Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[μ-1,1′-(Butane-1,4-diyl)di-1*H*-benzimidazole-κ^2N^3:$N^{3'}$]bis{[*N*,*N*′-bis(carboxymethyl)ethylenediamine-*N*,*N*′-diacetato-κ^5O,O',O'',N,N']mercury(II)} methanol disolvate

Xue-Wen Zhu,* Bo Xiao, Zhi-Gang Yin, Heng-Yu Qian and Gang-Sen Li

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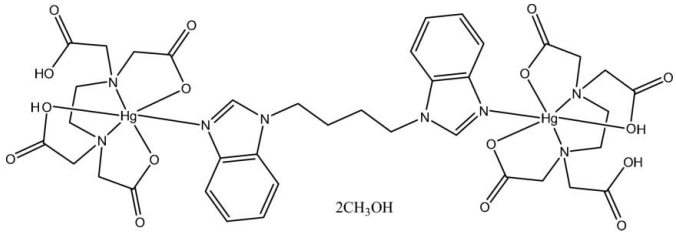
Received 24 May 2009; accepted 6 July 2009

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.011 Å; R factor = 0.045; wR factor = 0.121; data-to-parameter ratio = 14.2.

The binuclear title complex, $[Hg_2(C_{10}H_{14}N_2O_8)_2(C_{18}H_{18}N_4)]\cdot 2CH_3OH$, lies on an inversion center with the unique Hg^{II} ion coordinated in a disorted octahedral environment with one Hg—N bond significantly shorter than the other two. In the crystal structure, intermolecular O—H···O hydrogen bonds link complex and solvent molecules into a three-dimensional network.

Related literature

For the synthesis, see: Xiao *et al.* (2004); Xie *et al.* (2002). For bond lengths related mercury compounds, see: Guo & Dong (2009); Aghabozorg, *et al.* (2008).



Experimental

Crystal data

$[Hg_2(C_{10}H_{14}N_2O_8)_2(C_{18}H_{18}N_4)]\cdot 2CH_4O$
M_r = 1336.09
Monoclinic, $P2_1/n$
a = 10.274 (2) Å
b = 19.990 (3) Å
c = 11.4717 (17) Å
β = 104.035 (13)°
V = 2285.7 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 6.79 mm^{-1}
T = 291 K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.21, T_{max} = 0.29
14826 measured reflections
4397 independent reflections
3744 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.121
S = 1.04
4397 reflections
310 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −1.60 e Å^{-3}

Table 1
Selected bond lengths (Å).

Hg1—N1	2.138 (6)	Hg1—O3	2.473 (5)
Hg1—N4	2.364 (6)	Hg1—O5	2.547 (5)
Hg1—N3	2.390 (6)	Hg1—O1	2.604 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O5^{i}	0.82	1.74	2.534 (7)	164
O8—H8···O4^{ii}	0.82	1.84	2.462 (7)	131
O9—H9···O6^{iii}	0.82	2.00	2.744 (7)	150

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL*.

X-WZ thanks Zhengzhou University of Light Industry for research facilities

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2830).

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supporting information

Acta Cryst. (2009). E**65**, m912 [doi:10.1107/S1600536809026221]

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S1. Comment

Research of transition metal-organic polymers has been rapidly expanding because of their intriguing topologies and potential applications in catalysis, fluorescence, electrical conductivity and magnetism. As a result, the preparation of coordination polymers with fascinating frameworks has attracted considerable attention in recent years. For our group, metal-organic nonlinear optical (NLO) materials are of interest for various applications such as optical data processing and biological imaging (Xiao *et al.*, 2004). Some mercury complexes have already been synthesised (Guo, *et al.*, 2009; Aghabozorg *et al.*, 2008), and herein we present the synthesis and crystal structure of the title complex (I) using EDTA and bbbm (Xie, *et al.*, 2002) as ligands. The molecular structure of the title complex is shown in Fig. 1. The dinuclear complex lies on an inversion center with the unique Hg^{II} ion coordinated in a disorted octahedral coordination environment with one Hg—N bond significantly shorter than the other two, most likely, in part, as a results of steric effects from the bulky ligands. The Hg-O bond lengths are in agreement with those found in related Hg(II) complexes (Guo & Dong, 2009; Aghabozorg, *et al.,* 2008). The intramolecular Hg···Hg distance is ca. 12.21Å. In the crystal structure, intermolecular O-H···O hydrogen bonds link complex and solvent molecules into a three-dimensional network (Fig. 2). In addition there are weak $\pi\cdots\pi$ stacking interactions between benzimidazole rings related by inversion symmetry with a centroid to centroid distance of 3.556 (4)Å.

