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catena-Poly[[diiodidomercury(II)]-μ_2-2-aminopyrazine-$\kappa^2N^1:N^4$]

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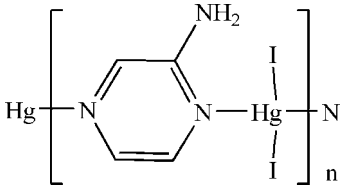
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.020 Å; disorder in main residue; R factor = 0.083; wR factor = 0.224; data-to-parameter ratio = 17.9.

In the crystal of the title polymeric compound, $[HgI_2(C_4H_5N_3)]_n$, the Hg^{II} cation is located on a twofold rotation axis and is coordinated by two I^- anions and two 2-aminopyrazine ligands in a distorted HgI_2N_2 tetrahedral geometry. In the crystal, the 2-aminopyrazine ligand is equally disordered over two positions about an inversion center, and bridges the Hg^{II} cations with pyrazine N atoms to form a polymeric chain running along the c axis. In the polymeric chain, the amino groups link to the coordinated I^- anions *via* intermolecular N—H···I hydrogen bonds.

Related literature

For related structures, see: Sun *et al.* (2009); Pagola *et al.* (2008); Boonmak *et al.* (2010); Gao & Ng (2011); Goher *et al.* (2008).



Experimental

Crystal data

$[HgI_2(C_4H_5N_3)]$
M_r = 549.50
Monoclinic, $C2/c$
a = 15.3389 (19) Å
b = 6.8791 (8) Å
c = 9.6239 (11) Å
β = 103.828 (10)°
V = 986.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 21.81 mm^{-1}
T = 298 K
0.50 × 0.05 × 0.04 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.275, T_{max} = 0.417
2648 measured reflections
933 independent reflections
911 reflections with $I > 2\sigma(I)$
R_{int} = 0.173

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.224
S = 1.08
933 reflections
52 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.67 e Å^{-3}
$\Delta\rho_{min}$ = −2.69 e Å^{-3}

Table 1
Selected bond lengths (Å).

Hg1—I1	2.6373 (13)	Hg1—N1^{i}	2.497 (11)

Symmetry code: (i) $-x, y, -z+\frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···I1^{i}	0.86	2.83	3.67 (3)	169

Symmetry code: (i) $-x, y, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We are grateful to the Islamic Azad University, Omidieh Branch, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5467).

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supplementary materials

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catena-Poly[[diiodidomercury(II)]-μ_2-2-aminopyrazine-$\kappa^2N^1:N^4$]

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Comment

2-Aminopyrazine is a good ligand and numerous complexes with 2-aminopyrazine have been prepared, such as that of silver (Sun *et al.*, 2009), copper (Pagola *et al.*, 2008), cobalt, iron and cadmium (Boonmak *et al.*, 2010) and zinc (Gao & Ng, 2011; Goher *et al.*, 2008). Here, we report the synthesis and structure of the title compound.

The asymmetric unit of the title compound, (Fig. 1), contains one half molecule. The Hg^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from two 2-aminopyrazine and two I atoms. The Hgd-I and Hg—N bond lengths angles are collected in Table 1.

Intermolecular N—H···I hydrogen bonds (Table 2) seem to be effective in the stabilization of the polymeric structure (Fig. 2).

Experimental

For the preparation of the title compound, a solution of 2-aminopyrazine (0.15 g, 1.50 mmol) in methanol (10 ml) was added to a solution of HgI_2 (0.55 g, 1.50 mmol) in methanol (10 ml) and the resulting colorless solution was stirred for 15 min at room temperature. This solution was left to evaporate slowly at room temperature. After one week, colorless needle crystals of the title compound were isolated (yield 0.63 g, 76.4%).

Refinement

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). In the crystal, the 2-aminopyrazine ring is equqlly disordered over two positions about an inversion center.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

