Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

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

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

Key indicators

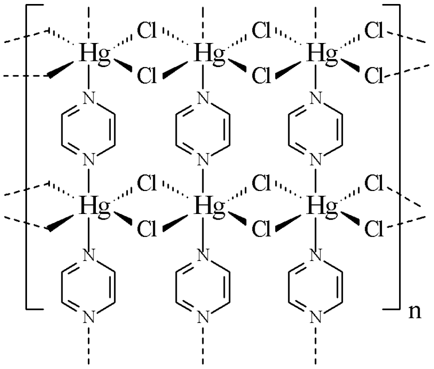
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.023
wR factor = 0.051
Data-to-parameter ratio = 13.6

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

In $[HgCl_2(Pyp)]_n$ (Pyp = pyrazine, $C_4H_4N_2$), chloride-bridged $HgCl_{4/2}$ strands are connected into layers by pyrazine molecules. The Hg atom is on a site of symmetry $2/m$, the unique Cl atom is on a mirror plane, the unique N atom is on a twofold rotation axis, and the unique C and H atoms are in general positions.

Comment

Many mercury(II) compounds, with their typical d^{10} closed-shell configuration together with relativistic effects (Pyykkö, 1978), tend to form strong bonds to nitrogen donors with highly covalent contributions (Grdenić, 1965; Breitinger & Brodersen, 1970). Because of this high affinity of mercury(II) for N-donor ligands, we have started a systematic structural study concerned with the formation of coordination polymers of mercuric compounds HgX_2 (with X = Cl, Br, I, NO_3, ClO_4 and CF_3) with N-donor ligands, especially with diazines (Nockemann, 2002; Meyer & Nockemann, 2003). The adducts of mercury(II) halides are particularly suitable for a comparative study.



(I)

The crystal structure of $[HgCl_2(Pyp)]_n$ (Pyp = pyrazine), (I), contains chloride-bridged edge-sharing $[HgCl_2N_2]$ octahedra. Each mercuric ion is coordinated by two pyrazine molecules. These connect the octahedra to give layers parallel to (001). The unique Hg—N distance is 2.510 (7) Å, almost the same as in the analogous adduct with pyrimidine [2.505 (14) Å; Nockemann, 2002], but longer than in the pyridazine compound [2.411 (5) Å; Nockemann & Meyer, 2004]. This is in accord with the low basicities of pyrazine and pyrimidine compared with pyridazine. There are two different Hg—Cl distances, *viz*. 2.503 (3) and 2.842 (4) Å. All N—Hg—Cl angles are exactly 90°. The distance between two contiguous layers is $a/2$ = 5.9485 (9) Å. The crystal structure of this

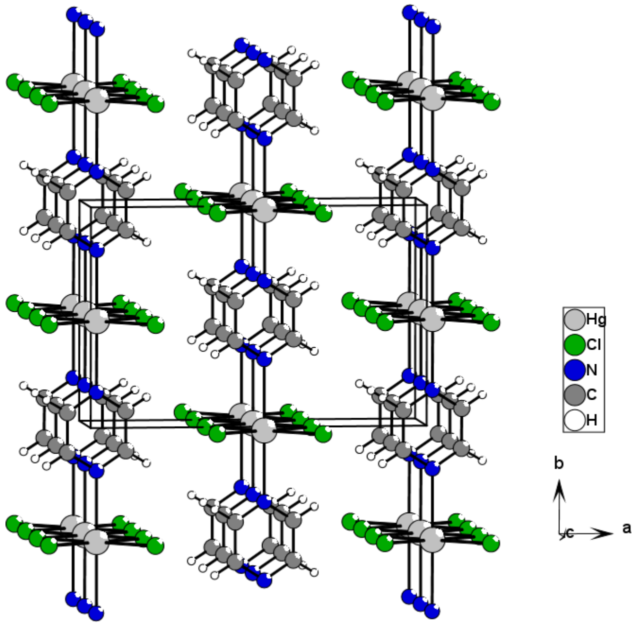


Figure 1
Packing diagram of $[HgCl_2(Pyp)]_n$, viewed approximately along the *c* axis.