S2. Experimental

Methanol solutions of $HgCl_2.2H_2O$ (76 mg, 0.2 mmol), Na_2edta (67 mg, 0.2 mmol) and 1, 1′-(1,4-butylidene)bis-1*H*-benzimidazole (15 mg, 0.1 mmol) were mixed in a 2:2:1 molar ratio, and the reaction mixture was stirred at about 300 K for 2 h. Colourless crystals ofthe title compound were obtained from the solution after three weeks at room temperature.

S3. Refinement

H atoms were placed in calculated positions with O-H = 0.82Å and C-H = 0.93-0.98Å and included in calculated postions with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$ for methyl H atoms.

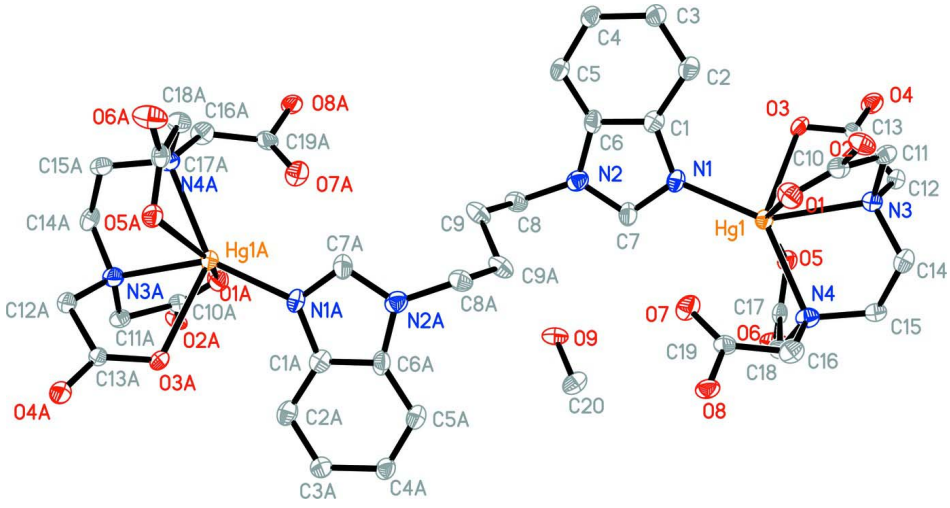

Figure 1

The molecular structure with ellipsoids shown at the 30% level. Symmetry code: (A) 1-x, 2-y, -z. The symmetry related solvent methanol molecule is not shown.

