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(μ_2-2-Methoxyethanol-κ^3O^1:O^1,O^3)(2-methoxyethanol-κO^1)tris(μ_2-3,4,5,6-tetrafluoro-*o*-phenylene-κ^2C^1:C^2)trimercury(II)

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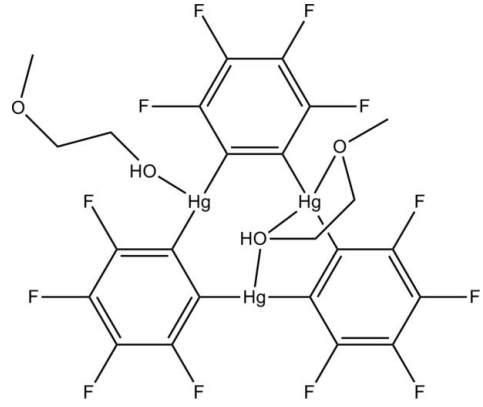
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.018 Å; R factor = 0.050; wR factor = 0.101; data-to-parameter ratio = 21.8.

In the title compound, $[Hg_3(C_6F_4)_3(C_3H_8O_2)_2]$, two O atoms from one 2-methoxyethanol ligand and one O atom from the second 2-methoxyethanol ligand coordinate three Hg^{II} atoms [Hg—O = 2.765 (7)–2.890 (8) Å] in the trimeric organomercurial Lewis acid (o-$C_6F_4Hg)_3$. The hydroxy groups are involved in formation of intra- and intermolecular O—H···O hydrogen bonds; the latter link two molecules into centrosymmetric dimers. An extensive net of weak intermolecular C—H···F interactions further consolidates the crystal packing.

Related literature

For the synthesis of trimeric perfluoro-*ortho*-phenylene mercury and its use as a catalyst, see: Sartori & Golloch (1968) and Lee *et al.* (1999), respectively. For the properties of organomercurial anticrowns, see: Taylor *et al.* (2007). For related crystal structures, see: Tikhonova *et al.* (2002, 2013).



Experimental

Crystal data

$[Hg_3(C_6F_4)_3(C_3H_8O_2)_2]$
M_r = 1198.14
Triclinic, $P\overline{1}$
a = 10.170 (4) Å
b = 12.623 (5) Å
c = 12.962 (5) Å
α = 113.450 (5)°
β = 110.411 (5)°
γ = 92.795 (5)°
V = 1396.3 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 16.56 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.979, T_{max} = 0.984
16463 measured reflections
8430 independent reflections
4880 reflections with $I > 2\sigma(I)$
R_{int} = 0.090

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.101
S = 0.91
8430 reflections
386 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 3.70 e Å^{-3}
$\Delta\rho_{min}$ = −2.93 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O3	0.84	2.04	2.771 (11)	145
O3—H3···O4^{i}	0.84	1.86	2.694 (10)	171
C21—H21B···F6^{ii}	0.99	2.52	3.480 (14)	162
C23—H23A···F10^{iii}	0.99	2.48	3.109 (12)	121
C23—H23B···F11^{iv}	0.99	2.47	3.301 (12)	141
C24—H24B···F5^{ii}	0.98	2.54	3.339 (14)	138
C24—H24C···F2^{v}	0.98	2.46	3.352 (15)	152
C19—H19B···F2^{vi}	0.98	2.53	3.207 (13)	126

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: CV5445).

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supporting information

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(μ_2-2-Methoxyethanol-κ^3O^1:O^1,O^3)(2-methoxyethanol-κO^1)tris(μ_2-3,4,5,6-tetrafluoro-*o*-phenylene-κ^2C^1:C^2)trimercury(II)

Raúl Castañeda, Sergiu Draguta, Andrey Yakovenko, Marina Fonari and Tatiana Timofeeva

S1. Comments

As an organomercurial compound trimeric perfluoro-*o*-phenylene mercury (**I**) has numerous adducts with aldehydes, ketones, amides, nitriles, phosphoramides, and sulfoxides (Taylor *et al.*, 2007). Formation of complexes involving **I** with oxygenated Lewis bases similar to 2-methoxyethanol (**II**) had been observed before (Tikhonova *et al.*, 2002). The studies of this type of coordination are important due the effect of **I** on the keto-enol tautomerism (Tikhonova *et al.*, 2013) as well on the activation of carbonyl compounds (Tikhonova *et al.*, 2002). Acting as Lewis acid **I** had proven catalyze the Diels-Alder reaction between thionoester and cyclopentadiene (Lee *et al.*, 1999). Besides **II** is not a strong Lewis base it exhibits shorter Hg···O contacts than the sum of the van der Walls radii (Hg = 1.7-2 Å, O = 1.52 Å).

