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catena-Poly[[bis(pyrazine-2-carboxamide-κN^4)mercury(II)]-di-μ-bromido]

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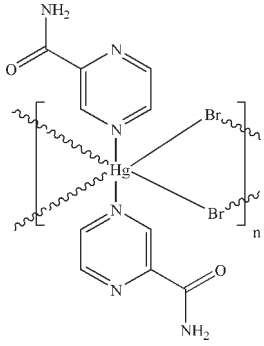
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.012 Å; R factor = 0.065; wR factor = 0.173; data-to-parameter ratio = 20.6.

In the crystal structure of the title compound, $[HgBr_2(C_5H_5N_3O)_2]_n$, the Hg^{II} cation is located on an inversion center and is coordinated by two N atoms from the pyrazine rings and four bridging Br^- anions in a distorted octahedral geometry. The Br^- anions bridge the Hg^{II} cations with significantly different Hg—Br bond distances of 2.4775 (8) and 3.1122 (8) Å, forming polymeric chains running along the *a* axis. Intermolecular N—H···O and N—H···N hydrogen bonds are effective in the stabilization of the crystal structure.

Related literature

For metal-binding properties of pyridine and pyrazine ligands, see: Sasan *et al.* (2008); Khavasi *et al.* (2009); Petro & Mukherjee (1999); Sigh & Mukherjee (2005). For the coordination modes of pyrazineamide, see: Hausmann & Brooker (2004); Cati & Stoeckli-Evans (2004); Miyazaki *et al.* (2007).



Experimental

Crystal data

$[HgBr_2(C_5H_5N_3O)_2]$
M_r = 606.63
Triclinic, $P\overline{1}$
a = 3.9628 (5) Å
b = 6.5162 (9) Å
c = 15.0388 (19) Å
α = 101.783 (10)°
β = 93.418 (11)°
γ = 95.214 (11)°
V = 377.36 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 15.50 mm^{-1}
T = 298 K
0.50 × 0.06 × 0.03 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: multi-scan (*X-RED* and *X-SHAPE*; Stoe & Cie, 2005)
T_{min} = 0.345, T_{max} = 0.630
4311 measured reflections
2002 independent reflections
1933 reflections with $I > 2\sigma(I)$
R_{int} = 0.144

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.173
S = 1.11
2002 reflections
97 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 3.93 e Å^{-3}
$\Delta\rho_{min}$ = −5.48 e Å^{-3}

Table 1
Selected bond lengths (Å).

Hg1—Br1	2.4775 (8)	Hg1—N2	2.758 (6)
Hg1—Br1^{i}	3.1122 (8)		

Symmetry code: (i) $x-1, y, z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1^{ii}	0.86	2.02	2.881 (11)	174
N3—H3B···N1^{iii}	0.86	2.53	3.214 (11)	137

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors wish to acknowledge Shahid Beheshti University, G·C., for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2716).

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supplementary materials

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catena-Poly[[bis(pyrazine-2-carboxamide-κN^4)mercury(II)]-di-μ-bromido]

B. Mir Mohammad Sadegh, A. Azhdari Tehrani and H. R. Khavasi

Comment

A large variety of pyridine and pyrazine amide ligands have been synthesized for investigating their metal-binding properties (Sasan *et al.*, 2008; Khavasi *et al.*, 2009; Petro & Mukherjee, 1999; Sigh & Mukherjee, 2005). The coordination chemistry of parazineamides is rich. Examples of coordination *via* the pyrazine N atoms, the carbonyl O atoms and the amide N atoms of the ligand in a non-, mono-, or bis-deprotonated form are known (Hausmann & Brooker, 2004; Cati & Stoeckli-Evans, 2004; Miyazaki *et al.*, 2007) and metal complexes of the ligands have been used extensively to mimic the properties of biologically active systems. Here we synthesized the title compound, (I), and report here its crystal structure.

The asymmetric unit of the title compound, (I), contains one half-molecule (Fig. 1). The Hg^{II} atom is six-coordinated in a distorted octahedral configuration by two N atoms from pyrazine amides and four bridging Br atoms. The bridging function of bromo atoms leads to a one-dimensional chain structure. The Hg—Br and Hg—N bond lengths and angles (Table 1) are within normal ranges. In the crystal structure (Fig. 2), intermolecular N—H···O and N—H···N hydrogen bonds (Table 2) result in the formation of a supramolecular structure, in which they may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, a solution of pyrazineamide (0.246 g, 2.0 mmol) in methanol (10 ml) was added to a solution of $HgBr_2$ (0.360 g, 1.0 mmol) in methanol (5 ml) at room temperature. The suitable crystals for X-ray analysis were obtained by slow evaporation from methanolic solution after one week (yield 0.500 g, 82.5%).