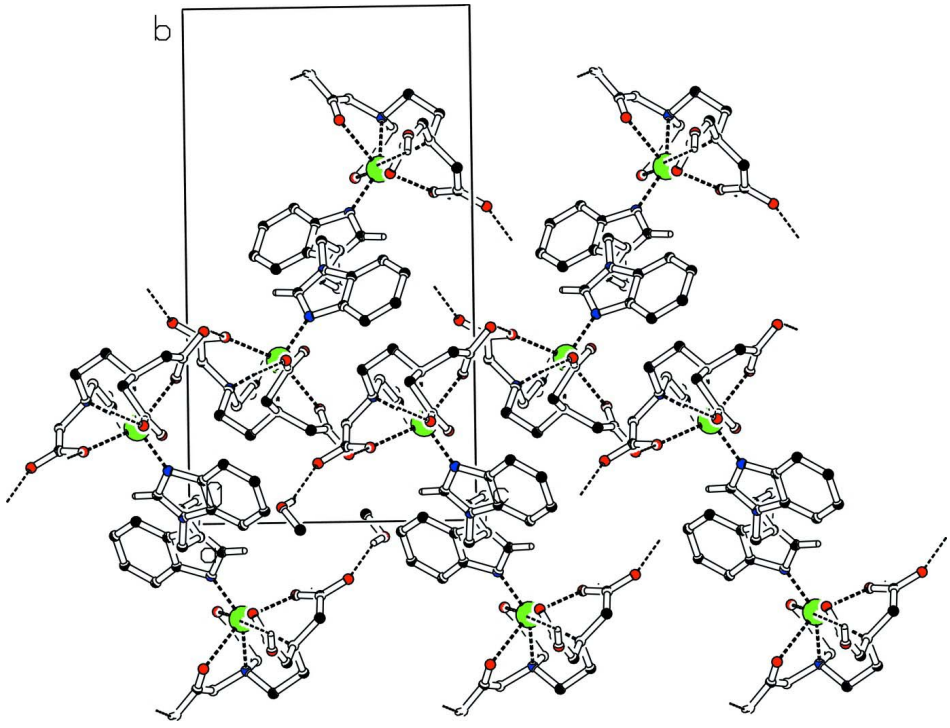

Figure 2

Part of the crystal structure with hydrogen bonds shown as dashed lines. Only H atoms included in the hydrogen bonds have been included.

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Hall symbol: -P 2yn
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$b = 19.990$ (3) Å
$c = 11.4717$ (17) Å
$\beta = 104.035$ (13)°
$V = 2285.7$ (7) Å^3
$Z = 2$
$F(000) = 1308$
$D_x = 1.941$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2608 reflections
$\theta = 2.4$–25.3°
$\mu = 6.79$ mm^{-1}
$T = 291$ K
Prism, colorless
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.21$, $T_{max} = 0.29$
14826 measured reflections
4397 independent reflections
3744 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.9°$
$h = -12\rightarrow12$
$k = -23\rightarrow24$
$l = -14\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.121$
$S = 1.04$
4397 reflections
310 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
$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 1.99P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.08$ e Å^{-3}
$\Delta\rho_{min} = -1.60$ e Å^{-3}
Absolute structure: Refinement

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}
C1	0.1031 (7)	0.0816 (3)	1.0464 (6)	0.0335 (15)
C2	0.0283 (8)	0.1117 (4)	1.1206 (6)	0.0395 (17)
H2A	−0.0216	0.1506	1.0997	0.047*

C3	0.0363 (8)	0.0778 (4)	1.2276 (7)	0.0421 (17)
H3	−0.0152	0.0924	1.2791	0.051*
C4	0.1222 (7)	0.0205 (4)	1.2612 (6)	0.0357 (15)
H4	0.1289	0.0008	1.3359	0.043*
C5	0.1937 (7)	−0.0058 (4)	1.1866 (6)	0.0370 (16)
H5	0.2490	−0.0428	1.2085	0.044*
C6	0.1803 (7)	0.0253 (4)	1.0767 (7)	0.0379 (16)
C7	0.1798 (7)	0.0552 (4)	0.8889 (7)	0.0419 (17)
