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Poly[[dibromomercury(II)]-di-μ-pyrazine-$\kappa^4N:N'$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.023
wR factor = 0.038
Data-to-parameter ratio = 17.8

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

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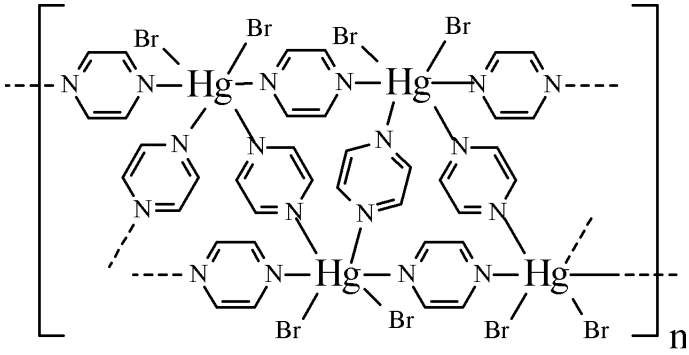
The crystal structure of $[HgBr_2(Pyp)_2]_n$ (Pyp = pyrazine, $C_4H_4N_2$) consists of almost linear $HgBr_2$ molecules which are linked by pyrazine molecules to form double strands of a coordination polymer in the [010] direction. The Hg and Br atoms lie on mirror planes.

Comment

The d^{10} closed-shell configuration and relativistic effects (Pyykkö, 1978) cause a pronounced preference of divalent mercury for 'soft' ligands and bonds with high covalent contributions. *N*-Donor ligands have been the focus of particular interest in the literature (*e.g.* Grdenić, 1965; Breitinger & Brodersen, 1970). In a systematic study, we have investigated the formation of coordination polymers of mercuric salts with *N*-donor ligands, especially with diazines (Nockemann, 2002; Meyer & Nockemann, 2003).



(I)

The structure of $[HgBr_2(Pyp)_2]_n$, (I), consists of $HgBr_2$ units, which lie on mirror planes and are connected to the 1 and 4 positions of four pyrazine molecules, with Hg—N distances of 2.719 (4) and 2.844 (4) Å. These slightly bent $HgBr_2$ molecules [Hg—Br = 2.4691 (10) and 2.4726 (9) Å; Br—Hg—Br = 167.78 (3)°] with a strongly deformed overall octahedral $[HgN_4Br_2]$ coordination of mercury are connected to give chains in the [010] direction by quite long Hg—N distances [2.844 (4) Å]. Further pyrazine molecules connect these chains to produce double strands, as shown in Fig. 1. Here, the Hg—N distance is 2.719 (4) Å. The two Hg—N distances are the longest bonds observed in diazine adducts with mercuric bromide. This correlation has also been found for adducts of $HgCl_2$, and is a result of the low basicity of pyrazine (Meyer & Nockemann, 2003).

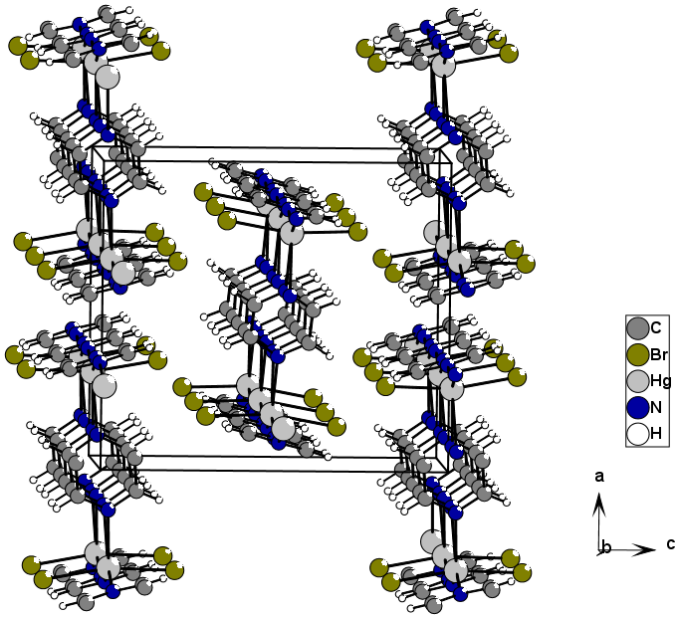


Figure 1
Packing diagram of $[HgBr_2(Pyp)_2]_n$, viewed approximately down the *b* axis.

