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{1,8-Bis[2-(1-benzyl-1*H*-imidazol-3-ylmethyl-κC^2)-phenoxy]-3,6-dioxaoctane-$\kappa^2 O^3,O^6$}mercury(**II**) bis(hexaflourophosphate) nitromethane solvate

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Key indicators

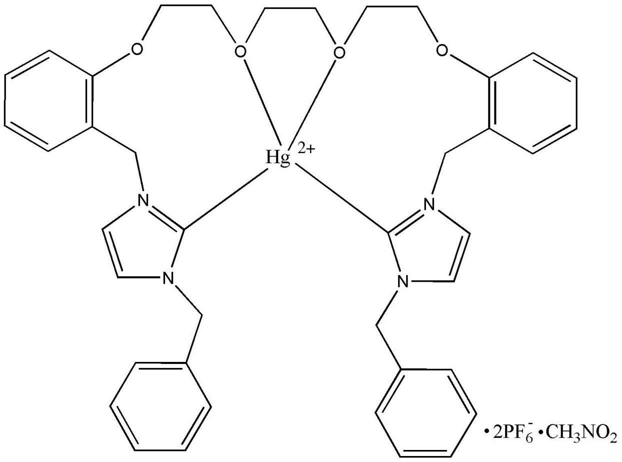
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.014 Å
R factor = 0.049
wR factor = 0.112
Data-to-parameter ratio = 13.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[\mathrm{Hg}(\mathrm{C}_{40}\mathrm{H}_{42}\mathrm{N}_4\mathrm{O}_4)](\mathrm{PF}_6)_2\cdot\mathrm{CH}_3\mathrm{NO}_2$, the geometry of the Hg coordination is distorted tetrahedral, formed by two C atoms [Hg—C = 2.076 (7) and 2.068 (7) Å] and two O atoms [Hg—O = 2.703 (5) and 2.934 (5) Å]. The crystal packing is stabilized by weak C—H···F and C—H···O interactions.

Comment

Metal complexes of carbenes based on imidazol-2-ylidene have received much attention in the past few years. *N*-heterocyclic carbenes can form stable carbene complexes with a wide range of metal ions (Herrman, 2002; Bourissou *et al.*, 2000). On the other hand, crown ethers can coordinate to metal ions and form various complexes (Onan *et al.*, 1983; Rebek *et al.*, 1985; Gabriela, 1980; Rogers *et al.*, 1993; Costero *et al.*, 1996). In continuation of our work on the chemistry of *N*-heterocyclic carbene complexes (Liu *et al.*, 2003), we report here the synthesis and crystal structure of the title mercury *N*-heterocyclic carbene complex, (I).



(I)

The structure of the cation of (I) is shown in Fig. 1. The X-ray analysis reveals that (I) is a 21-membered macrocyclic metal crown ether complex adopting a *trans*-conformation. The geometry of the Hg coordination is distorted tetrahedral (Table 1).

The crystal packing of (I) is stabilized by weak C—H···F and C—H···O interactions (Table 2).

Experimental

The title compound was prepared according to the reported procedure of Lee *et al.* (2001). Single crystals of (I) suitable for X-ray diffraction were obtained by recrystallization from diethyl ether–nitromethane (Ratio 1:1).

Crystal data

$[Hg(C_{40}H_{42}N_4O_4)](PF_6)_2\cdot CH_3NO_2$
$M_r = 1194.35$
Triclinic, $P\bar{1}$
$a = 10.729\ (3)$ Å
$b = 12.116\ (3)$ Å
$c = 19.552\ (6)$ Å
$\alpha = 89.721\ (5)^\circ$
$\beta = 85.328\ (6)^\circ$
$\gamma = 66.677\ (4)^\circ$
$V = 2325.1\ (11)$ Å^3
$Z = 2$
$D_x = 1.706$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 932 reflections
$\theta = 2.3$–22.3°
$\mu = 3.48$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
$0.24 \times 0.20 \times 0.16$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.428$, $T_{max} = 0.573$
12 192 measured reflections
8170 independent reflections
6318 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0^\circ$
$h = -12 \rightarrow 8$
$k = -14 \rightarrow 13$
$l = -22 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.112$
$S = 1.02$
8170 reflections
605 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.06$ e Å^{-3}
$\Delta\rho_{min} = -0.91$ e Å^{-3}
Extinction correction: none

Table 1
Selected geometric parameters (Å, °).