H7	0.1937	0.0537	0.8118	0.050*
C8	0.3271 (7)	−0.0452 (4)	0.9728 (7)	0.0393 (16)
H8A	0.3203	−0.0567	0.8894	0.047*
H8B	0.3010	−0.0842	1.0121	0.047*
C9	0.4721 (7)	−0.0270 (4)	1.0330 (7)	0.0414 (18)
H9A	0.4770	−0.0121	1.1144	0.050*
H9B	0.5275	−0.0667	1.0376	0.050*
C10	0.0718 (8)	0.3206 (4)	0.9820 (7)	0.0406 (17)
C11	−0.0801 (8)	0.3230 (3)	0.9266 (7)	0.0349 (16)
H11A	−0.1279	0.3025	0.9806	0.042*
H11B	−0.1098	0.3690	0.9130	0.042*
C12	−0.2518 (7)	0.2659 (4)	0.7742 (7)	0.0370 (15)
H12A	−0.2759	0.2549	0.6893	0.044*
H12B	−0.3076	0.3029	0.7873	0.044*
C13	−0.2778 (7)	0.2037 (4)	0.8490 (6)	0.0321 (15)
C14	−0.0796 (8)	0.3303 (3)	0.7160 (6)	0.0348 (15)
H14A	0.0002	0.3564	0.7497	0.042*
H14B	−0.1539	0.3611	0.6894	0.042*
C15	−0.0589 (8)	0.2912 (4)	0.6100 (7)	0.0385 (16)
H15A	−0.1428	0.2700	0.5699	0.046*
H15B	−0.0341	0.3218	0.5534	0.046*
C16	0.0334 (8)	0.1861 (3)	0.5512 (7)	0.0356 (15)
H16A	0.0232	0.2068	0.4731	0.043*
H16B	0.1149	0.1595	0.5675	0.043*
C17	−0.0798 (7)	0.1425 (3)	0.5481 (6)	0.0313 (14)
C18	0.1874 (7)	0.2721 (4)	0.6685 (7)	0.0415 (17)
H18A	0.2052	0.2850	0.5923	0.050*
H18B	0.1872	0.3124	0.7154	0.050*
C19	0.2947 (7)	0.2284 (4)	0.7319 (7)	0.0363 (15)
H20A	0.2877	0.0381	0.5581	0.055*
H20B	0.4119	0.0503	0.6662	0.055*
H20C	0.4187	−0.0043	0.5697	0.055*
C20	0.3614 (9)	0.0155 (4)	0.6152 (7)	0.0436 (18)
Hg1	0.02119 (3)	0.185765 (13)	0.82144 (2)	0.03426 (13)
N1	0.1043 (6)	0.1013 (3)	0.9279 (6)	0.0395 (14)
N2	0.2331 (6)	0.0113 (3)	0.9788 (6)	0.0385 (14)
N3	−0.1082 (6)	0.2859 (3)	0.8103 (6)	0.0375 (13)
N4	0.0466 (6)	0.2392 (3)	0.6444 (5)	0.0366 (13)
O1	0.1436 (5)	0.2817 (3)	0.9589 (5)	0.0465 (13)
O2	0.1103 (5)	0.3704 (3)	1.0576 (5)	0.0414 (12)