Refinement

All of the H atoms were positioned geometrically with C–H = 0.93 and N—H = 0.86 Å and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*). The largest peak and deepest hole are near to the Hg1 atom (0.90 and 0.79 Å, respectively).

Figures

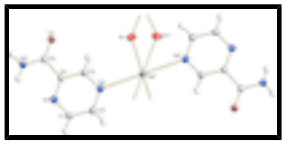

Fig. 1. The molecular structure with the atom-numbering scheme. Displacement ellipsoids are drawn at 30% probability level.

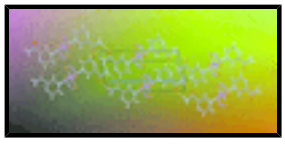

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[[bis(pyrazine-2-carboxamide-κN^4)mercury(II)]-\ di-μ-bromido]

Crystal data

$[HgBr_2(C_5H_5N_3O)_2]$	$Z = 1$
$M_r = 606.63$	$F(000) = 278$
Triclinic, $P\overline{1}$	$D_x = 2.669$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 3.9628$ (5) Å	Cell parameters from 765 reflections
$b = 6.5162$ (9) Å	$\theta = 3.2–29.1°$
$c = 15.0388$ (19) Å	$\mu = 15.50$ mm^{-1}
$\alpha = 101.783$ (10)°	$T = 298$ K
$\beta = 93.418$ (11)°	Needle, colorless
$\gamma = 95.214$ (11)°	0.5 × 0.06 × 0.03 mm
$V = 377.36$ (9) Å^3	

Data collection

Stoe IPDS II diffractometer	1933 reflections with $I > 2\sigma(I)$
rotation method scans	$R_{int} = 0.144$
Absorption correction: multi-scan (*X-RED* and *X-SHAPE*; Stoe & Cie, 2005)	$\theta_{max} = 29.1°$, $\theta_{min} = 3.2°$
$T_{min} = 0.345$, $T_{max} = 0.630$	$h = -5\rightarrow5$
4311 measured reflections	$k = -8\rightarrow8$
2002 independent reflections	$l = -20\rightarrow20$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.065$	$w = 1/[\sigma^2(F_o^2) + (0.1262P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.173$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.11$	$\Delta\rho_{max} = 3.93$ e Å^{-3}
2002 reflections	$\Delta\rho_{min} = -5.48$ e Å^{-3}
97 parameters	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.402 (2)	0.5193 (13)	0.7914 (6)	0.0456 (17)
H1	0.3215	0.6506	0.8064	0.055*
C2	0.400 (2)	0.4210 (13)	0.7010 (6)	0.0444 (16)
H2	0.3156	0.4876	0.6566	0.053*
C3	0.629 (2)	0.1448 (13)	0.7407 (5)	0.0414 (15)
H3	0.7049	0.0123	0.7252	0.05*
C4	0.638 (2)	0.2438 (14)	0.8329 (6)	0.0381 (15)
C5	0.790 (2)	0.1363 (13)	0.9029 (5)	0.0413 (15)
N1	0.519 (2)	0.4278 (10)	0.8588 (5)	0.0420 (14)
N2	0.5148 (18)	0.2350 (10)	0.6752 (4)	0.0422 (13)
N3	0.779 (2)	0.2309 (12)	0.9885 (5)	0.0525 (17)
H3A	0.8633	0.1766	1.0313	0.063*
H3B	0.6883	0.3471	1.0017	0.063*
O1	0.914 (2)	−0.0290 (12)	0.8783 (5)	0.0577 (19)
Hg1	0.5	0	0.5	0.0390 (2)
Br1	0.86218 (19)	−0.24778 (12)	0.55380 (6)	0.0394 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.065 (5)	0.036 (3)	0.038 (4)	0.015 (3)	−0.006 (3)	0.011 (3)
C2	0.055 (4)	0.042 (4)	0.037 (3)	0.004 (3)	−0.009 (3)	0.014 (3)
C3	0.056 (4)	0.039 (3)	0.030 (3)	0.013 (3)	−0.006 (3)	0.006 (3)
C4	0.048 (4)	0.037 (3)	0.028 (3)	0.006 (3)	−0.005 (3)	0.004 (3)
C5	0.055 (4)	0.041 (4)	0.029 (3)	0.011 (3)	−0.002 (3)	0.009 (3)
N1	0.062 (4)	0.031 (3)	0.032 (3)	0.007 (3)	−0.007 (3)	0.007 (2)
N2	0.057 (3)	0.040 (3)	0.029 (3)	0.007 (3)	−0.007 (2)	0.010 (2)
N3	0.085 (5)	0.045 (3)	0.030 (3)	0.023 (4)	−0.005 (3)	0.009 (3)
O1	0.095 (6)	0.049 (3)	0.031 (3)	0.032 (4)	−0.005 (3)	0.007 (2)
Hg1	0.0387 (3)	0.0433 (3)	0.0380 (3)	0.01479 (17)	−0.00149 (16)	0.01255 (19)
Br1	0.0390 (4)	0.0374 (4)	0.0453 (5)	0.0116 (3)	0.0000 (3)	0.0146 (3)