Hg1—C24	2.068 (7)	Hg1—O3	2.934 (5)
Hg1—C1	2.076 (7)	N2—C27	1.463 (10)
Hg1—O2	2.703 (5)	C2—C3	1.342 (13)
C24—Hg1—C1	168.3 (3)	C1—N1—C2	110.2 (7)
O2—Hg1—O3	61.5 (2)	C2—N1—C4	124.0 (8)
C1—Hg1—O2	89.5 (2)	C24—N4—C34	125.9 (6)
C24—Hg1—O2	100.8 (2)	N2—C1—Hg1	130.9 (6)
C1—Hg1—O3	104.6 (2)	N1—C1—Hg1	122.4 (5)
C24—Hg1—O3	85.3 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C3—H3⋯F7^{i}	0.93	2.32	3.233 (11)	166
C3—H3⋯F11^{i}	0.93	2.47	3.217 (10)	137
C20—H20⋯O6^{ii}	0.93	2.55	3.400 (11)	152
C23—H23A⋯F12^{ii}	0.97	2.52	3.444 (11)	159
C29—H29⋯F12^{ii}	0.93	2.53	3.401 (12)	156
C41—H41B⋯F1^{ii}	0.96	2.51	3.039 (13)	114

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

H atoms were placed in calculated positions, with C—H = 0.93, 0.96 or 0.97 Å, and included in the final cycles of refinement in a riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest peak is located at (0.2951, 0.1929, 0.2341).

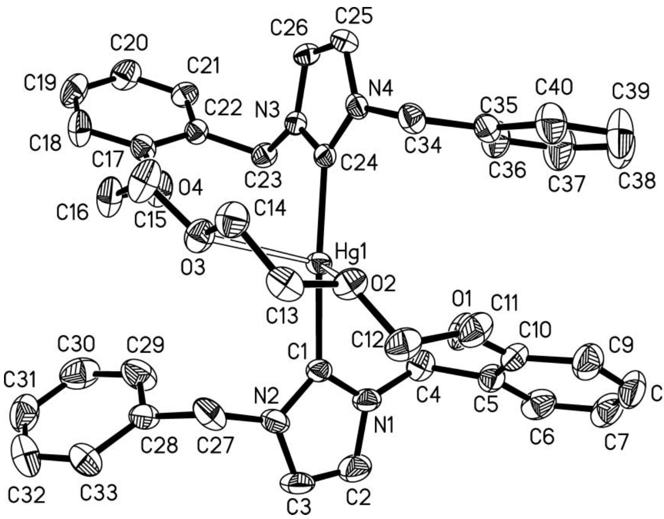


Figure 1
The cation of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms have been omitted for clarity.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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References

Bourissou, D., Guerret, O., Gabbaï, F. P. & Bertrand, G. (2000). *Chem. Rev.* **100**, 39–92.
Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Costero, A. M., Andreu, C., Monrabal, E., Tortajada, A., Ochando, L. E. & Amigó, J. M. (1996). *Tetrahedron*, **52**, 12499–12508.
Weber, G. (1980). *Acta Cryst.* B**36**, 2779–2781.
Herrman, W. A. (2002). *Angew. Chem. Int. Ed.* **41**, 1290–1309.
Lee, K.-M., Chen, J. C. C. & Lin, I. J. B. (2001). *J. Organomet. Chem.* **617–618**, 364–375.
Liu, Q. X., Xu, F. B., Li, Q. S., Zeng, X. S., Leng, X. B., Chou, Y. L. & Zhang, Z. Z. (2003). *Organometallics,* **22**, 309–314.
Onan, K., Rebek, J., Costello, T. & Marshall, L. (1983). *J. Am. Chem. Soc.* **105**, 6759–6760.
Rebek, J., Costello, T., Marshall, L., Wattley, R., Gadwood, R. C. & Onan, K. (1985). *J. Am. Chem. Soc.* **107**, 7481–7487.
Rogers, R. D., Bond., A. H. & Wolff, J. L. (1993). *J. Coord. Chem.* **29**, 187–207.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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