H2	0.1924	0.3733	1.0740	0.050*
O3	−0.1763 (5)	0.1700 (3)	0.9062 (5)	0.0412 (13)
O4	−0.3977 (6)	0.1878 (3)	0.8430 (5)	0.0443 (13)
O5	−0.1373 (5)	0.1400 (3)	0.6322 (5)	0.0380 (11)
O6	−0.1182 (6)	0.1106 (3)	0.4498 (5)	0.0502 (15)
O7	0.2823 (6)	0.1763 (3)	0.7841 (6)	0.0443 (13)
O8	0.4098 (5)	0.2491 (3)	0.7194 (5)	0.0401 (12)
H8	0.4604	0.2171	0.7225	0.048*
O9	0.3170 (5)	−0.0289 (3)	0.6776 (5)	0.0415 (12)
H9	0.2418	−0.0408	0.6411	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.040 (4)	0.027 (3)	0.029 (3)	−0.005 (3)	0.000 (3)	−0.007 (3)
C2	0.041 (4)	0.040 (4)	0.031 (4)	0.001 (3)	−0.004 (3)	−0.002 (3)
C3	0.041 (4)	0.042 (4)	0.046 (4)	0.004 (3)	0.015 (3)	0.010 (3)
C4	0.029 (3)	0.042 (4)	0.034 (4)	0.000 (3)	0.001 (3)	0.007 (3)
C5	0.042 (4)	0.032 (4)	0.033 (4)	0.004 (3)	0.000 (3)	0.001 (3)
C6	0.027 (3)	0.039 (4)	0.044 (4)	0.005 (3)	0.001 (3)	0.008 (3)
C7	0.038 (4)	0.040 (4)	0.046 (4)	0.010 (3)	0.007 (3)	0.006 (3)
C8	0.034 (4)	0.044 (4)	0.042 (4)	−0.005 (3)	0.014 (3)	−0.002 (3)
C9	0.032 (4)	0.046 (4)	0.050 (5)	−0.005 (3)	0.016 (3)	−0.013 (4)
C10	0.038 (4)	0.051 (5)	0.035 (4)	0.007 (3)	0.013 (3)	0.007 (3)
C11	0.039 (4)	0.030 (3)	0.038 (4)	−0.005 (3)	0.014 (3)	0.009 (3)
C12	0.040 (4)	0.036 (4)	0.037 (4)	0.011 (3)	0.013 (3)	0.009 (3)
C13	0.034 (4)	0.038 (4)	0.026 (3)	0.011 (3)	0.011 (3)	0.003 (3)
C14	0.037 (4)	0.030 (3)	0.031 (4)	−0.004 (3)	−0.005 (3)	0.000 (3)
C15	0.045 (4)	0.043 (4)	0.030 (4)	0.003 (3)	0.015 (3)	0.004 (3)
C16	0.036 (4)	0.035 (4)	0.038 (4)	−0.008 (3)	0.013 (3)	−0.002 (3)
C17	0.031 (3)	0.020 (3)	0.040 (4)	0.003 (3)	0.004 (3)	0.002 (3)
C18	0.041 (4)	0.036 (4)	0.047 (4)	−0.012 (3)	0.011 (3)	0.002 (3)
C19	0.031 (3)	0.038 (4)	0.045 (4)	−0.005 (3)	0.018 (3)	0.005 (3)
C20	0.062 (5)	0.029 (3)	0.037 (4)	−0.011 (3)	0.008 (4)	−0.001 (3)
Hg1	0.02994 (18)	0.03898 (19)	0.03433 (18)	0.00717 (11)	0.00868 (11)	0.00914 (11)
N1	0.033 (3)	0.047 (4)	0.035 (3)	0.010 (3)	0.001 (3)	0.010 (3)
N2	0.035 (3)	0.045 (3)	0.034 (3)	−0.004 (3)	0.005 (3)	0.004 (3)
N3	0.044 (3)	0.037 (3)	0.034 (3)	0.006 (3)	0.014 (3)	0.003 (3)
N4	0.032 (3)	0.045 (3)	0.032 (3)	−0.007 (3)	0.007 (2)	0.000 (3)
O1	0.036 (3)	0.061 (4)	0.039 (3)	0.005 (3)	0.001 (2)	−0.007 (3)
O2	0.028 (3)	0.053 (3)	0.049 (3)	−0.004 (2)	0.020 (2)	−0.002 (3)
O3	0.042 (3)	0.044 (3)	0.041 (3)	0.012 (2)	0.017 (2)	0.024 (2)
O4	0.033 (3)	0.057 (4)	0.042 (3)	0.002 (2)	0.008 (2)	0.015 (2)
O5	0.031 (2)	0.044 (3)	0.038 (3)	0.002 (2)	0.006 (2)	0.008 (2)
O6	0.050 (3)	0.056 (3)	0.050 (3)	−0.030 (3)	0.023 (3)	−0.018 (3)
O7	0.039 (3)	0.036 (3)	0.056 (4)	−0.012 (2)	0.009 (3)	0.011 (2)
O8	0.029 (2)	0.053 (3)	0.040 (3)	−0.005 (2)	0.012 (2)	0.014 (2)
O9	0.044 (3)	0.050 (3)	0.035 (3)	−0.015 (2)	0.018 (2)	−0.006 (2)