In the title compound (Fig. 1), the coordinating Hg···O contacts range from 2.765 (7) to 2.890 (8) Å. These short contacts are in the same range as those described for carbonyl compounds (Tikhonova *et al.*, 2002). The present complex [**I**·(**II**)$_2$] has two **II** molecules per one **I** molecule. The hydroxy groups are involved in formation of intra- and intermolecular O—H···O hydrogen bonds (Table 1), and the latter ones link two complex molecules into centrosymmetric dimers. An extensive net of weak intermolecular C—H···F interactions (Table 1) consolidate further the crystal packing. To the best of our knowledge this complex is the first coordination example of a non-cyclic ether with macrocycle **I**. That indicates a possibility of **I** to form complexes with non-cyclic ethers, like polyethylene glycol derivatives.

S2. Experimental

S2.1. Synthesis and crystallization

Trimeric perfluoro-o-phenylene mercury (**I**) was synthesized according to the known procedure (Sartori & Golloch, 1968). The title compound [**I**·(**II**)$_2$] was obtained by dissolving pure **I** in **II**, followed by slow evaporation of the solvent until single crystals were obtained.

S2.2. Refinement

All hydrogen atoms were placed in the calculated positions with O—H = 0.84 Å, C—H = 0.98–0.99 Å and refined as riding, with U_{iso}(H) = 1.2–1.5 U_{eq} of the parent atom.

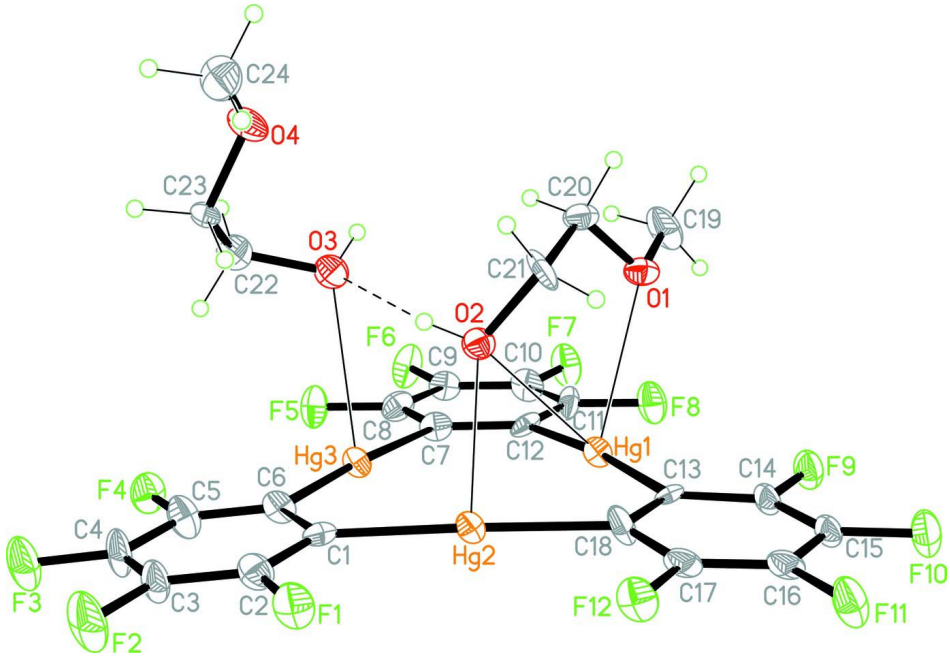

Figure 1

The molecular structure of the title compound showing the atomic numbering and 50% probability displacement ellipsoids. Dashed line denotes hydrogen bond.

