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Propane-1,3-diammonium bis[aquachlorido(4-hydroxypyridine-2,6-dicarboxylato-κ^3O^2,N,O^6)mercurate(II)] tetrahydrate

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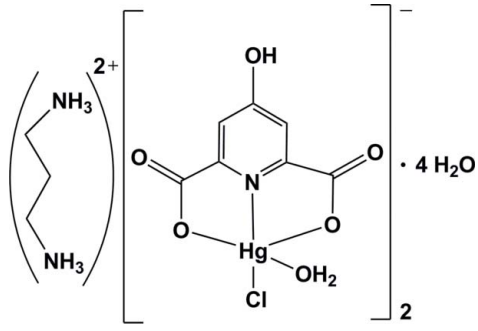
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.022; wR factor = 0.047; data-to-parameter ratio = 16.3.

The reaction of mercury(II) chloride dihydrate, propane-1,3-diamine and 4-hydroxypyridine-2,6-dicarboxylic acid in a 1:1:1 molar ratio in aqueous solution, resulted in the formation of the title compound, $(C_3H_{12}N_2)[Hg(C_7H_3NO_5)Cl(H_2O)]_2\cdot 4H_2O$ or $(pnH_2)[Hg(hypydc)Cl(H_2O)]_2\cdot 4H_2O$ (where pn is propane-1,3-diamine and hypydcH_2 is 4-hydroxypyridine-2,6-dicarboxylic acid). The metal atom is coordinated by one chloride group, one water molecule *cis* to the chloride ligand and one $(hypydc)^{2-}$ ligand. The coordinated water molecule is almost perpendicular to the plane of the aromatic ring of $(hypydc)^{2-}$. The geometry of the resulting $HgClNO_3$ coordination can be described as distorted square-pyramidal. This structure also contains propane-1,3-diammonium (site symmetry 2) as a counter-ion and four uncoordinated water molecules. There is a wide range of non-covalent interactions consisting of hydrogen bonding [of the types O—H···O, N—H···O and C—H···O, with $D\cdots A$ ranging from 2.548 (5) to 3.393 (6) Å] and ion pairing.

Related literature

For related literature, see: Aghabozorg *et al.* (2007, 2008); Aghabozorg, Ghadermazi & Attar Gharamaleki (2006); Aghabozorg, Ghadermazi & Ramezanipour (2006); Aghabozorg, Ghasemikhah *et al.* (2006); Ramezanipour *et al.* (2005).



Experimental

Crystal data

$(C_3H_{12}N_2)[Hg(C_7H_3NO_5)Cl(H_2O)]_2\cdot 4H_2O$
M_r = 1018.53
Monoclinic, $C2/c$
a = 29.2207 (13) Å
b = 6.7630 (3) Å
c = 15.4913 (7) Å
β = 114.5130 (10)°
V = 2785.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 11.28 mm^{-1}
T = 100 (2) K
0.11 × 0.08 × 0.07 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.284, T_{max} = 0.457
9362 measured reflections
3041 independent reflections
2632 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.047
S = 0.99
3041 reflections
187 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.84 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4^{i}	0.92	1.63	2.548 (5)	173
N2—H1C···O2W^{ii}	0.89	2.02	2.830 (5)	150
N2—H1D···O2W^{iii}	0.89	2.30	3.096 (6)	149
N2—H1E···O2W^{iv}	0.89	1.96	2.824 (6)	165
O1W—H1A···O5^{ii}	0.82	2.08	2.854 (5)	157
O1W—H1B···O2^{v}	0.82	2.06	2.837 (6)	157
O2W—H2B···O1	0.85	1.98	2.771 (6)	154
O2W—H2C···O2^{vi}	0.85	1.94	2.777 (5)	169
O3W—H3A···O3^{v}	0.85	2.30	3.019 (6)	142
O3W—H3B···O5	0.85	1.93	2.766 (6)	169
C8—H8B···O1	0.97	2.45	3.393 (6)	163

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *APEX2*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2244).

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supporting information

Acta Cryst. (2008). E**64**, m1065–m1066 [doi:10.1107/S1600536808022897]

Propane-1,3-diammonium bis[aquachlorido(4-hydroxypyridine-2,6-dicarboxylato-κ^3O^2,N,O^6)mercurate(II)] tetrahydrate

Hossein Aghabozorg, Sara Bagheri, Mohammad Heidari, Mohammad Ghadermazi and Jafar Attar Gharamaleki

S1. Comment

Recently, we have defined a plan to prepare water soluble proton-transfer compounds as novel self assembled systems that can function as suitable ligands in the synthesis of metal complexes. In this regard, we have reported cases in which protons transfer from pyridine-2,6-dicarboxylic acid, $pydcH_2$, and benzene-1,2,4,5-tetracarboxylicacid, $btcH_4$, to propane-1,3-diamine (pn) and 1,10-phenanthroline, (phen). These resulted in the formation of some novel proton transfer compounds such as $(pnH_2)(pydc).(pydcH_2).2.5H_2O$ (Aghabozorg, Ghadermazi, Ramezanipour, 2006), $(pnH_2)_2(btc).2H_2O$ (Aghabozorg, *et al.*, 2007) and $(phenH)_4(btcH_3)_2(btcH_2)$ (Aghabozorg, Ghadermazi, Attar Gharamaleki, 2006). For more details and related literature see our recent review article (Aghabozorg, *et al.*, 2008).

The molecular structure and crystal packing diagram of the title compound are presented in Figs. 1 and 2, respectively.