Geometric parameters (Å, º)

C1—C6	1.372 (10)	C13—O3	1.282 (9)
C1—C2	1.412 (11)	C14—N3	1.481 (9)
C1—N1	1.417 (9)	C14—C15	1.503 (11)
C2—C3	1.388 (10)	C14—H14A	0.9700
C2—H2A	0.9300	C14—H14B	0.9700
C3—C4	1.440 (10)	C15—N4	1.486 (10)
C3—H3	0.9300	C15—H15A	0.9700
C4—C5	1.361 (10)	C15—H15B	0.9700
C4—H4	0.9300	C16—C17	1.446 (9)
C5—C6	1.383 (10)	C16—N4	1.489 (9)
C5—H5	0.9300	C16—H16A	0.9700
C6—N2	1.389 (10)	C16—H16B	0.9700
C7—N1	1.348 (10)	C17—O5	1.248 (9)
C7—N2	1.364 (10)	C17—O6	1.271 (9)
C7—H7	0.9300	C18—C19	1.456 (11)
C8—N2	1.498 (10)	C18—N4	1.552 (9)
C8—C9	1.527 (10)	C18—H18A	0.9700
C8—H8A	0.9700	C18—H18B	0.9700
C8—H8B	0.9700	C19—O7	1.224 (9)
C9—C9^{i}	1.509 (15)	C19—O8	1.293 (8)
C9—H9A	0.9700	C20—O9	1.291 (9)
C9—H9B	0.9700	C20—H20A	0.9822
C10—O1	1.148 (10)	C20—H20B	0.9735
C10—O2	1.316 (10)	C20—H20C	0.9611
C10—C11	1.536 (11)	Hg1—N1	2.138 (6)
C11—N3	1.492 (10)	Hg1—N4	2.364 (6)
C11—H11A	0.9700	Hg1—N3	2.390 (6)
C11—H11B	0.9700	Hg1—O3	2.473 (5)
C12—N3	1.488 (10)	Hg1—O5	2.547 (5)
C12—C13	1.569 (10)	Hg1—O1	2.604 (6)
C12—H12A	0.9700	O2—H2	0.8200
C12—H12B	0.9700	O8—H8	0.8200
C13—O4	1.258 (9)	O9—H9	0.8200
C6—C1—C2	124.2 (7)	C17—C16—N4	112.3 (6)
C6—C1—N1	109.3 (6)	C17—C16—H16A	109.1
C2—C1—N1	126.3 (6)	N4—C16—H16A	109.1
C3—C2—C1	113.6 (7)	C17—C16—H16B	109.1
C3—C2—H2A	123.2	N4—C16—H16B	109.1
C1—C2—H2A	123.2	H16A—C16—H16B	107.9
C2—C3—C4	121.8 (7)	O5—C17—O6	124.2 (6)
C2—C3—H3	119.1	O5—C17—C16	122.2 (6)
C4—C3—H3	119.1	O6—C17—C16	113.5 (6)
C5—C4—C3	121.9 (7)	C19—C18—N4	113.2 (6)
C5—C4—H4	119.1	C19—C18—H18A	108.9
C3—C4—H4	119.1	N4—C18—H18A	108.9

C4—C5—C6	116.7 (7)	C19—C18—H18B	108.9
C4—C5—H5	121.6	N4—C18—H18B	108.9
C6—C5—H5	121.6	H18A—C18—H18B	107.7
C1—C6—C5	121.6 (7)	O7—C19—O8	122.2 (7)
C1—C6—N2	106.0 (6)	O7—C19—C18	126.9 (7)
C5—C6—N2	132.4 (7)	O8—C19—C18	110.8 (6)
N1—C7—N2	110.3 (7)	O9—C20—H20A	111.4
N1—C7—H7	124.9	O9—C20—H20B	111.5
N2—C7—H7	124.9	H20A—C20—H20B	106.6
N2—C8—C9	111.6 (6)	O9—C20—H20C	111.3
N2—C8—H8A	109.3	H20A—C20—H20C	107.5
C9—C8—H8A	109.3	H20B—C20—H20C	108.3
N2—C8—H8B	109.3	N1—Hg1—N4	137.4 (2)
C9—C8—H8B	109.3	N1—Hg1—N3	146.4 (2)
H8A—C8—H8B	108.0	N4—Hg1—N3	75.6 (2)
C9^{i}—C9—C8	113.0 (9)	N1—Hg1—O3	85.8 (2)
C9^{i}—C9—H9A	109.0	N4—Hg1—O3	131.86 (19)
C8—C9—H9A	109.0	N3—Hg1—O3	68.26 (19)
C9^{i}—C9—H9B	109.0	N1—Hg1—O5	106.7 (2)
C8—C9—H9B	109.0	N4—Hg1—O5	67.09 (18)
H9A—C9—H9B	107.8	N3—Hg1—O5	91.30 (19)
O1—C10—O2	123.9 (8)	O3—Hg1—O5	82.73 (18)
O1—C10—C11	124.8 (8)	N1—Hg1—O1	99.7 (2)
O2—C10—C11	111.3 (6)	N4—Hg1—O1	92.9 (2)
N3—C11—C10	108.2 (6)	N3—Hg1—O1	66.2 (2)
N3—C11—H11A	110.1	O3—Hg1—O1	100.25 (19)
C10—C11—H11A	110.1	O5—Hg1—O1	153.57 (18)
N3—C11—H11B	110.1	C7—N1—C1	105.6 (6)
C10—C11—H11B	110.1	C7—N1—Hg1	122.1 (5)
H11A—C11—H11B	108.4	C1—N1—Hg1	132.2 (5)
N3—C12—C13	110.5 (6)	C7—N2—C6	108.5 (6)
N3—C12—H12A	109.5	C7—N2—C8	126.6 (6)
C13—C12—H12A	109.5	C6—N2—C8	124.9 (6)
N3—C12—H12B	109.5	C14—N3—C12	108.5 (6)
C13—C12—H12B	109.5	C14—N3—C11	109.0 (5)
H12A—C12—H12B	108.1	C12—N3—C11	110.2 (6)
O4—C13—O3	124.0 (7)	C14—N3—Hg1	109.5 (4)
O4—C13—C12	117.8 (6)	C12—N3—Hg1	106.9 (4)
O3—C13—C12	118.1 (6)	C11—N3—Hg1	112.6 (4)
N3—C14—C15	111.8 (6)	C15—N4—C16	112.1 (6)
N3—C14—H14A	109.2	C15—N4—C18	109.8 (6)
C15—C14—H14A	109.2	C16—N4—C18	110.4 (6)
N3—C14—H14B	109.2	C15—N4—Hg1	108.6 (4)
C15—C14—H14B	109.2	C16—N4—Hg1	106.5 (4)
H14A—C14—H14B	107.9	C18—N4—Hg1	109.3 (4)
N4—C15—C14	112.7 (6)	C10—O1—Hg1	113.3 (6)
N4—C15—H15A	109.1	C10—O2—H2	109.5
C14—C15—H15A	109.1	C13—O3—Hg1	112.0 (4)