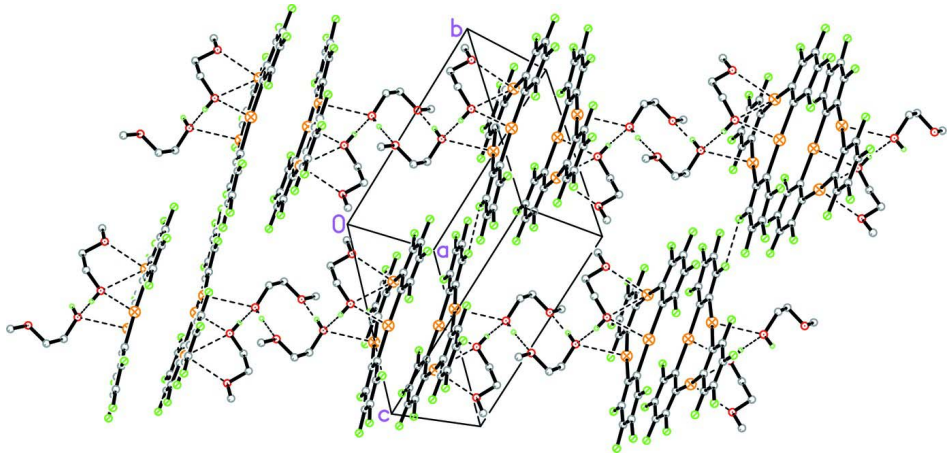

Figure 2

The crystal packing.

(μ_2-2-Methoxyethanol-κ^3O^1:O^1,O^3)(2-methoxyethanol-κO^1)tris(μ_2-3,4,5,6-tetrafluoro-*o*-phenylene-κ^2C^1:C^2)trimercury(II)

Crystal data

$[Hg_3(C_6F_4)_3(C_3H_8O_2)_2]$	α = 113.450 (5)°
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Triclinic, $P\overline{1}$	γ = 92.795 (5)°
a = 10.170 (4) Å	V = 1396.3 (9) Å^3
b = 12.623 (5) Å	Z = 2
c = 12.962 (5) Å	$F(000)$ = 1080

D_x = 2.850 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 16.56 mm^{-1}

T = 100 K
Prism, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.979, T_{max} = 0.984

16463 measured reflections
8430 independent reflections
4880 reflections with $I > 2\sigma(I)$
R_{int} = 0.090
θ_{max} = 30.7°, θ_{min} = 4.4°
h = −14→14
k = −17→18
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.101
S = 0.91
8430 reflections
386 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
$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 3.70 e Å^{-3}
$\Delta\rho_{min}$ = −2.93 e Å^{-3}

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.
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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Hg1	0.34545 (4)	1.01863 (4)	0.29484 (4)	0.01824 (11)
Hg2	0.22471 (4)	0.98504 (4)	0.51393 (4)	0.01800 (11)
Hg3	0.41210 (4)	0.77523 (4)	0.36850 (4)	0.01824 (11)
F1	0.1682 (7)	0.9075 (6)	0.7026 (6)	0.0307 (16)
F2	0.2340 (9)	0.7301 (7)	0.7630 (7)	0.048 (2)
F3	0.3741 (8)	0.5752 (7)	0.6553 (6)	0.0408 (19)
F4	0.4452 (7)	0.5942 (6)	0.4792 (6)	0.0303 (16)
F5	0.5756 (7)	0.6279 (6)	0.2121 (6)	0.0310 (17)
F6	0.6681 (7)	0.6575 (6)	0.0508 (6)	0.0323 (17)
F7	0.6287 (7)	0.8460 (6)	0.0030 (6)	0.0331 (17)
F8	0.4924 (7)	1.0048 (6)	0.1120 (6)	0.0316 (17)
F9	0.2731 (7)	1.2533 (6)	0.2847 (6)	0.0279 (16)
F10	0.1551 (7)	1.4209 (6)	0.4062 (6)	0.0328 (17)