The Hg^{II} atom is five-coordinated by one chloro group, one water molecule and one 4-hydroxypyridine-2,6-dicarboxylate, or $(hypydc)^{2-}$, group which is coordinated through one pyridine N atom and two carboxylate O atoms. These distances are in good agreement with our two recently reported Hg^{II} structures (Aghabozorg, Ghasemikhah, Ghadermazi, *et al.*, 2006; Ramezanipour *et al.*, 2005).

The sum of the Cl1—Hg1—O1, O1—Hg1—N1, N1—Hg1—O4 and O4—Hg1—Cl1 bond angles equals 361.33 °, which indicates that these four atoms are almost located in the plane. As it can be seen, the O1W atom of the coordinated water molecule occupies the axial position, while the O1, O4, N1 and Cl1 atoms form the equatorial plane of the square pyramid. The O1W—Hg1—Cl1, O1W—Hg1—N1, O1W—Hg1—O1 and O1W—Hg1—O4 angles are 94.63 (7), 96.83 (11), 91.72 (9) and 82.81 (9)°, respectively, indicating that the coordinated water molecule is located at *cis* position to the chloro ligand and is also almost perpendicular to the square plane of the pyramid. Therefore, the geometry of the resulting $HgClNO_3$ coordination can be described as distorted square pyramidal. The molecular structure of the title compound also contains propane-1,3-diammonium (site symmetry 2) as counter-ion and four uncoordinated water molecules. In the crystal structure, there is a wide range of non-covalent interactions consisting of hydrogen bonding (of the type O—H···O, N—H···O and C—H···O with D···A ranging from 2.548 (5) Å to 3.393 (6) Å) and ion pairing (Table 1).

S2. Experimental

Aqueous solutions of $HgCl_2.2H_2O$ (76 mg, 0.2 mmol), propane-1,3-diamine (18 mg, 0.2 mmol) and 4-hydroxypyridine-2,6-dicarboxylic acid (72 mg, 0.2 mmol) were mixed in a 1:1:1 molar ratio, and the reaction mixture was heated at about 313 K for 2 h. Colourless crystals of the title compound were obtained from the solution after three weeks at room temperature.

S3. Refinement

The hydrogen atoms of the NH_3 and OH groups, and also H atoms of water molecules were found in difference Fourier synthesis. The H(C) atom positions were calculated. All H(N) and H(O) atoms were refined in isotropic approximation in rigid model, the H(C) atoms were refined in isotropic approximation in riding model with with the U_{iso}(H) parameters equal to 1.2 U_{eq}(Ci) and 1.5 U_{eq}(Cii) for OH, NH3 group and water molecules, where U(C) are the equivalent thermal parameters of the atoms to which corresponding H atoms are bonded.

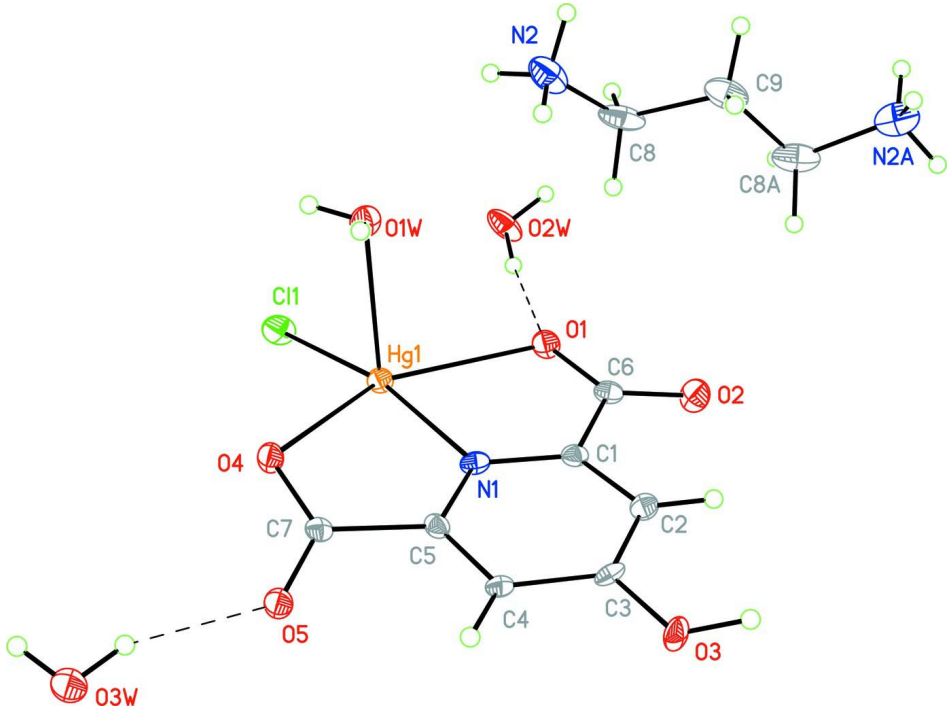

Figure 1

The molecular structure of the title compound, displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. Symmetry code A: -*x* + 1, *y*, -*z* + 3/2.