N4—C15—H15B	109.1	C17—O5—Hg1	108.7 (4)
C14—C15—H15B	109.1	C19—O8—H8	109.5
H15A—C15—H15B	107.8	C20—O9—H9	109.5
C6—C1—C2—C3	−1.8 (11)	O5—Hg1—N3—C14	−76.7 (5)
N1—C1—C2—C3	173.8 (7)	O1—Hg1—N3—C14	89.0 (5)
C1—C2—C3—C4	4.6 (11)	N1—Hg1—N3—C12	−83.0 (6)
C2—C3—C4—C5	−4.0 (12)	N4—Hg1—N3—C12	106.5 (4)
C3—C4—C5—C6	0.1 (11)	O3—Hg1—N3—C12	−41.0 (4)
C2—C1—C6—C5	−1.9 (11)	O5—Hg1—N3—C12	40.6 (4)
N1—C1—C6—C5	−178.2 (7)	O1—Hg1—N3—C12	−153.7 (5)
C2—C1—C6—N2	178.3 (7)	N1—Hg1—N3—C11	38.1 (7)
N1—C1—C6—N2	2.0 (8)	N4—Hg1—N3—C11	−132.3 (5)
C4—C5—C6—C1	2.7 (11)	O3—Hg1—N3—C11	80.1 (5)
C4—C5—C6—N2	−177.5 (8)	O5—Hg1—N3—C11	161.8 (4)
N2—C8—C9—C9^{i}	−67.0 (10)	O1—Hg1—N3—C11	−32.5 (4)
O1—C10—C11—N3	−21.5 (10)	C14—C15—N4—C16	159.3 (6)
O2—C10—C11—N3	156.8 (6)	C14—C15—N4—C18	−77.6 (8)
N3—C12—C13—O4	168.5 (6)	C14—C15—N4—Hg1	41.9 (7)
N3—C12—C13—O3	−15.8 (9)	C17—C16—N4—C15	−72.5 (8)
N3—C14—C15—N4	−54.6 (8)	C17—C16—N4—C18	164.8 (6)
N4—C16—C17—O5	−16.4 (10)	C17—C16—N4—Hg1	46.2 (7)
N4—C16—C17—O6	159.9 (6)	C19—C18—N4—C15	165.0 (6)
N4—C18—C19—O7	−14.0 (12)	C19—C18—N4—C16	−71.0 (8)
N4—C18—C19—O8	161.4 (6)	C19—C18—N4—Hg1	45.9 (7)
N2—C7—N1—C1	−4.4 (8)	N1—Hg1—N4—C15	171.9 (5)
N2—C7—N1—Hg1	172.8 (5)	N3—Hg1—N4—C15	−15.9 (5)
C6—C1—N1—C7	1.4 (8)	O3—Hg1—N4—C15	26.0 (6)
C2—C1—N1—C7	−174.8 (7)	O5—Hg1—N4—C15	81.8 (5)
C6—C1—N1—Hg1	−175.4 (5)	O1—Hg1—N4—C15	−80.5 (5)
C2—C1—N1—Hg1	8.4 (11)	N1—Hg1—N4—C16	51.0 (6)
N4—Hg1—N1—C7	−12.1 (8)	N3—Hg1—N4—C16	−136.8 (5)
N3—Hg1—N1—C7	−178.3 (5)	O3—Hg1—N4—C16	−94.9 (5)
O3—Hg1—N1—C7	143.1 (6)	O5—Hg1—N4—C16	−39.1 (4)
O5—Hg1—N1—C7	62.0 (6)	O1—Hg1—N4—C16	158.6 (4)
O1—Hg1—N1—C7	−117.2 (6)	N1—Hg1—N4—C18	−68.3 (6)
N4—Hg1—N1—C1	164.2 (5)	N3—Hg1—N4—C18	103.8 (5)
N3—Hg1—N1—C1	−2.0 (9)	O3—Hg1—N4—C18	145.8 (4)
O3—Hg1—N1—C1	−40.6 (6)	O5—Hg1—N4—C18	−158.5 (5)
O5—Hg1—N1—C1	−121.7 (6)	O1—Hg1—N4—C18	39.3 (5)
O1—Hg1—N1—C1	59.1 (7)	O2—C10—O1—Hg1	174.3 (6)
N1—C7—N2—C6	5.8 (9)	C11—C10—O1—Hg1	−7.6 (10)
N1—C7—N2—C8	−177.3 (6)	N1—Hg1—O1—C10	−125.7 (6)
C1—C6—N2—C7	−4.7 (8)	N4—Hg1—O1—C10	95.2 (6)
C5—C6—N2—C7	175.6 (8)	N3—Hg1—O1—C10	22.3 (6)
C1—C6—N2—C8	178.3 (6)	O3—Hg1—O1—C10	−38.2 (6)
C5—C6—N2—C8	−1.4 (13)	O5—Hg1—O1—C10	56.1 (8)
C9—C8—N2—C7	100.6 (9)	O4—C13—O3—Hg1	153.3 (6)