F11	0.0669 (7)	1.3997 (6)	0.5718 (6)	0.0336 (18)
F12	0.0954 (6)	1.2102 (6)	0.6197 (6)	0.0274 (16)
O1	0.1057 (7)	0.9283 (7)	0.0754 (6)	0.0220 (17)
O2	0.1230 (7)	0.8390 (7)	0.2563 (7)	0.0221 (17)
H2	0.1125	0.7678	0.2434	0.033*
O3	0.1619 (8)	0.6097 (7)	0.1593 (7)	0.0262 (18)
H3	0.1431	0.5953	0.0860	0.039*
O4	−0.1110 (8)	0.4592 (8)	0.0789 (6)	0.0261 (19)
C1	0.2690 (11)	0.8440 (10)	0.5548 (9)	0.020 (2)
C2	0.2353 (11)	0.8292 (11)	0.6427 (10)	0.025 (3)
C3	0.2689 (14)	0.7414 (11)	0.6758 (10)	0.030 (3)
C4	0.3408 (14)	0.6609 (11)	0.6203 (11)	0.030 (3)
C5	0.3735 (12)	0.6747 (11)	0.5329 (11)	0.028 (3)
C6	0.3446 (11)	0.7621 (10)	0.4967 (9)	0.018 (2)
C7	0.4814 (11)	0.8017 (10)	0.2454 (9)	0.019 (2)
C8	0.5518 (11)	0.7228 (11)	0.1895 (11)	0.026 (3)
C9	0.6030 (11)	0.7385 (10)	0.1068 (10)	0.020 (2)
C10	0.5808 (12)	0.8336 (11)	0.0835 (10)	0.025 (3)
C11	0.5103 (11)	0.9119 (10)	0.1372 (11)	0.023 (3)
C12	0.4586 (10)	0.8986 (9)	0.2192 (10)	0.018 (2)
C13	0.2464 (10)	1.1399 (9)	0.3867 (9)	0.016 (2)
C14	0.2302 (11)	1.2401 (10)	0.3691 (9)	0.0193 (17)
C15	0.1701 (11)	1.3265 (10)	0.4274 (9)	0.0193 (17)
C16	0.1251 (12)	1.3143 (11)	0.5125 (10)	0.024 (3)
C17	0.1416 (11)	1.2187 (11)	0.5344 (9)	0.020 (2)
C18	0.1981 (12)	1.1268 (11)	0.4728 (10)	0.024 (3)
C19	0.1318 (14)	0.9019 (13)	−0.0342 (11)	0.036 (3)
H19A	0.0444	0.8993	−0.0996	0.055*
H19B	0.1587	0.8250	−0.0606	0.055*
H19C	0.2100	0.9634	−0.0165	0.055*
C20	0.0035 (11)	0.8364 (10)	0.0569 (10)	0.024 (3)
H20A	0.0308	0.7599	0.0220	0.028*
H20B	−0.0917	0.8328	−0.0025	0.028*
C21	−0.0059 (12)	0.8555 (12)	0.1742 (11)	0.030 (3)
H21A	−0.0190	0.9368	0.2149	0.036*
H21B	−0.0907	0.7993	0.1573	0.036*
C22	0.1456 (12)	0.4994 (11)	0.1684 (11)	0.029 (3)
H22A	0.2294	0.5029	0.2386	0.034*
H22B	0.1416	0.4333	0.0926	0.034*
C23	0.0117 (11)	0.4786 (11)	0.1859 (9)	0.024 (3)
H23A	0.0071	0.4087	0.2025	0.029*
H23B	0.0120	0.5480	0.2576	0.029*
C24	−0.2418 (12)	0.4380 (13)	0.0905 (12)	0.036 (3)
H24A	−0.3226	0.4258	0.0152	0.055*
H24B	−0.2444	0.5063	0.1603	0.055*
H24C	−0.2490	0.3673	0.1040	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0181 (2)	0.0224 (3)	0.0180 (2)	0.00763 (18)	0.00949 (17)	0.0103 (2)
Hg2	0.0193 (2)	0.0209 (3)	0.0173 (2)	0.00739 (18)	0.00843 (17)	0.01047 (19)
Hg3	0.0176 (2)	0.0230 (3)	0.0186 (2)	0.00700 (18)	0.00915 (17)	0.0115 (2)
F1	0.047 (4)	0.031 (4)	0.024 (4)	0.019 (4)	0.025 (3)	0.012 (3)
F2	0.087 (6)	0.050 (5)	0.037 (5)	0.032 (5)	0.043 (4)	0.031 (4)