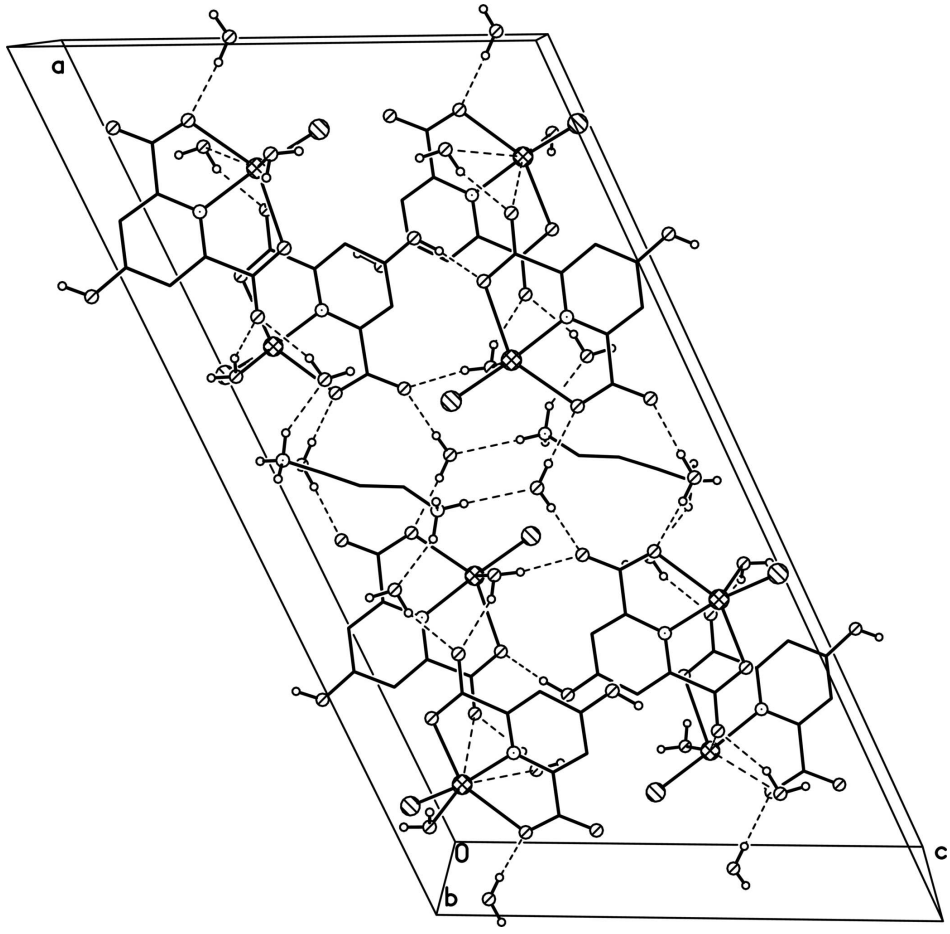

Figure 2

The crystal packing of the title compound viewed down the *b* axis, hydrogen bonds are shown as dashed lines.

Propane-1,3-diammonium bis[aquachlorido(4-hydroxypyridine-2,6- dicarboxylato-κ^3O^2,N,O^6)mercurate(II)] tetrahydrate

Crystal data

$(C_3H_{12}N_2)[Hg(C_7H_3NO_5)Cl(H_2O)]_2\cdot 4H_2O$
M_r = 1018.53
Monoclinic, *C*2/*c*
a = 29.2207 (13) Å
b = 6.7630 (3) Å
c = 15.4913 (7) Å
β = 114.513 (1)°
V = 2785.5 (2) Å^3
Z = 4
F(000) = 1928
D_x = 2.429 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 2868 reflections
θ = 3–27°
μ = 11.28 mm^{-1}
T = 100 K
Prism, colourless
0.11 × 0.08 × 0.07 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.284, T_{max} = 0.457
9362 measured reflections
3041 independent reflections

2632 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.5°$
$h = -37 \rightarrow 36$
$k = -8 \rightarrow 8$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.047$
$S = 0.99$
3041 reflections
187 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.84$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.360437 (6)	0.72342 (2)	0.843452 (11)	0.01284 (6)
Cl1	0.40073 (4)	0.88117 (16)	0.98816 (7)	0.0205 (2)
O1	0.41510 (10)	0.6883 (4)	0.7583 (2)	0.0163 (6)
O2	0.40827 (11)	0.6472 (5)	0.6102 (2)	0.0200 (7)
O3	0.22507 (10)	0.4439 (4)	0.43123 (19)	0.0161 (6)
H3	0.2422	0.4065	0.3956	0.024*
O4	0.27295 (10)	0.6300 (4)	0.8299 (2)	0.0159 (6)
O5	0.19566 (10)	0.6269 (5)	0.7138 (2)	0.0173 (6)
N1	0.31418 (12)	0.6356 (5)	0.7000 (2)	0.0115 (7)
C1	0.33511 (15)	0.6083 (6)	0.6378 (3)	0.0118 (8)
C2	0.30679 (15)	0.5421 (6)	0.5469 (3)	0.0135 (9)
H2A	0.3218	0.5200	0.5053	0.016*
C3	0.25554 (15)	0.5084 (6)	0.5177 (3)	0.0118 (9)
C4	0.23390 (15)	0.5464 (6)	0.5813 (3)	0.0120 (8)
H4A	0.1994	0.5324	0.5627	0.014*
C5	0.26445 (15)	0.6044 (6)	0.6713 (3)	0.0113 (8)
C6	0.39097 (15)	0.6514 (6)	0.6713 (3)	0.0130 (8)
C7	0.24210 (15)	0.6239 (6)	0.7438 (3)	0.0106 (8)
N2	0.47091 (14)	0.1672 (6)	0.8789 (3)	0.0266 (9)
H1C	0.4384	0.1443	0.8438	0.040*
H1D	0.4744	0.2326	0.9311	0.040*
H1E	0.4873	0.0528	0.8949	0.040*