Geometric parameters (Å, °)

C1—N1	1.356 (10)	C5—O1	1.224 (11)
C1—C2	1.378 (12)	C5—N3	1.313 (10)
C1—H1	0.93	N3—H3A	0.86
C2—N2	1.325 (11)	N3—H3B	0.86
C2—H2	0.93	Hg1—Br1	2.4775 (8)
C3—N2	1.323 (9)	Hg1—Br1^{i}	2.4775 (8)
C3—C4	1.402 (11)	Hg1—Br1^{ii}	3.1122 (8)
C3—H3	0.93	Hg1—Br1^{iii}	3.1122 (8)
C4—N1	1.321 (12)	Hg1—N2	2.758 (6)
C4—C5	1.505 (12)	Hg1—N2^{i}	2.758 (6)

N1—C1—C2	121.2 (8)	N3—C5—C4	116.1 (8)
N1—C1—H1	119.4	C4—N1—C1	116.5 (7)
C2—C1—H1	119.4	C3—N2—C2	116.8 (7)
N2—C2—C1	122.2 (7)	C5—N3—H3A	120
N2—C2—H2	118.9	C5—N3—H3B	120
C1—C2—H2	118.9	H3A—N3—H3B	120
N2—C3—C4	121.7 (8)	Br1—Hg1—Br1^{i}	180.00 (4)
N2—C3—H3	119.1	Br1—Hg1—Br1^{ii}	90.44 (2)
C4—C3—H3	119.1	Br1^{i}—Hg1—Br1^{ii}	89.56 (2)
N1—C4—C3	121.5 (8)	Br1—Hg1—Br1^{iii}	89.56 (2)
N1—C4—C5	120.1 (7)	Br1^{i}—Hg1—Br1^{iii}	90.44 (2)
C3—C4—C5	118.4 (8)	Br1^{ii}—Hg1—Br1^{iii}	180.000 (17)
O1—C5—N3	124.2 (8)	Hg1—Br1—Hg1^{iv}	89.56 (2)
O1—C5—C4	119.7 (7)		
N1—C1—C2—N2	−0.7 (15)	C3—C4—C5—N3	−177.2 (9)
N2—C3—C4—N1	2.9 (14)	C3—C4—N1—C1	−2.6 (12)
N2—C3—C4—C5	−176.4 (8)	C5—C4—N1—C1	176.7 (9)
N1—C4—C5—O1	−176.4 (8)	C2—C1—N1—C4	1.6 (13)
C3—C4—C5—O1	3.0 (14)	C4—C3—N2—C2	−1.9 (12)
N1—C4—C5—N3	3.4 (13)	C1—C2—N2—C3	0.8 (13)

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+2, −*y*, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O1^{v}	0.86	2.02	2.881 (11)	174
N3—H3B···N1^{vi}	0.86	2.53	3.214 (11)	137

Symmetry codes: (v) −*x*+2, −*y*, −*z*+2; (vi) −*x*+1, −*y*+1, −*z*+2.

Fig. 1

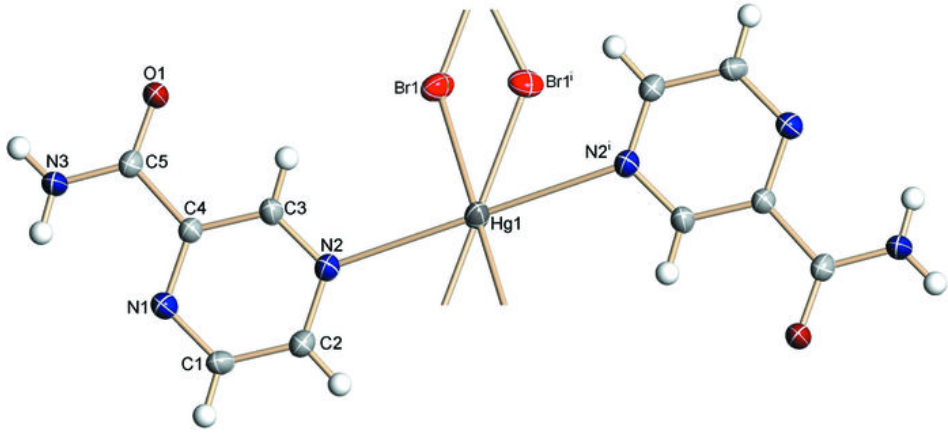

Fig. 2