F3	0.071 (5)	0.041 (5)	0.037 (4)	0.029 (4)	0.036 (4)	0.029 (4)
F4	0.034 (4)	0.026 (4)	0.035 (4)	0.015 (3)	0.017 (3)	0.014 (3)
F5	0.036 (4)	0.028 (4)	0.046 (5)	0.017 (3)	0.025 (3)	0.024 (4)
F6	0.039 (4)	0.028 (4)	0.053 (5)	0.019 (3)	0.037 (4)	0.022 (4)
F7	0.042 (4)	0.043 (5)	0.042 (4)	0.022 (4)	0.034 (4)	0.030 (4)
F8	0.042 (4)	0.037 (5)	0.036 (4)	0.018 (4)	0.026 (3)	0.026 (4)
F9	0.040 (4)	0.026 (4)	0.026 (4)	0.013 (3)	0.016 (3)	0.016 (3)
F10	0.052 (4)	0.030 (4)	0.032 (4)	0.023 (4)	0.023 (3)	0.021 (4)
F11	0.051 (4)	0.039 (5)	0.029 (4)	0.029 (4)	0.024 (3)	0.023 (4)
F12	0.034 (4)	0.035 (4)	0.025 (4)	0.012 (3)	0.020 (3)	0.017 (3)
O1	0.021 (4)	0.023 (5)	0.017 (4)	0.004 (3)	0.006 (3)	0.005 (4)
O2	0.019 (4)	0.022 (5)	0.023 (4)	0.006 (3)	0.007 (3)	0.009 (4)
O3	0.034 (4)	0.028 (5)	0.018 (4)	0.004 (4)	0.012 (4)	0.011 (4)
O4	0.023 (4)	0.043 (6)	0.016 (4)	0.008 (4)	0.010 (3)	0.015 (4)
C1	0.021 (5)	0.016 (6)	0.014 (6)	−0.001 (5)	0.003 (5)	0.002 (5)
C2	0.021 (6)	0.028 (7)	0.025 (6)	0.007 (5)	0.008 (5)	0.014 (6)
C3	0.057 (8)	0.023 (7)	0.020 (6)	0.016 (6)	0.022 (6)	0.013 (6)
C4	0.054 (8)	0.030 (8)	0.032 (7)	0.020 (7)	0.030 (6)	0.024 (6)
C5	0.029 (6)	0.037 (8)	0.033 (7)	0.019 (6)	0.019 (6)	0.023 (7)
C6	0.022 (5)	0.025 (7)	0.014 (5)	0.010 (5)	0.015 (5)	0.007 (5)
C7	0.022 (6)	0.023 (7)	0.016 (6)	0.006 (5)	0.014 (5)	0.006 (5)
C8	0.021 (6)	0.024 (7)	0.030 (7)	0.000 (5)	0.011 (5)	0.009 (6)
C9	0.018 (5)	0.026 (7)	0.021 (6)	0.010 (5)	0.014 (5)	0.007 (5)
C10	0.026 (6)	0.036 (8)	0.022 (6)	0.007 (5)	0.019 (5)	0.015 (6)
C11	0.024 (6)	0.018 (7)	0.033 (7)	0.004 (5)	0.012 (5)	0.016 (6)
C12	0.010 (5)	0.011 (6)	0.025 (6)	0.000 (4)	0.007 (4)	0.000 (5)
C13	0.017 (5)	0.009 (6)	0.011 (5)	−0.002 (4)	0.002 (4)	−0.001 (4)
C14	0.028 (4)	0.021 (5)	0.014 (4)	0.009 (4)	0.009 (3)	0.011 (4)
C15	0.028 (4)	0.021 (5)	0.014 (4)	0.009 (4)	0.009 (3)	0.011 (4)
C16	0.029 (6)	0.028 (7)	0.018 (6)	0.016 (6)	0.013 (5)	0.008 (5)
C17	0.024 (6)	0.025 (7)	0.004 (5)	0.005 (5)	0.003 (4)	0.001 (5)
C18	0.033 (6)	0.029 (7)	0.023 (6)	0.018 (6)	0.014 (5)	0.019 (6)
C19	0.053 (8)	0.049 (9)	0.022 (7)	0.026 (7)	0.020 (6)	0.023 (7)
C20	0.020 (6)	0.021 (7)	0.020 (6)	0.004 (5)	0.003 (5)	0.003 (5)
C21	0.023 (6)	0.048 (9)	0.033 (7)	0.013 (6)	0.006 (5)	0.034 (7)
C22	0.033 (6)	0.026 (7)	0.025 (7)	0.010 (6)	0.012 (5)	0.008 (6)
C23	0.037 (7)	0.020 (7)	0.007 (5)	0.000 (5)	0.003 (5)	0.004 (5)
C24	0.030 (7)	0.042 (9)	0.043 (8)	0.005 (6)	0.016 (6)	0.024 (7)