C8	0.49190 (17)	0.2877 (7)	0.8234 (3)	0.0254 (11)
H8A	0.5237	0.3455	0.8659	0.030*
H8B	0.4689	0.3945	0.7916	0.030*
C9	0.5000	0.1595 (9)	0.7500	0.0249 (15)
H9A	0.4711	0.0763	0.7190	0.030*
O1W	0.38232 (10)	0.3754 (4)	0.91250 (19)	0.0169 (6)
H1A	0.3582	0.3001	0.8895	0.025*
H1B	0.3848	0.3976	0.9663	0.025*
O2W	0.50594 (11)	0.7731 (4)	0.9089 (2)	0.0245 (7)
H2B	0.4842	0.7451	0.8535	0.037*
H2C	0.5315	0.7479	0.8977	0.037*
O3W	0.12234 (11)	0.6629 (5)	0.7822 (2)	0.0245 (7)
H3A	0.1428	0.6436	0.8395	0.037*
H3B	0.1438	0.6364	0.7600	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.00977 (9)	0.01538 (9)	0.01123 (8)	−0.00051 (7)	0.00222 (6)	−0.00185 (7)
Cl1	0.0158 (5)	0.0230 (6)	0.0160 (5)	0.0004 (4)	−0.0002 (4)	−0.0066 (4)
O1	0.0102 (15)	0.0221 (16)	0.0141 (15)	−0.0007 (12)	0.0025 (12)	−0.0031 (13)
O2	0.0127 (16)	0.0302 (17)	0.0187 (16)	−0.0032 (13)	0.0082 (13)	0.0011 (14)
O3	0.0106 (15)	0.0279 (17)	0.0084 (14)	−0.0034 (12)	0.0026 (12)	−0.0056 (12)
O4	0.0095 (15)	0.0257 (17)	0.0120 (15)	−0.0008 (12)	0.0038 (12)	−0.0012 (13)
O5	0.0103 (16)	0.0285 (17)	0.0128 (15)	0.0006 (13)	0.0044 (13)	−0.0003 (13)
N1	0.0085 (17)	0.0113 (16)	0.0103 (17)	−0.0020 (13)	−0.0004 (14)	−0.0009 (14)
C1	0.012 (2)	0.010 (2)	0.012 (2)	0.0019 (15)	0.0034 (17)	0.0010 (16)
C2	0.017 (2)	0.011 (2)	0.014 (2)	0.0006 (16)	0.0073 (18)	0.0031 (16)
C3	0.013 (2)	0.011 (2)	0.008 (2)	−0.0001 (16)	0.0018 (18)	0.0040 (15)
C4	0.008 (2)	0.015 (2)	0.009 (2)	0.0020 (16)	0.0006 (17)	0.0015 (16)
C5	0.010 (2)	0.011 (2)	0.014 (2)	0.0012 (15)	0.0068 (18)	0.0022 (16)
C6	0.012 (2)	0.0094 (19)	0.016 (2)	0.0002 (16)	0.0040 (18)	0.0009 (17)
C7	0.012 (2)	0.0068 (19)	0.012 (2)	0.0007 (15)	0.0039 (17)	−0.0015 (15)
N2	0.018 (2)	0.028 (2)	0.031 (2)	0.0039 (17)	0.0067 (18)	−0.0086 (18)
C8	0.013 (2)	0.017 (2)	0.033 (3)	0.0037 (18)	−0.004 (2)	−0.003 (2)
C9	0.013 (3)	0.017 (3)	0.040 (4)	0.000	0.005 (3)	0.000
O1W	0.0174 (17)	0.0173 (15)	0.0139 (15)	−0.0014 (12)	0.0046 (13)	−0.0020 (12)
O2W	0.0126 (16)	0.0283 (18)	0.0305 (18)	0.0014 (13)	0.0067 (14)	−0.0098 (15)
O3W	0.0126 (16)	0.039 (2)	0.0191 (16)	0.0034 (14)	0.0037 (14)	0.0031 (15)

Geometric parameters (Å, º)

Hg1—N1	2.151 (3)	C2—H2A	0.9300
Hg1—Cl1	2.3151 (10)	C3—C4	1.397 (5)
Hg1—O1	2.469 (3)	C4—C5	1.365 (6)
Hg1—O1W	2.555 (3)	C4—Hg1^{ii}	4.049 (4)
Hg1—O4	2.556 (3)	C4—H4A	0.9300
Hg1—C1	3.058 (4)	C5—C7	1.521 (5)

Hg1—C5	3.069 (4)	C7—Hg1^{ii}	3.844 (4)
Hg1—O5^{i}	3.117 (3)	N2—C8	1.489 (6)
Hg1—C6	3.182 (4)	N2—H1C	0.8900
Hg1—C7	3.219 (4)	N2—H1D	0.8900
Hg1—O3W^{i}	3.700 (3)	N2—H1E	0.8900
Hg1—C7^{i}	3.844 (4)	C8—C9	1.524 (6)
O1—C6	1.261 (5)	C8—H8A	0.9700
O2—C6	1.244 (5)	C8—H8B	0.9700
O3—C3	1.337 (5)	C9—C8^{iii}	1.524 (6)
O3—H3	0.9220	C9—H9A	0.9601
O4—C7	1.263 (5)	O1W—H1A	0.8205
O5—C7	1.239 (5)	O1W—H1B	0.8199
O5—Hg1^{ii}	3.117 (3)	O2W—H2B	0.8500
N1—C5	1.348 (5)	O2W—H2C	0.8499
N1—C1	1.351 (5)	O3W—Hg1^{ii}	3.700 (3)
C1—C2	1.379 (6)	O3W—H3A	0.8501
C1—C6	1.522 (5)	O3W—H3B	0.8501
C2—C3	1.392 (6)		