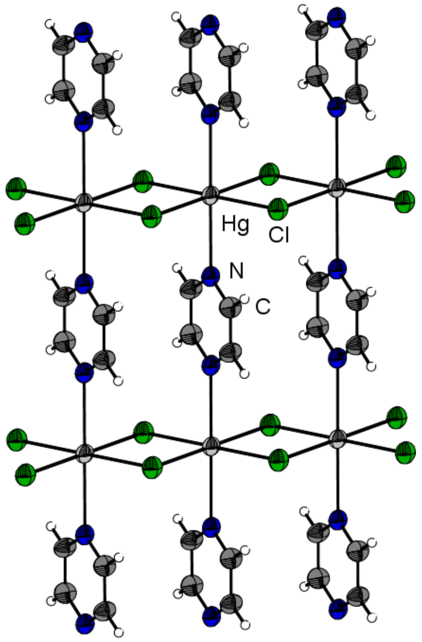


Figure 2
View of a part of the $[HgCl_2(Pyp)]_n$ coordination polymer, showing 50% probability displacement ellipsoids and the atom-numbering scheme for the asymmetric unit.

coordination polymer, $[HgCl_2(Pyp)]$, is quite similar to that of the copper(I) compound [CuCl(Pyp)] (Näther *et al.*, 2001), again with a closed-shell d^{10}-configuration of the central metal ion but with half the chloride bridges missing.

The Hg atoms and the pyrazine ligands lie in positions with $2/m$ site symmetry, and Cl atoms are on mirror planes.

Experimental

Mercury(II) chloride (0.272 g, 1 mmol) and an excess of pyrazine (3 g, 37.5 mmol) were sealed in a glass ampoule under dry argon. This ampoule was heated to 398 K at a heating rate of 10 K h^{-1} and kept at that temperature for 7 d, after which it was cooled at a rate of 5 K h^{-1}. $[HgCl_2(Pyp)]_n$ crystallized as colorless prisms and could easily be separated from excess pyrazine, which sublimed off to the cooler parts of the ampoule. Attempts to crystallize the product from aqueous or methanolic solutions led to twinned or poor-quality crystals.

Crystal data

$[HgCl_2(C_4H_4N_2)]$
$M_r = 349.57$
Monoclinic, $C2/m$
$a = 11.8970$ (17) Å
$b = 7.783$ (3) Å
$c = 3.840$ (7) Å
$\beta = 90.99$ (6)°
$V = 355.6$ (7) Å^3
$Z = 2$
$D_x = 3.265$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1625 reflections
$\theta = 3.4$–25.9°
$\mu = 22.30$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.2 × 0.2 × 0.2 mm

Data collection

Stoe IPDS-I diffractometer
φ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
$T_{min} = 0.150$, $T_{max} = 0.399$
1625 measured reflections
354 independent reflections
354 reflections with $I > 2\sigma(I)$
$R_{int} = 0.079$
$\theta_{max} = 25.9°$
$h = -14 \rightarrow 14$
$k = -9 \rightarrow 9$
$l = -4 \rightarrow 4$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.051$
$S = 1.09$
354 reflections
26 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -1.28$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0103 (13)

Table 1
Selected geometric parameters (Å, °).

$Hg—Cl^{i}$	2.503 (3)	N—C	1.326 (7)
Hg—N	2.510 (7)	$C—C^{ii}$	1.404 (12)
Hg—Cl	2.842 (4)		
$Cl^{i}—Hg—Cl^{iii}$	180	$N—Hg—Cl^{iv}$	90
$Cl^{i}—Hg—N$	90	$Hg^{v}—Cl—Hg$	91.65 (12)
$N^{iv}—Hg—N$	180	$C—N—C^{vi}$	118.3 (7)
$Cl^{i}—Hg—Cl^{iv}$	88.35 (12)	C—N—Hg	120.9 (4)

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

The highest peak and deepest hole were located 0.99 and 0.85 Å, respectively, from Hg. The H atom was visible in a difference map and was treated as a riding atom, 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.

References

Brandenburg, K. (1999). *DIAMOND*. Version 2.1c. Crystal Impact GbR, Bonn, Germany.
Breitinger, D. & Brodersen, K. (1970). *Angew. Chem. Int. Ed. Engl.* **9**, 357–367.
Grdenić, D. (1965). *Quart. Rev.* **19**, 303–327.
Meyer, G. & Nockemann, P. (2003). *Z. Anorg. Allg. Chem.* **629**, 1447–1461.

Näther, C., Greve, J. & Jeß, I. (2001). *Polyhedron*, **20**, 1017–1022.

Nockemann, P. (2002). Dissertation, Universität zu Köln, Germany.

Nockemann, P. & Meyer, G. (2004). *Acta Cryst.* E**60**, m751–m752.

Pyykkö, P. (1978). *Adv. Quantum Chem.* **11**, 353–409.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Stoe & Cie (1998). *X-SHAPE*. Stoe & Cie, Darmstadt, Germany.

Stoe & Cie (2000). *X-STEP*32. Version 1.06f. Stoe & Cie, Darmstadt, Germany.

Stoe & Cie (2001). *X-AREA* (Version 1.15) and *X-RED*32 (Version 1.22). Stoe & Cie, Darmstadt, Germany.