Geometric parameters (Å, º)

Hg1—C13	2.076 (10)	O2—C21	1.457 (12)
Hg1—C12	2.087 (10)	O3—C22	1.450 (14)
Hg1—O1	2.765 (7)	O4—C24	1.415 (13)
Hg1—O2	2.844 (9)	O4—C23	1.427 (12)
Hg2—C18	2.065 (11)	C1—C2	1.374 (15)
Hg2—C1	2.078 (11)	C1—C6	1.446 (14)
Hg2—O2	2.850 (8)	C2—C3	1.357 (15)
Hg3—C6	2.064 (10)	C3—C4	1.395 (15)
Hg3—C7	2.083 (10)	C4—C5	1.356 (15)
Hg3—O3	2.890 (8)	C5—C6	1.368 (15)
F1—C2	1.366 (12)	C7—C8	1.374 (14)
F2—C3	1.352 (13)	C7—C12	1.404 (15)
F3—C4	1.345 (13)	C8—C9	1.418 (15)
F4—C5	1.383 (12)	C9—C10	1.360 (16)
F5—C8	1.355 (13)	C10—C11	1.358 (15)
F6—C9	1.350 (11)	C11—C12	1.399 (15)
F7—C10	1.353 (11)	C13—C14	1.379 (14)
F8—C11	1.341 (12)	C13—C18	1.427 (14)
F9—C14	1.373 (11)	C14—C15	1.366 (14)
F10—C15	1.330 (12)	C15—C16	1.389 (15)
F11—C16	1.350 (12)	C16—C17	1.351 (16)
F12—C17	1.380 (12)	C17—C18	1.400 (14)
O1—C20	1.404 (13)	C20—C21	1.480 (15)
O1—C19	1.447 (12)	C22—C23	1.484 (15)
C13—Hg1—C12	174.4 (4)	C11—C10—F7	121.1 (11)
C18—Hg2—C1	175.0 (4)	C11—C10—C9	121.2 (10)
C6—Hg3—C7	175.8 (4)	F7—C10—C9	117.6 (10)
C20—O1—C19	111.1 (9)	F8—C11—C10	118.9 (10)
C24—O4—C23	112.5 (8)	F8—C11—C12	119.7 (9)
C2—C1—C6	117.7 (10)	C10—C11—C12	121.4 (10)
C2—C1—Hg2	121.4 (8)	C7—C12—C11	118.4 (9)
C6—C1—Hg2	120.8 (8)	C7—C12—Hg1	121.8 (8)
C3—C2—F1	117.8 (10)	C11—C12—Hg1	119.8 (8)
C3—C2—C1	122.9 (11)	C14—C13—C18	117.4 (9)
F1—C2—C1	119.3 (10)	C14—C13—Hg1	120.0 (8)
C2—C3—F2	121.0 (10)	C18—C13—Hg1	122.5 (8)
C2—C3—C4	120.4 (11)	C15—C14—F9	117.1 (9)
F2—C3—C4	118.6 (10)	C15—C14—C13	124.5 (10)
F3—C4—C5	123.8 (10)	F9—C14—C13	118.4 (9)
F3—C4—C3	119.3 (10)	F10—C15—C14	122.3 (10)
C5—C4—C3	116.9 (11)	F10—C15—C16	119.7 (9)
C4—C5—C6	125.6 (11)	C14—C15—C16	118.0 (10)
C4—C5—F4	116.0 (10)	C17—C16—F11	122.0 (10)
C6—C5—F4	118.4 (10)	C17—C16—C15	119.5 (10)
C5—C6—C1	116.5 (10)	F11—C16—C15	118.5 (10)

C5—C6—Hg3	120.4 (8)	C16—C17—F12	117.5 (9)
C1—C6—Hg3	123.1 (8)	C16—C17—C18	123.7 (10)
C8—C7—C12	119.4 (10)	F12—C17—C18	118.7 (10)
C8—C7—Hg3	119.1 (9)	C17—C18—C13	116.9 (10)
C12—C7—Hg3	121.5 (7)	C17—C18—Hg2	121.6 (8)
F5—C8—C7	121.3 (10)	C13—C18—Hg2	121.3 (8)
F5—C8—C9	117.7 (10)	O1—C20—C21	110.6 (10)
C7—C8—C9	121.0 (11)	O2—C21—C20	111.5 (9)
F6—C9—C10	122.0 (10)	O3—C22—C23	109.9 (9)
F6—C9—C8	119.4 (10)	O4—C23—C22	110.2 (8)
C10—C9—C8	118.6 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3	0.84	2.04	2.771 (11)	145
O3—H3···O4^{i}	0.84	1.86	2.694 (10)	171
C21—H21*B*···F6^{ii}	0.99	2.52	3.480 (14)	162
C23—H23*A*···F10^{iii}	0.99	2.48	3.109 (12)	121
C23—H23*B*···F11^{iv}	0.99	2.47	3.301 (12)	141
C24—H24*B*···F5^{ii}	0.98	2.54	3.339 (14)	138
C24—H24*C*···F2^{v}	0.98	2.46	3.352 (15)	152
C19—H19*B*···F2^{vi}	0.98	2.53	3.207 (13)	126

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