N1—Hg1—Cl1	167.66 (9)	C3—O3—H3	112.8
N1—Hg1—O1	71.94 (11)	C7—O4—Hg1	110.2 (2)
Cl1—Hg1—O1	112.32 (7)	C7—O5—Hg1^{ii}	117.2 (2)
N1—Hg1—O1W	96.83 (11)	C5—N1—C1	119.2 (3)
Cl1—Hg1—O1W	94.63 (7)	C5—N1—Hg1	120.9 (3)
O1—Hg1—O1W	91.72 (9)	C1—N1—Hg1	119.9 (3)
N1—Hg1—O4	70.64 (11)	N1—C1—C2	121.0 (4)
Cl1—Hg1—O4	106.43 (7)	N1—C1—C6	118.0 (3)
O1—Hg1—O4	141.18 (9)	C2—C1—C6	121.0 (4)
O1W—Hg1—O4	82.81 (9)	C2—C1—Hg1	158.4 (3)
N1—Hg1—C1	22.53 (11)	C6—C1—Hg1	80.5 (2)
Cl1—Hg1—C1	158.80 (8)	C1—C2—C3	119.6 (4)
O1—Hg1—C1	49.41 (10)	C1—C2—H2A	120.2
O1W—Hg1—C1	96.44 (10)	C3—C2—H2A	120.2
O4—Hg1—C1	92.87 (10)	O3—C3—C2	123.9 (4)
N1—Hg1—C5	22.16 (11)	O3—C3—C4	117.3 (4)
Cl1—Hg1—C5	151.22 (8)	C2—C3—C4	118.8 (4)
O1—Hg1—C5	94.09 (10)	C5—C4—C3	118.5 (4)
O1W—Hg1—C5	95.85 (10)	C5—C4—Hg1^{ii}	95.5 (2)
O4—Hg1—C5	48.81 (9)	C3—C4—Hg1^{ii}	131.7 (3)
C1—Hg1—C5	44.68 (10)	C5—C4—H4A	120.7
N1—Hg1—O5^{i}	85.23 (10)	C3—C4—H4A	120.7
Cl1—Hg1—O5^{i}	82.43 (6)	N1—C5—C4	122.7 (4)
O1—Hg1—O5^{i}	108.22 (8)	N1—C5—C7	118.5 (3)
O1W—Hg1—O5^{i}	159.50 (8)	C4—C5—C7	118.7 (3)
O4—Hg1—O5^{i}	78.64 (8)	C4—C5—Hg1	159.7 (3)
C1—Hg1—O5^{i}	93.15 (9)	C7—C5—Hg1	81.6 (2)
C5—Hg1—O5^{i}	78.42 (9)	O2—C6—O1	126.5 (4)
N1—Hg1—C6	50.66 (11)	O2—C6—C1	116.9 (4)

Cl1—Hg1—C6	132.49 (8)	O1—C6—C1	116.6 (3)
O1—Hg1—C6	21.38 (10)	O2—C6—Hg1	169.9 (3)
O1W—Hg1—C6	95.82 (9)	O1—C6—Hg1	45.54 (19)
O4—Hg1—C6	120.80 (10)	C1—C6—Hg1	71.4 (2)
C1—Hg1—C6	28.14 (10)	O5—C7—O4	125.9 (4)
C5—Hg1—C6	72.81 (10)	O5—C7—C5	117.6 (3)
O5^{i}—Hg1—C6	101.11 (9)	O4—C7—C5	116.5 (3)
N1—Hg1—C7	50.00 (11)	O5—C7—Hg1	165.4 (3)
Cl1—Hg1—C7	125.05 (7)	O4—C7—Hg1	48.15 (19)
O1—Hg1—C7	121.87 (9)	C5—C7—Hg1	70.6 (2)
O1W—Hg1—C7	92.32 (9)	O5—C7—Hg1^{ii}	46.1 (2)
O4—Hg1—C7	21.60 (9)	O4—C7—Hg1^{ii}	120.3 (3)
C1—Hg1—C7	72.52 (10)	C5—C7—Hg1^{ii}	101.0 (2)
C5—Hg1—C7	27.86 (9)	Hg1—C7—Hg1^{ii}	147.28 (12)
O5^{i}—Hg1—C7	73.33 (9)	C8—N2—H1C	109.5
C6—Hg1—C7	100.66 (10)	C8—N2—H1D	109.5
N1—Hg1—O3W^{i}	80.95 (10)	H1C—N2—H1D	109.5
Cl1—Hg1—O3W^{i}	90.78 (6)	C8—N2—H1E	109.5
O1—Hg1—O3W^{i}	62.42 (8)	H1C—N2—H1E	109.5
O1W—Hg1—O3W^{i}	153.57 (8)	H1D—N2—H1E	109.5
O4—Hg1—O3W^{i}	120.33 (8)	N2—C8—C9	110.3 (4)
C1—Hg1—O3W^{i}	71.54 (9)	N2—C8—H8A	109.6
C5—Hg1—O3W^{i}	91.63 (9)	C9—C8—H8A	109.6
O5^{i}—Hg1—O3W^{i}	46.93 (7)	N2—C8—H8B	109.6
C6—Hg1—O3W^{i}	62.32 (9)	C9—C8—H8B	109.6
C7—Hg1—O3W^{i}	105.62 (8)	H8A—C8—H8B	108.1
N1—Hg1—C7^{i}	76.55 (11)	C8—C9—C8^{iii}	110.6 (5)
Cl1—Hg1—C7^{i}	91.42 (6)	C8—C9—H9A	109.3
O1—Hg1—C7^{i}	117.56 (9)	C8^{iii}—C9—H9A	109.6
O1W—Hg1—C7^{i}	145.03 (9)	Hg1—O1W—H1A	111.7
O4—Hg1—C7^{i}	62.49 (9)	Hg1—O1W—H1B	99.1
C1—Hg1—C7^{i}	89.81 (9)	H1A—O1W—H1B	104.6
C5—Hg1—C7^{i}	65.25 (9)	Hg1—O2W—H2B	56.6
O5^{i}—Hg1—C7^{i}	16.66 (8)	Hg1—O2W—H2C	150.6
C6—Hg1—C7^{i}	105.18 (9)	H2B—O2W—H2C	95.7
C7—Hg1—C7^{i}	56.86 (4)	Hg1^{ii}—O3W—H3A	103.6
O3W^{i}—Hg1—C7^{i}	60.36 (7)	Hg1^{ii}—O3W—H3B	48.2
C6—O1—Hg1	113.1 (2)	H3A—O3W—H3B	94.0

