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catena-Poly[[(1*H*-benzimidazole-κN)iodomercury(II)]-μ-iodo]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.013 Å
R factor = 0.033
wR factor = 0.067
Data-to-parameter ratio = 17.9

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

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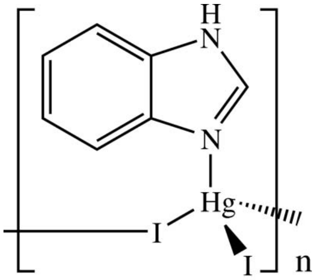
In the title polymeric complex, $[HgI_2(C_7H_6N_2)]_n$, the Hg^{II} atom is coordinated by one benzimidazole (bzim) and three I^- anions with a distorted tetrahedral geometry; one I^- anion is in a monodentate coordination mode and the other two are bridging. The two bridging Hg—I bond distances differ significantly [2.7420 (7) and 3.0543 (7) Å]. The face-to-face separation of 3.31 (3) Å between the mean planes of parallel bzim ligands and the partially overlapped arrangement indicate the existence of π–π stacking.

Comment

As π–π stacking between aromatic rings plays an important role for the electron-transfer process in some biological systems (Desenhofer & Michel, 1989), we are interested in the nature of π–π stacking. A series of metal complexes incorporating different aromatic ligands has been prepared in our laboratory (Pan & Xu, 2004; Luo *et al.*, 2004; Li *et al.*, 2005). In order to study the effect of the central metal ion on π–π stacking in metal complexes, the title Hg^{II} complex, (I), with the benzimidazole ligand (bzim) has been prepared and its structure is presented here.



(I)

A segment of the polymeric structure of (I) is illustrated in Fig. 1. The Hg^{II} atom is coordinated by one bzim and three I^- anions with a distorted tetrahedral geometry. While atom I1 coordinates as monodentate to the Hg^{II} atom with a shorter bond distance (Table 1), atoms I2 and $I2^i$ bridge neighbouring Hg^{II} atoms to form a zigzag polymeric chain, propagating along the *a* axis. The Hg—I2 bond is longer than the Hg—$I2^i$ bond by 0.312 (10) Å, which is comparable with the value of 0.424 (8) Å found in the only other μ_2-iodo–Hg^{II} complex published to date, bis[di-μ_2-iodo-diiodobis(diphenyltelluro)dimercury(II)] (Einstein *et al.*, 1983). The I1—Hg—$I2^i$ bond angle is larger than the I1—Hg—I2 bond angle by 29.23 (3)° [symmetry code: (i) $1 + x, y, z$], showing the degree of distortion of the coordination geometry from normal tetrahedral (Table 1).

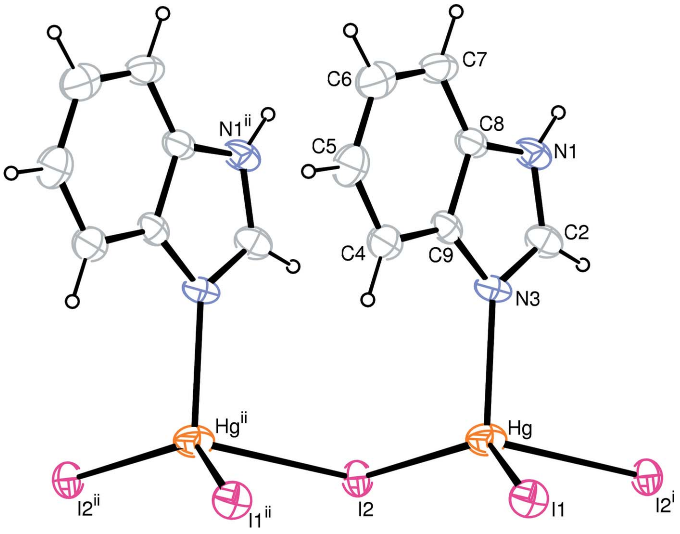


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids [symmetry codes: (i) $1 + x, y, z$; (ii) $-1 + x, y, z$].

The packing of (I) is shown in Fig. 2. Adjacent polymeric chains are linked by N—H⋯I hydrogen bonds (Table 2) to form two-dimensional supramolecular layers. A partially overlapped arrangement is observed between neighbouring bzim ligands, and the short face-to-face separation of 3.31 (3) Å between the mean planes of the bzim and bzim^{ii} ligands [symmetry code: (ii) $-1 + x, y, z$] clearly suggests the existence of π–π stacking in the crystal structure of (I).