C9—C8—N2—C6	−82.9 (9)	C12—C13—O3—Hg1	−22.1 (8)
C15—C14—N3—C12	−79.7 (7)	N1—Hg1—O3—C13	−166.5 (5)
C15—C14—N3—C11	160.2 (6)	N4—Hg1—O3—C13	−9.0 (6)
C15—C14—N3—Hg1	36.6 (7)	N3—Hg1—O3—C13	35.3 (5)
C13—C12—N3—C14	163.5 (6)	O5—Hg1—O3—C13	−59.1 (5)
C13—C12—N3—C11	−77.1 (7)	O1—Hg1—O3—C13	94.4 (5)
C13—C12—N3—Hg1	45.5 (6)	O6—C17—O5—Hg1	163.8 (6)
C10—C11—N3—C14	−80.9 (7)	C16—C17—O5—Hg1	−20.2 (8)
C10—C11—N3—C12	160.1 (6)	N1—Hg1—O5—C17	−101.6 (5)
C10—C11—N3—Hg1	40.9 (6)	N4—Hg1—O5—C17	33.4 (4)
N1—Hg1—N3—C14	159.6 (5)	N3—Hg1—O5—C17	107.1 (5)
N4—Hg1—N3—C14	−10.8 (4)	O3—Hg1—O5—C17	175.0 (5)
O3—Hg1—N3—C14	−158.4 (5)	O1—Hg1—O5—C17	76.6 (6)

Symmetry code: (i) −*x*+1, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O5^{ii}	0.82	1.74	2.534 (7)	164
O8—H8···O4^{iii}	0.82	1.84	2.462 (7)	131
O9—H9···O6^{iv}	0.82	2.00	2.744 (7)	150

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