N1—Hg1—O1—C6	5.0 (3)	C7—Hg1—C5—C4	−175.8 (9)
Cl1—Hg1—O1—C6	−162.6 (3)	O3W^{i}—Hg1—C5—C4	62.7 (8)
O1W—Hg1—O1—C6	101.6 (3)	C7^{i}—Hg1—C5—C4	118.8 (8)
O4—Hg1—O1—C6	21.0 (3)	N1—Hg1—C5—C7	177.6 (4)
C1—Hg1—O1—C6	4.6 (3)	Cl1—Hg1—C5—C7	−26.9 (3)
C5—Hg1—O1—C6	5.7 (3)	O1—Hg1—C5—C7	176.0 (2)
O5^{i}—Hg1—O1—C6	−73.5 (3)	O1W—Hg1—C5—C7	83.9 (2)
C7—Hg1—O1—C6	7.8 (3)	O4—Hg1—C5—C7	8.77 (19)
O3W^{i}—Hg1—O1—C6	−84.1 (3)	C1—Hg1—C5—C7	177.1 (3)

C7^{i}—Hg1—O1—C6	−58.5 (3)	O5^{i}—Hg1—C5—C7	−76.2 (2)
N1—Hg1—O4—C7	−15.6 (3)	C6—Hg1—C5—C7	178.2 (2)
Cl1—Hg1—O4—C7	151.8 (2)	O3W^{i}—Hg1—C5—C7	−121.5 (2)
O1—Hg1—O4—C7	−31.7 (3)	C7^{i}—Hg1—C5—C7	−65.42 (19)
O1W—Hg1—O4—C7	−115.5 (3)	Hg1—O1—C6—O2	171.9 (3)
C1—Hg1—O4—C7	−19.3 (3)	Hg1—O1—C6—C1	−7.9 (4)
C5—Hg1—O4—C7	−11.2 (2)	N1—C1—C6—O2	−172.1 (4)
O5^{i}—Hg1—O4—C7	73.3 (3)	C2—C1—C6—O2	8.4 (6)
C6—Hg1—O4—C7	−22.9 (3)	Hg1—C1—C6—O2	−173.9 (4)
O3W^{i}—Hg1—O4—C7	50.9 (3)	N1—C1—C6—O1	7.8 (5)
C7^{i}—Hg1—O4—C7	69.0 (2)	C2—C1—C6—O1	−171.7 (4)
Cl1—Hg1—N1—C5	−69.5 (6)	Hg1—C1—C6—O1	6.0 (3)
O1—Hg1—N1—C5	178.3 (3)	N1—C1—C6—Hg1	1.8 (3)
O1W—Hg1—N1—C5	88.7 (3)	C2—C1—C6—Hg1	−177.7 (4)
O4—Hg1—N1—C5	8.9 (3)	N1—Hg1—C6—O2	145.7 (18)
C1—Hg1—N1—C5	179.1 (5)	Cl1—Hg1—C6—O2	−18.5 (18)
O5^{i}—Hg1—N1—C5	−70.8 (3)	O1—Hg1—C6—O2	−40.5 (16)
C6—Hg1—N1—C5	−179.3 (4)	O1W—Hg1—C6—O2	−120.2 (17)
C7—Hg1—N1—C5	1.4 (3)	O4—Hg1—C6—O2	154.7 (17)
O3W^{i}—Hg1—N1—C5	−117.9 (3)	C1—Hg1—C6—O2	147.0 (18)
C7^{i}—Hg1—N1—C5	−56.4 (3)	C5—Hg1—C6—O2	145.4 (17)
Cl1—Hg1—N1—C1	111.5 (4)	O5^{i}—Hg1—C6—O2	71.4 (17)
O1—Hg1—N1—C1	−0.8 (3)	C7—Hg1—C6—O2	146.3 (17)
O1W—Hg1—N1—C1	−90.3 (3)	O3W^{i}—Hg1—C6—O2	44.1 (17)
O4—Hg1—N1—C1	−170.2 (3)	C7^{i}—Hg1—C6—O2	88.0 (17)
C5—Hg1—N1—C1	−179.1 (5)	N1—Hg1—C6—O1	−173.8 (3)
O5^{i}—Hg1—N1—C1	110.2 (3)	Cl1—Hg1—C6—O1	22.0 (3)
C6—Hg1—N1—C1	1.6 (3)	O1W—Hg1—C6—O1	−79.8 (3)
C7—Hg1—N1—C1	−177.6 (4)	O4—Hg1—C6—O1	−164.8 (2)
O3W^{i}—Hg1—N1—C1	63.1 (3)	C1—Hg1—C6—O1	−172.5 (4)
C7^{i}—Hg1—N1—C1	124.6 (3)	C5—Hg1—C6—O1	−174.1 (3)
C5—N1—C1—C2	−2.5 (6)	O5^{i}—Hg1—C6—O1	111.9 (3)
Hg1—N1—C1—C2	176.6 (3)	C7—Hg1—C6—O1	−173.2 (3)
C5—N1—C1—C6	178.0 (3)	O3W^{i}—Hg1—C6—O1	84.6 (3)
Hg1—N1—C1—C6	−2.9 (5)	C7^{i}—Hg1—C6—O1	128.5 (3)
C5—N1—C1—Hg1	−179.1 (5)	N1—Hg1—C6—C1	−1.3 (2)
Cl1—Hg1—C1—N1	−146.6 (3)	Cl1—Hg1—C6—C1	−165.48 (17)
O1—Hg1—C1—N1	179.0 (3)	O1—Hg1—C6—C1	172.5 (4)
O1W—Hg1—C1—N1	92.3 (3)	O1W—Hg1—C6—C1	92.8 (2)
O4—Hg1—C1—N1	9.2 (3)	O4—Hg1—C6—C1	7.7 (2)
C5—Hg1—C1—N1	0.5 (3)	C5—Hg1—C6—C1	−1.6 (2)
O5^{i}—Hg1—C1—N1	−69.5 (3)	O5^{i}—Hg1—C6—C1	−75.6 (2)
C6—Hg1—C1—N1	−177.4 (4)	C7—Hg1—C6—C1	−0.7 (2)
C7—Hg1—C1—N1	1.9 (3)	O3W^{i}—Hg1—C6—C1	−102.9 (2)
O3W^{i}—Hg1—C1—N1	−111.8 (3)	C7^{i}—Hg1—C6—C1	−59.0 (2)
C7^{i}—Hg1—C1—N1	−53.2 (3)	Hg1^{ii}—O5—C7—O4	−99.8 (4)
N1—Hg1—C1—C2	−8.0 (7)	Hg1^{ii}—O5—C7—C5	78.1 (4)
Cl1—Hg1—C1—C2	−154.6 (6)	Hg1^{ii}—O5—C7—Hg1	−160.3 (10)