Experimental

An aqueous solution (10 ml) of oxydiacetatic acid (1 mmol) and Na_2CO_3 (1 mmol) was mixed with a water–ethanol solution (10 ml, 1:1) of bzim (2 mmol), and then HgI_2 (1 mmol) was added to the solution. The resulting red mixture was refluxed for 2 h and a red precipitate appeared. The precipitate was separated by filtration, and the red filtrate was refluxed again until the colour of the solution changed to bright yellow. After cooling to room temperature, the solution was filtered. Single crystals of (I) were obtained from the filtrate after 2 d.

Crystal data

$[HgI_2(C_7H_6N_2)]$
$M_r = 572.53$
Monoclinic, $P2_1/n$
$a = 4.4079$ (4) Å
$b = 13.3559$ (11) Å
$c = 18.6196$ (16) Å
$\beta = 96.136$ (12)°
$V = 1089.88$ (16) Å^3
$Z = 4$
$D_x = 3.489$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7029 reflections
$\theta = 2.0$–25.0°
$\mu = 19.74$ mm^{-1}
$T = 295$ (2) K
Prism, yellow
0.12 × 0.08 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.095$, $T_{max} = 0.298$
7910 measured reflections
1955 independent reflections
1768 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.2°$
$h = -5 \rightarrow 4$
$k = -16 \rightarrow 16$
$l = -22 \rightarrow 22$

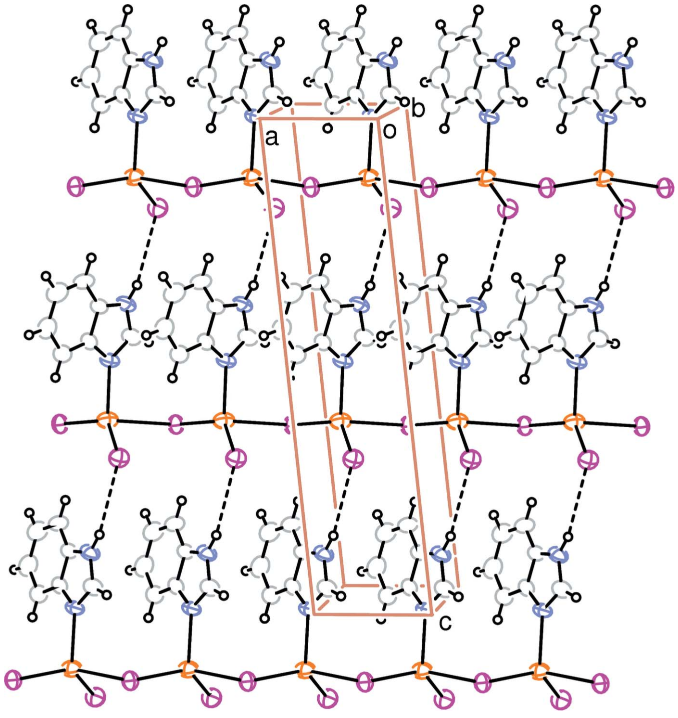


Figure 2
A packing diagram for (I), showing the hydrogen bonding (dashed lines) between polymeric chains.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.067$
$S = 1.20$
1955 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0191P)^2 + 7.8058P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.27$ e Å^{-3}
$\Delta\rho_{min} = -1.41$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg—I1	2.6322 (7)	Hg—I2	3.0543 (7)
Hg—I2^i	2.7420 (7)	Hg—N3	2.289 (6)
I1—Hg—I2	105.53 (2)	N3—Hg—I2^i	101.12 (17)
I1—Hg—I2^i	134.76 (2)	I2^i—Hg—I2	98.87 (2)
I1—Hg—N3	113.29 (17)	Hg^{ii}—I2—Hg	98.87 (2)
I2—Hg—N3	95.93 (18)		

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯I1^{iii}	0.86	3.01	3.820 (7)	158

Symmetry code: (iii) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and included in the final cycles of refinement in

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the riding model, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atom. The highest peak and deepest hole in the final difference Fourier map are 0.87 and 0.77 Å from the Hg atom, respectively.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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