Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[mercury(II)-di-μ-chloro-μ-pyridazine-κ^2N:N']

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Received 29 March 2004
Accepted 29 April 2004
Online 8 May 2004

Key indicators

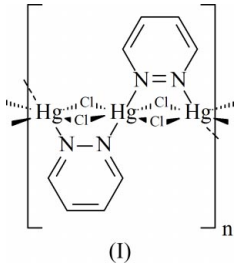
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.022
wR factor = 0.030
Data-to-parameter ratio = 15.4

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

The crystal structure of $[HgCl_2(Pyo)]_n$ (Pyo = pyridazine, $C_4H_4N_2$) consists of chloride-bridged strands of octahedrally coordinated mercuric centers, connected by the two neighboring N atoms of pyridazine molecules. All atoms lie in special positions: Hg with site symmetry 2/m and the others on mirror planes.

Comment

N-Donor ligands generate a wide variety of coordination compounds with mercury (*e.g.* Grdenić, 1965; Breitinger & Brodersen, 1970). We have carried out a systematic study of the affinity of mercury towards *N*-donor ligands (Nockemann, 2002; Meyer & Nockemann, 2003).



(I)

The crystal structure of $[HgCl_2(Pyo)]_n$ (Pyo = pyridazine), (I), consists of strands of octahedrally coordinated mercuric

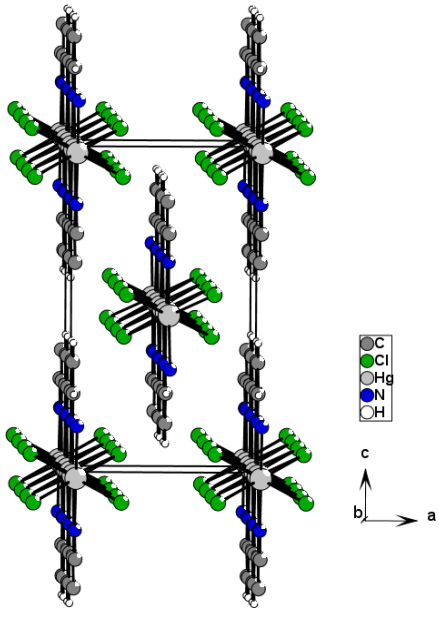


Figure 1
Packing diagram of $[HgCl_2(Pyo)]_n$, viewed approximately down the *b* axis.

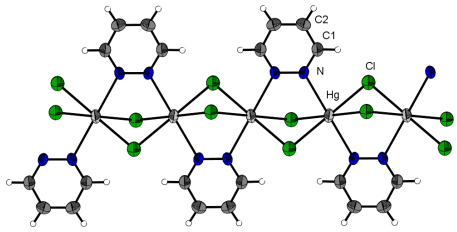


Figure 2
View of a part of the $[HgCl_2(Pyo)]_n$ coordination polymer, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

centers symmetrically bridged by chloride, with four equal Hg—Cl distances of 2.6819 (16) Å. Neighboring mercuric centers are connected by the two adjacent N atoms of pyridazine molecules, with two Hg—N distances of 2.411 (5) Å. This is the shortest Hg—N bond observed in diazine adducts of mercuric chloride and results from the high basicity of pyridazine (Meyer & Nockemann, 2003). The Cl—Hg—Cl angle within the Hg_2Cl_2 rings in the strands in the [010] direction is 82.80 (8)°.

The Hg atom has 2/*m* site symmetry and all other atoms lie on mirror planes.

Experimental

Crystals of $[HgCl_2(Pyo)]_n$ were obtained by adding a solution of 1 g (12.5 mmol) pyridazine in 20 ml methanol dropwise and slowly to 10 ml of a 0.1 *N* aqueous solution of mercury(II) chloride without stirring. This solution was allowed to stand for 7 d, during which colorless prismatic crystals appeared.

Crystal data

$[HgCl_2(C_4H_4N_2)]$
M_r = 351.58
Orthorhombic, *Imma*
a = 7.458 (2) Å
b = 7.1667 (16) Å
c = 13.136 (4) Å
V = 702.1 (3) Å^3
Z = 4
D_x = 3.326 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2760 reflections
θ = 3.1–27.0°
μ = 22.59 mm^{-1}
T = 293 (2) K
Prism, colorless
0.3 × 0.2 × 0.1 mm

Data collection

Stoe IPDS-I diffractometer
φ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
T_{min} = 0.249, T_{max} = 0.617
2760 measured reflections
448 independent reflections
296 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 27.0°
$h = -9 \rightarrow 9$
$k = -9 \rightarrow 8$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.030
S = 0.97
448 reflections
29 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0107P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg—N	2.411 (5)	N—N^{i}	1.334 (9)
Hg—Cl	2.6819 (16)	C1—C2	1.391 (9)
N—C1	1.316 (8)	C2—C2^{i}	1.359 (14)
N—Hg—N^{ii}	180	C1—N—N^{i}	119.5 (3)
N—Hg—Cl	89.43 (9)	C1—N—Hg	122.7 (4)
Cl^{ii}—Hg—Cl	180	N^{i}—N—Hg	117.81 (11)
N—Hg—Cl^{iii}	90.57 (9)	N—C1—C2	123.4 (6)
Cl—Hg—Cl^{i}	82.80 (8)		

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

The highest peak and deepest hole were located 1.85 Å from H2 and 1.80 Å from Cl1, respectively. H atoms were visible in a difference map and were treated as riding atoms, with a C—H distance of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-STEP*32 (Stoe & Cie, 2000); data reduction: *X-RED*32 (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL*97.

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