7	0.4474 (4)	0.4743 (3)	0.2765 (2)	0.0161 (7)
C8	0.4008 (4)	0.3863 (3)	0.3008 (2)	0.0173 (7)
C9	0.4501 (4)	0.2987 (3)	0.2762 (3)	0.0189 (8)
N1	0.6254 (4)	0.6785 (3)	0.3521 (2)	0.0213 (7)
N2	0.9176 (4)	0.5836 (3)	0.5355 (3)	0.0289 (8)
C10	0.7588 (4)	0.7081 (3)	0.4799 (2)	0.0165 (7)
C11	0.6861 (4)	0.6895 (3)	0.4081 (2)	0.0174 (7)
C12	0.8478 (4)	0.6369 (3)	0.5080 (2)	0.0198 (7)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Hg1	0.01452 (9)	0.01481 (10)	0.01793 (10)	0.000	0.00398 (7)	0.000
Hg2	0.01430 (7)	0.01349 (8)	0.01709 (8)	0.00109 (4)	0.00400 (5)	0.00000 (5)
F1	0.0273 (13)	0.0178 (12)	0.0327 (14)	-0.0010 (10)	0.0092 (11)	0.0003 (10)
F2	0.0296 (14)	0.0186 (13)	0.0321 (14)	0.0050 (10)	0.0088 (11)	-0.0055 (10)
F3	0.0209 (12)	0.0275 (14)	0.0277 (13)	0.0033 (10)	0.0111 (10)	-0.0001 (11)
F4	0.0243 (13)	0.0192 (12)	0.0308 (14)	-0.0003 (10)	0.0110 (10)	0.0012 (10)
F5	0.0237 (13)	0.0204 (13)	0.0281 (13)	-0.0003 (10)	0.0139 (10)	0.0032 (10)
F6	0.0251 (13)	0.0132 (12)	0.0333 (14)	-0.0026 (9)	0.0073 (11)	0.0029 (10)
C1	0.0174 (18)	0.0188 (19)	0.0195 (18)	0.0010 (14)	0.0016 (14)	0.0010 (14)
C2	0.0200 (19)	0.0171 (19)	0.0225 (19)	0.0003 (14)	0.0045 (15)	-0.0001 (15)
C3	0.0190 (18)	0.0184 (19)	0.0223 (19)	0.0091 (14)	0.0018 (15)	-0.0041 (15)
C4	0.0142 (17)	0.023 (2)	0.0206 (18)	0.0024 (14)	0.0054 (14)	-0.0003 (15)
C5	0.0181 (18)	0.0180 (18)	0.0171 (17)	0.0014 (14)	0.0023 (14)	0.0010 (14)

C6	0.0142 (16)	0.0158 (18)	0.0161 (17)	0.0034 (13)	0.0031 (13)	-0.0007 (13)
C7	0.0148 (17)	0.0149 (17)	0.0186 (17)	0.0038 (13)	0.0053 (14)	0.0002 (14)
C8	0.0159 (17)	0.0188 (19)	0.0173 (17)	0.0026 (14)	0.0035 (14)	0.0019 (14)
C9	0.0177 (18)	0.0161 (18)	0.0228 (19)	-0.0020 (14)	0.0001 (15)	0.0018 (15)
N1	0.0216 (17)	0.0193 (17)	0.0231 (17)	-0.0011 (13)	0.0044 (13)	0.0001 (13)
N2	0.028 (2)	0.028 (2)	0.031 (2)	0.0051 (16)	0.0072 (16)	0.0016 (16)
C10	0.0143 (16)	0.0169 (18)	0.0184 (17)	-0.0012 (13)	0.0030 (13)	0.0010 (14)
C11	0.0182 (18)	0.0166 (18)	0.0174 (17)	-0.0001 (14)	0.0036 (14)	-0.0011 (14)
C12	0.0196 (18)	0.0195 (19)	0.0205 (18)	0.0001 (15)	0.0030 (14)	-0.0006 (15)

