Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[mercury(II)-di-μ-bromo-μ-pyridazine-$\kappa^2N:N'$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(N–N) = 0.017 Å
R factor = 0.066
wR factor = 0.165
Data-to-parameter ratio = 18.8

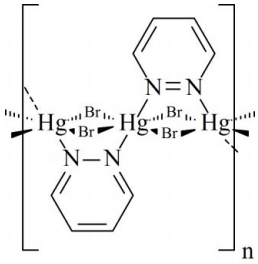
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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

The crystal structure of $[HgBr_2(Pyo)]_n$ (Pyo = pyridazine, $C_4H_4N_2$) consists of strands of octahedrally coordinated mercuric centers asymmetrically bridged by bromide and connected by the two neighboring N atoms of pyridazine molecules to complete the octahedral coordination of mercury. The Hg atoms lie on inversion centers.

Comment

N-Donor ligands exhibit 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 $[HgBr_2(Pyo)]_n$ (Pyo = pyridazine) consists of strands of octahedrally coordinated mercuric centers asymmetrically bridged by bromide, with two short Hg—Br distances of 2.5962 (15) Å and two longer at 3.0280 (16) Å. Adjacent $[HgN_2Br_4]$ octahedra are linked by two neighboring N atoms of a pyridazine molecule, with Hg—N distances of 2.532 (11) Å. This is the shortest Hg—N bond observed in diazine adducts of mercuric bromide, and results from the high basicity of pyridazine (Meyer & Nockemann, 2003). The Br—Hg—Br angle in the Hg_2Br_2 rings in the strands in the [010] direction is 84.34 (5)°. The two different Hg—Br distances are concomitant with a reduction of the symmetry from space group *Imma* for $[HgCl_2(Pyo)]_n$, with four symmetrical chloride bridges (Nockemann & Meyer, 2004), to *C*2/*c* for $[HgBr_2(Pyo)]_n$.

Hg atoms lie on inversion centers; all other atoms are in general positions.

Experimental

Crystals of $[HgBr_2(Pyo)]_n$ were obtained by adding a solution of 1 g (12.5 mmol) pyridazine (1,2-diazine) in 20 ml methanol dropwise and slowly to 10 ml of a 0.1 *N* aqueous solution of mercury(II) bromide without stirring. This solution was allowed to stand for 7 d, during which colorless prismatic crystals appeared.

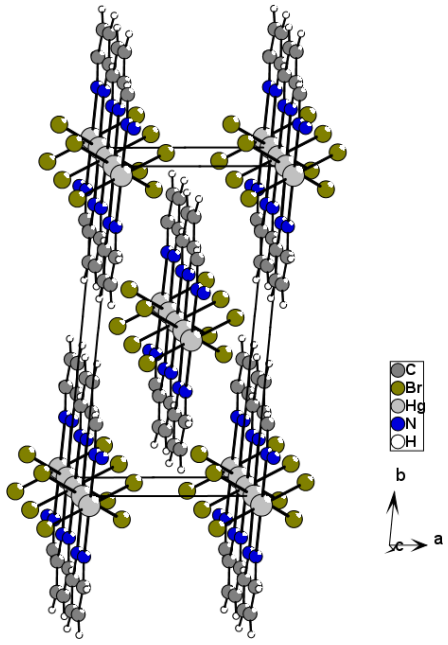


Figure 1
Packing diagram of $[HgBr_2(Pyo)]_n$, viewed approximately down the *c* axis.

Crystal data

$[HgBr_2(C_4H_4N_2)]$	D_x = 3.754 Mg m^{-3}
M_r = 440.50	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3625 reflections
a = 10.178 (3) Å	θ = 3.0–32.2°
b = 13.653 (3) Å	μ = 29.92 mm^{-1}
c = 7.438 (2) Å	T = 293 (2) K
β = 131.061 (18)°	Prism, colorless
V = 779.3 (4) Å^3	0.3 × 0.2 × 0.2 mm
Z = 4	

Data collection

Stoe IPDS-I diffractometer	637 reflections with $I > 2\sigma(I)$
φ scans	R_{int} = 0.270
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)	θ_{max} = 26.0°
T_{min} = 0.004, T_{max} = 0.068	$h = -12 \rightarrow 12$
3824 measured reflections	$k = -16 \rightarrow 16$
771 independent reflections	$l = -8 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0896P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.066	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.165	$\Delta\rho_{max}$ = 1.76 e Å^{-3}
S = 0.98	$\Delta\rho_{min}$ = −3.93 e Å^{-3}
771 reflections	Extinction correction: *SHELXL*
41 parameters	Extinction coefficient: 0.0013 (5)
H-atom parameters constrained	

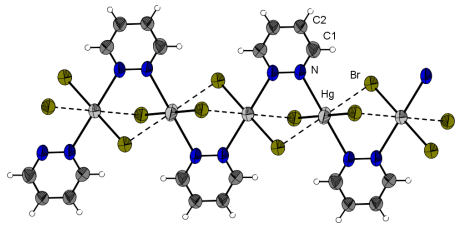


Figure 2
View of a part of the $[HgBr_2(Pyo)]_n$ coordination polymer, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Table 1
Selected geometric parameters (Å, °).

Hg—N	2.532 (11)	N—N^{iii}	1.332 (18)
Hg—Br^{i}	2.5962 (15)	N—C1	1.339 (14)
Hg—Br	3.0280 (16)	C1—C2	1.360 (19)
Hg—Br^{ii}	3.0280 (16)		
N^{ii}—Hg—N	180	Hg^{iii}—Br—Hg	82.41 (4)
N^{ii}—Hg—Br^{iii}	88.8 (3)	N^{iii}—N—C1	118.0 (6)
N—Hg—Br^{iii}	91.2 (3)	N^{iii}—N—Hg	117.8 (2)
Br^{iii}—Hg—Br^{i}	180	C1—N—Hg	123.7 (7)
N^{ii}—Hg—Br	92.6 (2)	N—C1—C2	124.4 (6)
Br^{iii}—Hg—Br	84.34 (5)	C2^{iii}—C2—C1	117.5 (6)
Br^{i}—Hg—Br	95.66 (5)		

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

The highest peak and deepest hole were located 1.05 and 0.95 Å, respectively, from Hg1. 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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