O1—Hg1—C1—C2	171.0 (8)	Hg1—O4—C7—O5	−162.9 (3)
O1W—Hg1—C1—C2	84.3 (8)	Hg1—O4—C7—C5	19.2 (4)
O4—Hg1—C1—C2	1.2 (8)	Hg1—O4—C7—Hg1^{ii}	141.68 (15)
C5—Hg1—C1—C2	−7.5 (7)	N1—C5—C7—O5	168.5 (4)
O5^{i}—Hg1—C1—C2	−77.5 (8)	C4—C5—C7—O5	−14.8 (5)
C6—Hg1—C1—C2	174.6 (9)	Hg1—C5—C7—O5	166.9 (3)
C7—Hg1—C1—C2	−6.1 (7)	N1—C5—C7—O4	−13.4 (5)
O3W^{i}—Hg1—C1—C2	−119.9 (8)	C4—C5—C7—O4	163.3 (4)
C7^{i}—Hg1—C1—C2	−61.2 (8)	Hg1—C5—C7—O4	−15.0 (3)
N1—Hg1—C1—C6	177.4 (4)	N1—C5—C7—Hg1	1.6 (3)
Cl1—Hg1—C1—C6	30.7 (4)	C4—C5—C7—Hg1	178.3 (4)
O1—Hg1—C1—C6	−3.58 (19)	N1—C5—C7—Hg1^{ii}	−145.6 (3)
O1W—Hg1—C1—C6	−90.3 (2)	C4—C5—C7—Hg1^{ii}	31.2 (4)
O4—Hg1—C1—C6	−173.4 (2)	Hg1—C5—C7—Hg1^{ii}	−147.18 (11)
C5—Hg1—C1—C6	177.9 (3)	N1—Hg1—C7—O5	−128.0 (12)
O5^{i}—Hg1—C1—C6	107.8 (2)	Cl1—Hg1—C7—O5	37.8 (12)
C7—Hg1—C1—C6	179.3 (2)	O1—Hg1—C7—O5	−131.5 (11)
O3W^{i}—Hg1—C1—C6	65.5 (2)	O1W—Hg1—C7—O5	135.1 (11)
C7^{i}—Hg1—C1—C6	124.2 (2)	O4—Hg1—C7—O5	71.4 (11)
N1—C1—C2—C3	2.0 (6)	C1—Hg1—C7—O5	−128.9 (11)
C6—C1—C2—C3	−178.5 (4)	C5—Hg1—C7—O5	−126.8 (12)
Hg1—C1—C2—C3	7.7 (10)	O5^{i}—Hg1—C7—O5	−30.0 (11)
C1—C2—C3—O3	−179.8 (4)	C6—Hg1—C7—O5	−128.6 (11)
C1—C2—C3—C4	1.1 (6)	O3W^{i}—Hg1—C7—O5	−64.6 (11)
O3—C3—C4—C5	177.3 (4)	C7^{i}—Hg1—C7—O5	−27.3 (10)
C2—C3—C4—C5	−3.6 (6)	N1—Hg1—C7—O4	160.7 (3)
O3—C3—C4—Hg1^{ii}	48.2 (5)	Cl1—Hg1—C7—O4	−33.6 (3)
C2—C3—C4—Hg1^{ii}	−132.7 (3)	O1—Hg1—C7—O4	157.2 (2)
C1—N1—C5—C4	−0.2 (6)	O1W—Hg1—C7—O4	63.7 (3)
Hg1—N1—C5—C4	−179.2 (3)	C1—Hg1—C7—O4	159.7 (3)
C1—N1—C5—C7	176.4 (3)	C5—Hg1—C7—O4	161.8 (4)
Hg1—N1—C5—C7	−2.7 (5)	O5^{i}—Hg1—C7—O4	−101.4 (3)
C1—N1—C5—Hg1	179.1 (5)	C6—Hg1—C7—O4	160.1 (3)
C3—C4—C5—N1	3.2 (6)	O3W^{i}—Hg1—C7—O4	−135.9 (2)
Hg1^{ii}—C4—C5—N1	147.6 (3)	C7^{i}—Hg1—C7—O4	−98.7 (3)
C3—C4—C5—C7	−173.3 (3)	N1—Hg1—C7—C5	−1.2 (2)
Hg1^{ii}—C4—C5—C7	−29.0 (4)	Cl1—Hg1—C7—C5	164.56 (18)
C3—C4—C5—Hg1	1.9 (10)	O1—Hg1—C7—C5	−4.7 (2)
Hg1^{ii}—C4—C5—Hg1	146.3 (7)	O1W—Hg1—C7—C5	−98.1 (2)
Cl1—Hg1—C5—N1	155.4 (3)	O4—Hg1—C7—C5	−161.8 (4)
O1—Hg1—C5—N1	−1.6 (3)	C1—Hg1—C7—C5	−2.1 (2)
O1W—Hg1—C5—N1	−93.8 (3)	O5^{i}—Hg1—C7—C5	96.8 (2)
O4—Hg1—C5—N1	−168.9 (3)	C6—Hg1—C7—C5	−1.8 (2)
C1—Hg1—C5—N1	−0.5 (3)	O3W^{i}—Hg1—C7—C5	62.2 (2)
O5^{i}—Hg1—C5—N1	106.2 (3)	C7^{i}—Hg1—C7—C5	99.5 (2)
C6—Hg1—C5—N1	0.5 (3)	N1—Hg1—C7—Hg1^{ii}	78.7 (2)
C7—Hg1—C5—N1	−177.6 (4)	Cl1—Hg1—C7—Hg1^{ii}	−115.6 (2)
O3W^{i}—Hg1—C5—N1	60.9 (3)	O1—Hg1—C7—Hg1^{ii}	75.2 (2)