*Geometric parameters (Å, °)*

Hg1—C1	2.087 (4)	C2—C3	1.389 (6)
Hg1—N1	3.030 (4)	C3—C4	1.385 (6)
Hg2—C6	2.071 (4)	C4—C5	1.382 (6)
Hg2—C7	2.077 (4)	C5—C6	1.394 (5)
Hg2—N1	2.990 (4)	C7—C8	1.375 (6)
F1—C2	1.351 (5)	C7—C7 <sup>i</sup>	1.429 (7)
F2—C3	1.348 (5)	C8—C9	1.384 (6)
F3—C4	1.340 (4)	C9—C9 <sup>i</sup>	1.377 (8)
F4—C5	1.347 (5)	N1—C11	1.140 (6)
F5—C8	1.363 (5)	N2—C12	1.136 (6)
F6—C9	1.339 (5)	C10—C10 <sup>ii</sup>	1.355 (8)
C1—C2	1.387 (6)	C10—C12	1.437 (6)
C1—C6	1.415 (6)	C10—C11	1.441 (6)
C1—Hg1—C1 <sup>i</sup>	173.9 (2)	C1—C6—Hg2	123.7 (3)
C6—Hg2—C7	176.24 (16)	C8—C7—C7 <sup>i</sup>	117.8 (2)
C2—C1—C6	118.4 (4)	C8—C7—Hg2	120.8 (3)
C2—C1—Hg1	120.0 (3)	C7 <sup>i</sup> —C7—Hg2	121.39 (11)
C6—C1—Hg1	121.6 (3)	F5—C8—C7	119.9 (3)
F1—C2—C1	121.1 (4)	F5—C8—C9	116.7 (4)
F1—C2—C3	116.8 (4)	C7—C8—C9	123.4 (4)
C1—C2—C3	122.1 (4)	F6—C9—C9 <sup>i</sup>	120.0 (2)
F2—C3—C4	118.9 (4)	F6—C9—C8	121.2 (4)
F2—C3—C2	121.4 (4)	C9 <sup>i</sup> —C9—C8	118.8 (2)
C4—C3—C2	119.7 (4)	C11—N1—Hg2	136.2 (3)
F3—C4—C5	121.7 (4)	C11—N1—Hg1	127.4 (3)
F3—C4—C3	119.5 (4)	Hg2—N1—Hg1	74.82 (9)
C5—C4—C3	118.9 (4)	C10 <sup>ii</sup> —C10—C12	121.1 (5)
F4—C5—C4	117.3 (4)	C10 <sup>ii</sup> —C10—C11	119.4 (5)
F4—C5—C6	120.3 (4)	C12—C10—C11	119.5 (4)
C4—C5—C6	122.4 (4)	N1—C11—C10	176.9 (5)
C5—C6—C1	118.6 (4)	N2—C12—C10	175.2 (5)
C5—C6—Hg2	117.7 (3)		
C6—C1—C2—F1	-179.0 (4)	F4—C5—C6—C1	179.4 (4)
Hg1—C1—C2—F1	-0.2 (6)	C4—C5—C6—C1	-0.6 (6)

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C6—C1—C2—C3	0.3 (6)	F4—C5—C6—Hg2	-2.5 (5)
Hg1—C1—C2—C3	179.1 (3)	C4—C5—C6—Hg2	177.5 (3)
F1—C2—C3—F2	-1.9 (6)	C2—C1—C6—C5	0.7 (6)
C1—C2—C3—F2	178.8 (4)	Hg1—C1—C6—C5	-178.1 (3)
F1—C2—C3—C4	177.9 (4)	C2—C1—C6—Hg2	-177.2 (3)
C1—C2—C3—C4	-1.4 (7)	Hg1—C1—C6—Hg2	4.0 (5)
F2—C3—C4—F3	2.0 (6)	C7 <sup>i</sup> —C7—C8—F5	179.2 (4)
C2—C3—C4—F3	-177.8 (4)	Hg2—C7—C8—F5	-1.1 (5)
F2—C3—C4—C5	-178.7 (4)	C7 <sup>i</sup> —C7—C8—C9	-0.4 (7)
C2—C3—C4—C5	1.5 (6)	Hg2—C7—C8—C9	179.3 (3)
F3—C4—C5—F4	-1.2 (6)	F5—C8—C9—F6	-1.2 (6)
C3—C4—C5—F4	179.5 (4)	C7—C8—C9—F6	178.4 (4)
F3—C4—C5—C6	178.8 (4)	F5—C8—C9—C9 <sup>i</sup>	179.5 (5)
C3—C4—C5—C6	-0.5 (6)	C7—C8—C9—C9 <sup>i</sup>	-0.8 (8)

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Symmetry codes: (i)  $-x+1, y, -z+1/2$ ; (ii)  $-x+3/2, -y+3/2, -z+1$ .