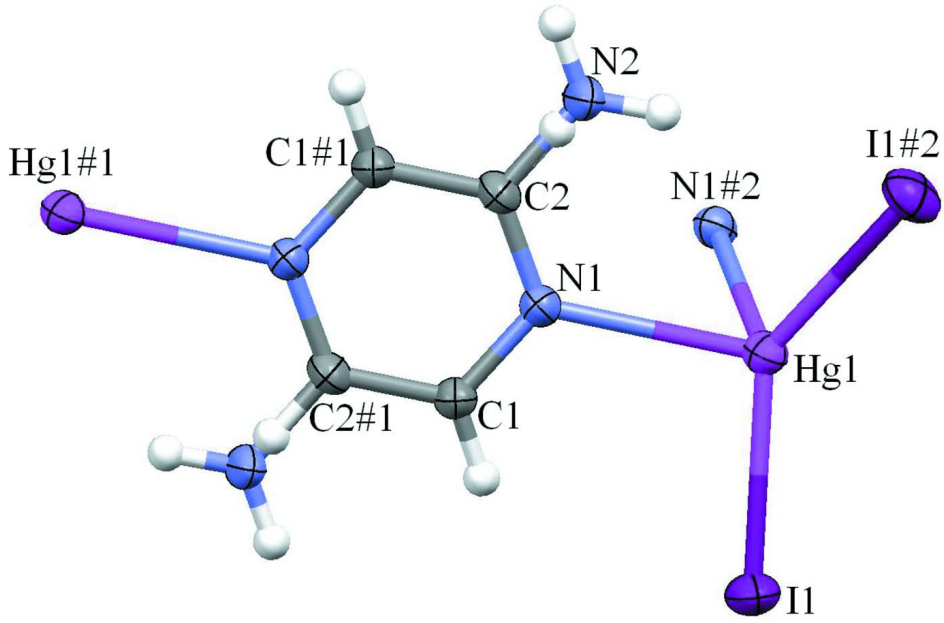

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: #1: -*x*, 1 - *y*, 1 - *z*; #2: -*x*, *y*, 3/2 - *z*].

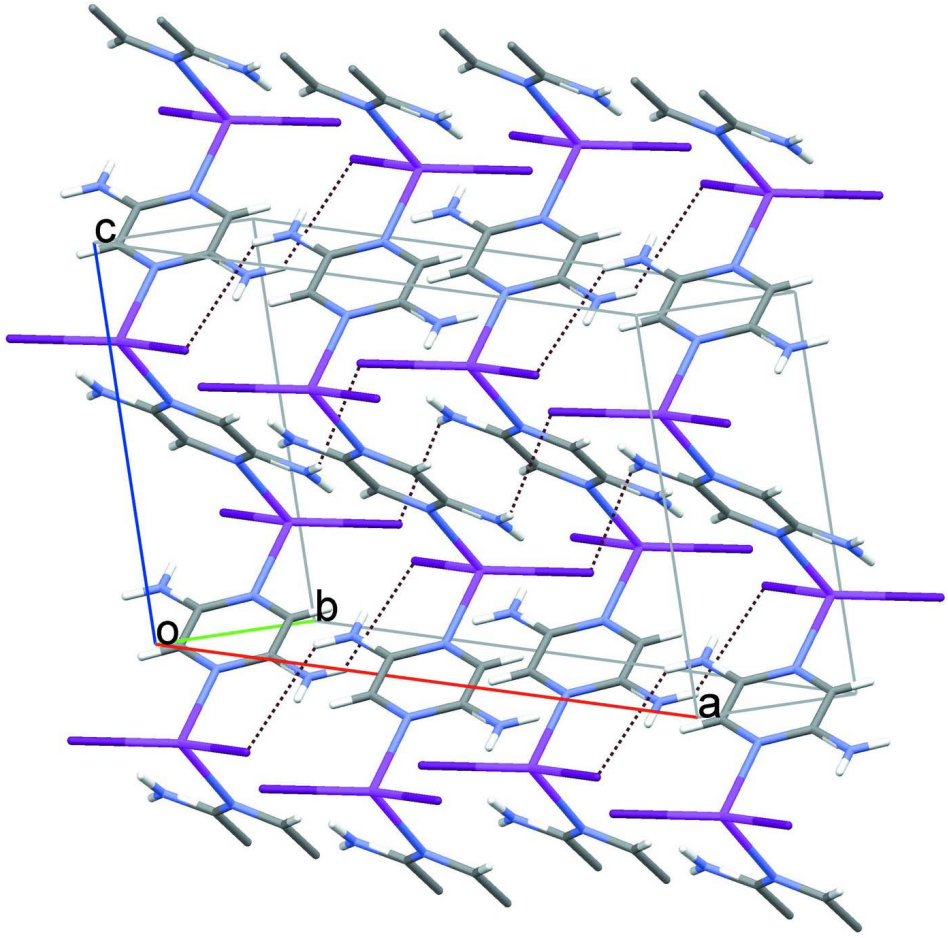

Figure 2

A packing diagram of the title complex. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[HgI_2(C_4H_5N_3)]$
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Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 15.3389 (19) Å
b = 6.8791 (8) Å
c = 9.6239 (11) Å
β = 103.828 (10)°
V = 986.1 (2) Å^3
Z = 4
F(000) = 944
D_x = 3.701 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 2648 reflections
θ = 2.7–26.0°
μ = 21.81 mm^{-1}
T = 298 K
Needle, colorless
0.50 × 0.05 × 0.04 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.275, T_{max} = 0.417
2648 measured reflections
933 independent reflections
911 reflections with $I > 2\sigma(I)$