C7^{i}—Hg1—C5—N1	116.9 (3)	O1W—Hg1—C7—Hg1^{ii}	−18.3 (2)
N1—Hg1—C5—C4	1.9 (7)	O4—Hg1—C7—Hg1^{ii}	−82.0 (3)
Cl1—Hg1—C5—C4	157.3 (7)	C1—Hg1—C7—Hg1^{ii}	77.8 (2)
O1—Hg1—C5—C4	0.2 (8)	C5—Hg1—C7—Hg1^{ii}	79.9 (3)
O1W—Hg1—C5—C4	−91.9 (8)	O5^{i}—Hg1—C7—Hg1^{ii}	176.6 (2)
O4—Hg1—C5—C4	−167.0 (9)	C6—Hg1—C7—Hg1^{ii}	78.1 (2)
C1—Hg1—C5—C4	1.3 (8)	O3W^{i}—Hg1—C7—Hg1^{ii}	142.1 (2)
O5^{i}—Hg1—C5—C4	108.0 (8)	C7^{i}—Hg1—C7—Hg1^{ii}	179.4 (3)
C6—Hg1—C5—C4	2.4 (8)	N2—C8—C9—C8^{iii}	165.1 (4)

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+3/2; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iii) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4^{iv}	0.92	1.63	2.548 (5)	173
N2—H1*C*···O3*W*^{ii}	0.89	2.03	2.830 (5)	150
N2—H1*D*···O2*W*^{v}	0.89	2.30	3.096 (6)	149
N2—H1*E*···O2*W*^{vi}	0.89	1.96	2.824 (6)	165
O1*W*—H1*A*···O5^{ii}	0.82	2.08	2.854 (5)	157
O1*W*—H1*B*···O2^{vii}	0.82	2.07	2.837 (6)	157
O2*W*—H2*B*···O1	0.85	1.98	2.771 (6)	154
O2*W*—H2*C*···O2^{iii}	0.85	1.94	2.777 (5)	169
O3*W*—H3*A*···O3^{vii}	0.85	2.30	3.019 (6)	142
O3*W*—H3*B*···O5	0.85	1.93	2.766 (6)	169
C8—H8*B*···O1	0.97	2.45	3.393 (6)	163

Symmetry codes: (ii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iii) −*x*+1, *y*, −*z*+3/2; (iv) *x*, −*y*+1, *z*−1/2; (v) −*x*+1, −*y*+1, −*z*+2; (vi) *x*, *y*−1, *z*; (vii) *x*, −*y*+1, *z*+1/2.