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μ-Pyrazine-κ^2N:N'-bis[diiodomercury(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.040 Å
R factor = 0.059
wR factor = 0.171
Data-to-parameter ratio = 23.9

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

In [Hg_2I_4(Pyp)] (Pyp = pyrazine, $C_4H_4N_2$), centrosymmetric molecules consist of two HgI_2 units connected by a pyrazine molecule.

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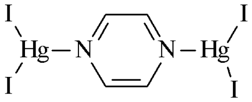
Comment

The coordination chemistry of divalent mercury with N-donor ligands has been reviewed several times (*e.g.* Grdenić, 1965; Breitinger & Brodersen, 1970). In a systematic structural study, we have used diazines as N-donor ligands to mercuric halides (Nockemann, 2002; Meyer & Nockemann, 2003).



(I)

The structure of [Hg_2I_4(Pyp)], (I), consists of two HgI_2 molecules, which are connected by the 1 and 4 positions of a pyrazine molecule. The complete discrete molecule is centrosymmetric. The Hg—N bond length [2.511 (18) Å] is shorter than in the adduct of pyrazine with mercuric bromide $HgBr_2$ (Nockemann & Meyer, 2004*b*), indicating somewhat stronger covalent contributions. This affects also the I—Hg—I angle, which is bent to 163.41 (7)°, smaller than that of the bromide at 167.78 (3)°. The Hg—I bond lengths are 2.6036 (19) and 2.6278 (19) Å, comparable to those in mercury(II) iodide itself in its metastable orange modification, at 2.612 Å (Jeffrey & Vlasse, 1967), but shorter than in the

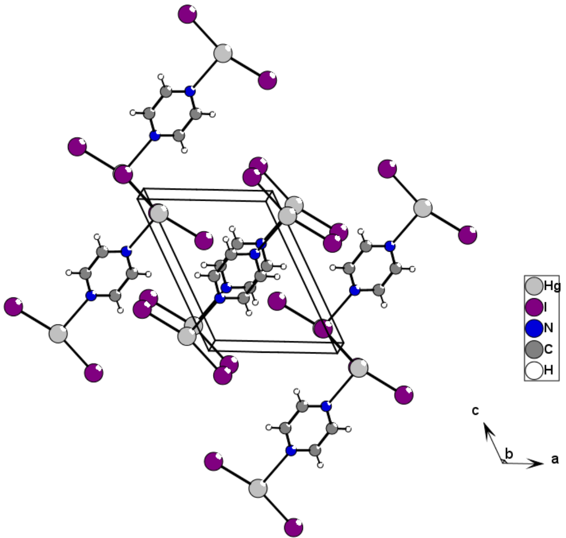


Figure 1
Packing diagram of [Hg_2I_4(Pyp)], viewed approximately down the b axis.

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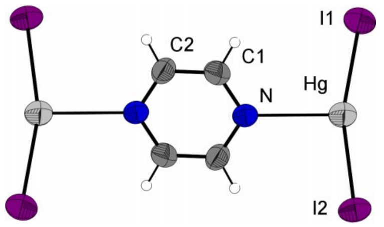

Figure 2
View of the $[Hg_2I_4(Pyp)]$ molecule, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

room-temperature modification, at 2.784 Å (Turner & Harmon, 1989).

There are no significant interactions between the molecules in the crystal structure. Thus, a molecular compound with a 2:1 ratio of HgI_2 to pyrazine is formed, even though the synthesis employed a large excess of pyrazine. The series of adducts of pyrazine with $HgCl_2$, $HgBr_2$ and HgI_2 exhibits a tendency to depolymerization in this order (Nockemann & Meyer, 2004*a*,*b*).

Experimental

$[Hg_2I_4(Pyp)]$ was obtained by adding a solution of an excess of pyrazine (2.0 g, 25 mmol) in ethanol to an ethanolic solution of mercury(II) iodide (2.27 g, 5 mmol) in a Schlenk vessel under an argon atmosphere. Yellow crystals were obtained by slow evaporation of the ethanol into a second vessel, cooled with dry ice. Exposure of the crystals to moist air results in their decomposition after a few hours.

Crystal data

$[HgI_4(C_4H_4N_2)]$
$M_r = 988.87$
Triclinic, $P\bar{1}$
$a = 7.107$ (2) Å
$b = 7.114$ (3) Å
$c = 8.436$ (3) Å
$\alpha = 95.72$ (3)°
$\beta = 109.30$ (2)°
$\gamma = 113.14$ (2)°
$V = 357.0$ (2) Å^3
$Z = 1$
$D_x = 4.600$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2831 reflections
$\theta = 5.3$–59.3°
$\mu = 30.09$ mm^{-1}
$T = 293$ (2) K
Prism, yellow
0.2 × 0.2 × 0.2 mm

Data collection

Stoe IPDS-I diffractometer
φ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
$T_{\min} = 0.113$, $T_{\max} = 0.261$
2831 measured reflections
1340 independent reflections
996 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.063$
$\theta_{\max} = 26.0°$
$h = -8 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.171$
$S = 1.03$
1340 reflections
56 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1031P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 4.22$ e Å^{-3}
$\Delta\rho_{\min} = -1.49$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.020 (2)

Table 1
Selected geometric parameters (Å, °).

Hg—N	2.511 (18)	N—C1	1.33 (3)
Hg—I1	2.6036 (19)	C1—C2$^{\rm i}$	1.38 (3)
Hg—I2	2.6278 (19)	C2—C1$^{\rm i}$	1.38 (3)
N—C2	1.32 (3)		
N—Hg—I1	99.5 (4)	C2—N—Hg	123.3 (14)
N—Hg—I2	97.1 (4)	C1—N—Hg	121.9 (15)
I1—Hg—I2	163.41 (7)	N—C1—C2$^{\rm i}$	124 (2)
C2—N—C1	114.8 (19)	N—C2—C1$^{\rm i}$	121 (2)
I2—Hg—N—C2	33.2 (16)	I1—Hg—N—C1	31.7 (17)

Symmetry code: (i) $1 - x, 2 - y, 1 - z$.

The highest peak and deepest hole were located 1.39 Å from I2 and 0.86 Å from Hg, respectively. H atoms were visible in a difference map and were treated as riding atoms, with a C—H distance of 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

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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