R_{int} = 0.173
θ_{max} = 26.0°, θ_{min} = 2.7°
h = −18→18
k = −8→8
l = −11→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.224
S = 1.08
933 reflections
52 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1405P)^2 + 17.0935P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 2.67 e Å^{-3}
$\Delta\rho_{min}$ = −2.69 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.015 (2)

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.0725 (10)	0.383 (2)	0.5415 (17)	0.042 (3)	
H1	0.1234	0.3063	0.5710	0.050*	
C2	−0.0746 (11)	0.455 (2)	0.542 (2)	0.044 (3)	
H2C	−0.1274	0.4240	0.5694	0.054*	0.50
N1	−0.0046 (8)	0.3371 (17)	0.5809 (12)	0.040 (2)	
N2	−0.154 (2)	0.409 (5)	0.578 (4)	0.059 (8)	0.50
H2A	−0.1586	0.3048	0.6251	0.071*	0.50
H2B	−0.1999	0.4856	0.5531	0.071*	0.50
Hg1	0.0000	0.05992 (11)	0.7500	0.0451 (6)	
I1	0.16288 (9)	−0.07523 (19)	0.76493 (17)	0.0629 (7)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.038 (7)	0.040 (7)	0.051 (7)	0.005 (6)	0.016 (6)	0.008 (7)
C2	0.034 (7)	0.046 (8)	0.055 (9)	−0.003 (5)	0.016 (6)	0.005 (6)
N1	0.039 (6)	0.035 (5)	0.050 (6)	0.002 (4)	0.018 (5)	0.004 (5)
N2	0.054 (17)	0.062 (17)	0.070 (17)	0.020 (14)	0.032 (15)	0.034 (14)
Hg1	0.0390 (8)	0.0411 (8)	0.0576 (8)	0.000	0.0164 (5)	0.000
I1	0.0484 (10)	0.0655 (10)	0.0793 (11)	0.0199 (5)	0.0241 (7)	0.0154 (5)

Geometric parameters (Å, º)

C1—N1	1.363 (19)	N1—Hg1	2.497 (11)
C1—C2^{i}	1.38 (2)	N2—H2A	0.8600
C1—H1	0.9300	N2—H2B	0.8600
C2—N1	1.33 (2)	Hg1—I1^{ii}	2.6372 (13)
C2—H2C	0.9300	Hg1—I1	2.6373 (13)
C2—C1^{i}	1.38 (2)	Hg1—N1^{ii}	2.497 (11)
C2—N2	1.38 (4)		
N1—C1—C2^{i}	119.6 (14)	C1—N1—Hg1	117.9 (10)
N1—C1—H1	120.2	C2—N2—H2A	120.0
C2^{i}—C1—H1	120.2	C2—N2—H2B	120.0
C1^{i}—C2—H2C	119.0	H2A—N2—H2B	120.0
N1^{i}—C2—H2C	149.0	N1^{ii}—Hg1—N1	80.4 (5)
N1—C2—C1^{i}	121.6 (15)	N1^{ii}—Hg1—I1^{ii}	100.6 (3)
N1—C2—N2	120.0 (17)	N1—Hg1—I1^{ii}	110.8 (3)
C1^{i}—C2—N2	118.2 (18)	N1^{ii}—Hg1—I1	110.8 (3)
C2—N1—C1	118.6 (13)	N1—Hg1—I1	100.6 (3)
C2—N1—Hg1	122.9 (10)	I1^{ii}—Hg1—I1	138.71 (7)
C1^{i}—C2—N1—C1	3 (3)	C2—N1—Hg1—N1^{ii}	−68.8 (12)
N2—C2—N1—C1	179 (2)	C1—N1—Hg1—N1^{ii}	102.6 (12)
C1^{i}—C2—N1—Hg1	174.4 (13)	C2—N1—Hg1—I1^{ii}	29.0 (13)
N2—C2—N1—Hg1	−10 (3)	C1—N1—Hg1—I1^{ii}	−159.7 (10)
C2^{i}—C1—N1—C2	−3 (3)	C2—N1—Hg1—I1	−178.4 (12)
C2^{i}—C1—N1—Hg1	−174.8 (12)	C1—N1—Hg1—I1	−7.0 (11)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···I1^{ii}	0.86	2.83	3.67 (3)	169

Symmetry code: (ii) −*x*, *y*, −*z*+3/2.