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(2,2-Bipyridine *N*,*N*′-dioxide-κ^2O,O')dichloromercury(II)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.022 Å
R factor = 0.054
wR factor = 0.135
Data-to-parameter ratio = 14.6

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

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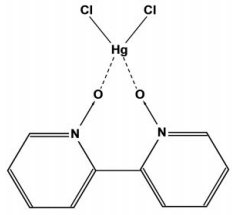
In the crystal structure of the title compound, $[HgCl_2(C_{10}H_8N_2O_2)]$, the Hg atom has severely distorted tetrahedral coordination by two Cl atoms and by two O atoms of the chelating ligand. Additional weak Hg···Cl bonds link the molecules into a chain.

Comment

Although the existence of (2,2-bipyridine *N*,*N*′-dioxide)dichloromercury(II), $[HgCl_2(C_{10}H_8N_2O_2)]$, (I), has been recognized for many decades, its crystal structure remained undetermined. Crystal growth at low temperatures has now yielded crystalline specimens of (I) that have allowed us to determine the crystal structure for the first time. According to Ahuja & Singh (1973), the halide–mercury complexes of 2,2-bipyridine *N*,*N*′-dioxide ($BipyO_2$) are characterized as pseudotetrahedral structures on the basis of IR data. Our results from X-ray crystallography confirm these findings.



(I)

The title structure consists of $[HgCl_2(C_{10}H_8N_2O_2)]$ complex molecules, as depicted in Fig. 1. The Hg atom is bonded to two Cl atoms and two O atoms of the chelating 2,2-bipyridine *N*,*N*′-dioxide ligand and has strongly distorted coordination geometry (Table 1). In addition to the two strong Hg—Cl bonds, each Hg atom forms two longer Hg···Cl bonds that cap the O/Cl1/Cl2 face of the tetrahedron. These bonds [$Hg\cdots Cl1^{ii}$ = 3.433 (4) Å and $Hg\cdots Cl2^{i}$ = 3.416 (4) Å; see Table 1] are much weaker and about 1.1 Å longer than the intramolecular Hg—Cl bonds. They play an important role, however, in the structure and bind the complex molecules into a chain along the *b* axis (Fig. 2). Thus the $HgCl_2$ groups form a step-like double chain such that the longer Hg···Cl bonds lie along the chain and the short Hg—Cl bonds lie across it. The Hg···Hg distances along the chain are 4.139 (2) and 4.394 (2) Å. The bis(oxypyridine) ligand is chelating and has a propeller configuration, with an angle of 61.0 (3)° between the rings.

Experimental

Caution: mercury(II) chloride sublimes to emit poisonous fumes. The experiment should only be performed in chemical fume hoods. The

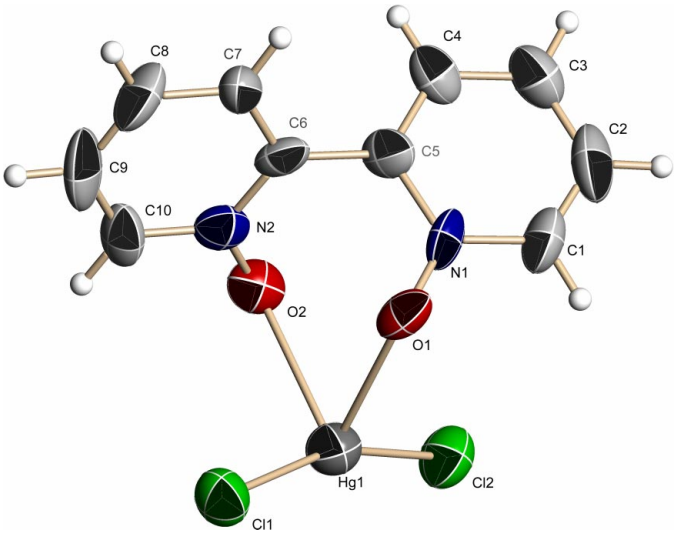


Figure 1
A view of a molecule of (I), showing the atom-numbering scheme employed. Anisotropic atomic displacement ellipsoids for the non-H atoms are shown at the 50% probability level. H atoms are displayed with arbitrarily small radii.

chemicals used to prepare this compound were at least of reagent grade. 2,2′-Bipyridine was oxidized to bipyO$_2$ by the method described by Simpson *et al.* (1963). [$HgCl_2(C_{10}H_8N_2O_2)$] crystals were obtained from the procedure detailed by Ahuja & Singh (1973).

Crystal data

[$HgCl_2(C_{10}H_8N_2O_2)$]
M_r = 459.67
Monoclinic, $P2_1/n$
a = 9.728 (3) Å
b = 8.064 (3) Å
c = 15.746 (5) Å
β = 94.492 (6)°
V = 1231.4 (7) Å^3
Z = 4
D_x = 2.479 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1650 reflections
θ = 2.4–21.0°
μ = 12.92 mm^{-1}
T = 296 (2) K
Needle, colorless
0.24 × 0.04 × 0.03 mm

Data collection

Bruker SMART diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.386, T_{max} = 0.679
9792 measured reflections
2255 independent reflections
1356 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 25.3°
$h = -11 \rightarrow 11$
$k = -9 \rightarrow 9$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.136
S = 1.00
2255 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.005P)^2 + 5P]$, where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

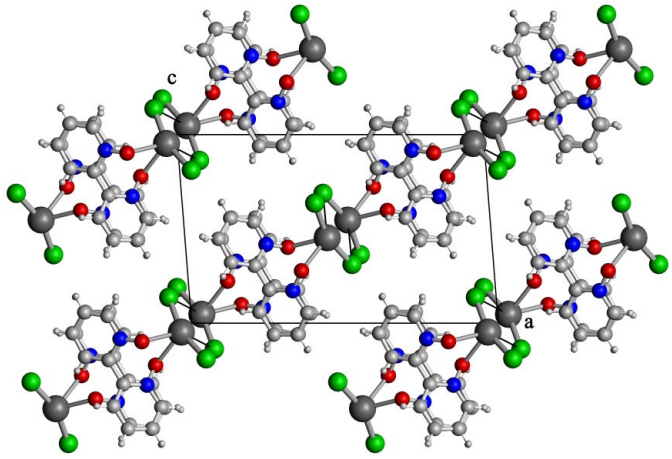


Figure 2
A view of the molecular packing for (I). Dark thin lines show weak Hg···Cl bonds.

Table 1
Selected geometric parameters (Å, °).

Hg1—Cl1	2.305 (4)	Hg1—O2	2.472 (9)
Hg1—Cl2	2.320 (4)	Hg1···Cl2^{i}	3.416 (4)
Hg1—O1	2.466 (9)	Hg1···Cl1^{ii}	3.433 (4)
Cl1—Hg1—Cl2	161.24 (14)	Cl2—Hg1—O2	95.8 (2)
Cl1—Hg1—O1	91.5 (2)	O1—Hg1—O2	71.6 (3)
Cl2—Hg1—O1	103.4 (2)	Cl2^{i}—Hg1—Cl1^{ii}	144.96 (9)
Cl1—Hg1—O2	99.8 (2)		

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

H atoms were treated as riding, with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 1999); software used to prepare material for publication: *SHELXL*97.

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