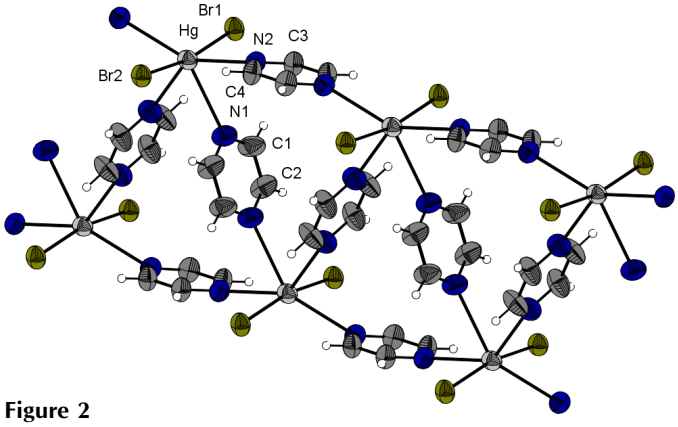


Figure 2
View of a part of the $[HgBr_2(Pyp)_2]_n$ coordination polymer, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

Mercury(II) bromide (0.360 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 with 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}. $[HgBr_2(Pyp)_2]_n$ crystallized as brown prisms and could easily be separated from excess pyrazine, which sublimed off to the cooler parts of the ampoule. Attempts to crystallize this compound from aqueous or methanolic solutions led to twinned or poor-quality crystals.

Crystal data

$[HgBr_2(C_4H_4N_2)]$
M_r = 520.59
Orthorhombic, *Pnma*
a = 11.5603 (10) Å
b = 8.3073 (19) Å
c = 12.9906 (16) Å
V = 1247.6 (3) Å^3
Z = 4
D_x = 2.772 Mg m^{-3}
Cell parameters from 12170 reflections
θ = 2.4–24.0°
μ = 18.72 mm^{-1}
T = 293 (2) K
Prism, brown
0.3 × 0.2 × 0.2 mm

Data collection

Stoe IPDS-I diffractometer
φ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
T_{min} = 0.229, T_{max} = 0.539
15175 measured reflections
1316 independent reflections
916 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 26.0°
h = −14 → 14
k = −9 → 10
l = −16 → 16

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.038
S = 0.85
1316 reflections
74 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0115P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00104 (6)

Table 1
Selected geometric parameters (Å, °).

Hg—Br2	2.4691 (10)	N2—C3	1.324 (7)
Hg—Br1	2.4726 (9)	N2—C4	1.335 (7)
Hg—N1	2.719 (4)	C1—C2^{ii}	1.372 (8)
Hg—N2^{i}	2.844 (4)	C3—C3^{i}	1.362 (12)
N1—C1	1.309 (8)	C4—C4^{i}	1.368 (13)
N1—C2	1.310 (8)		
Br2—Hg—Br1	167.78 (3)	C1—N1—C2	114.5 (5)
Br2—Hg—N1	96.27 (12)	C1—N1—Hg	123.6 (4)
Br1—Hg—N1	93.89 (12)	C2—N1—Hg	121.1 (4)
Br2—Hg—N1^{iii}	96.27 (12)	C3—N2—C4	115.0 (5)
Br1—Hg—N1^{iii}	93.89 (12)	C3—N2—Hg^{v}	118.5 (4)
N1—Hg—N1^{iii}	67.4 (2)	C4—N2—Hg^{v}	124.7 (4)
Br2—Hg—N2^{i}	87.93 (11)	N1—C1—C2^{ii}	122.5 (6)
Br1—Hg—N2^{i}	89.07 (11)	N1—C2—C1^{ii}	123.0 (5)
N1—Hg—N2^{i}	70.56 (14)	N2—C3—C3^{i}	122.7 (3)
N1^{iii}—Hg—N2^{i}	137.95 (13)	N2—C4—C4^{i}	122.3 (3)
N2^{i}—Hg—N2^{iv}	151.49 (16)		

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

The highest peak and deepest hole were located 1.15 Å from Hg1 and 2.06 Å from H2, respectively. H atoms were visible in difference maps 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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