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Crystal structure of catena-poly[tetraiodido-(μ_2 -1,4-bis(2-methyl-1*H*-imidazol-1-yl)benzene- $\kappa^2N:N'$)dimercury(II)], $C_{14}H_{14}Hg_2I_4N_4$

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Abstract

$C_{14}H_{14}Hg_2I_4N_4$, monoclinic, $P2_1/c$, $a = 4.3592(11)$ Å, $b = 20.116(5)$ Å, $c = 12.713(3)$ Å, $\beta = 96.838(5)^\circ$, $Z = 2$, $V = 1106.9(5)$ Å³, $R_{gt}(F) = 0.0362$, $wR_{ref}(F^2) = 0.0863$, $T = 296(2)$ K.

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Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.25 × 0.22 × 0.19 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	19.4 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	25.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	6289, 2054, 0.041
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1799
$N(param)_{refined}$:	110
Programs:	SHELX [1, 2], CrysAlis ^{PRO} [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Hg1	0.39779(12)	0.31347(2)	0.46968(4)	0.04825(16)
C1	0.126(2)	0.4790(5)	0.0992(8)	0.032(2)
C2	−0.030(3)	0.5385(5)	0.0869(8)	0.039(2)
H2	−0.0487	0.5649	0.1458	0.047*
C3	0.158(2)	0.4406(5)	0.0114(8)	0.035(2)
H3	0.2665	0.4007	0.0188	0.042*
C4	0.038(3)	0.3416(6)	0.2018(9)	0.050(3)
H4A	−0.0167	0.3131	0.2573	0.075*
H4B	0.1550	0.3168	0.1559	0.075*
H4C	−0.1470	0.3583	0.1618	0.075*
C5	0.225(2)	0.3978(5)	0.2486(8)	0.036(2)
C6	0.518(3)	0.4601(5)	0.3574(8)	0.042(3)
H6	0.6445	0.4738	0.4175	0.050*
C7	0.440(3)	0.4974(5)	0.2720(8)	0.041(2)
H7	0.4979	0.5413	0.2621	0.049*
I1	0.60515(18)	0.20475(4)	0.38664(7)	0.0480(2)
I2	0.00610(16)	0.35980(4)	0.60039(6)	0.0457(2)
N1	0.383(2)	0.3981(5)	0.3440(7)	0.043(2)
N2	0.2585(19)	0.4585(4)	0.2018(6)	0.0331(18)

Source of material

A mixture of 1,4-bis(2-methyl-1*H*-imidazol-1-yl)benzene (23.8 mg, 0.1 mmol), mercury(II) iodide (136.3 mg, 0.3 mmol), 1 mL ethanol and 6 mL distilled water were added in a Teflon-lined autoclave and then heated to 140 °C for 72 h before cooled to room temperature. Yellow block crystals were obtained in 63% yield (based on 1,4-bis(2-methyl-1*H*-imidazol-1-yl)benzene), washed with deionized water, and dried in air. Anal. Calcd. for C₇H₇HgI₂N₂ (573.54): C, 14.66; H, 1.23; N, 4.88%. Found: C, 14.21; H, 1.20; N, 4.96%.

Experimental details

All hydrogen atoms were placed at calculated positions and refined with a riding model, with $d(C-H) = 0.93 \text{ \AA}$ and $0.96 \text{ \AA}$ (CH₃). U_{iso} parameters of hydrogen atoms were set to $1.5U_{eq}(C)$ for methyl groups and $1.2U_{eq}(C)$ otherwise.

Comment

Coordination polymers (CPs) have attracted great attention because of their molecular topologies, properties, and potential applications in the fields of materials [3–7]. Imidazole derivatives have been widely used as ligands in bioinorganic chemistry, cluster science, and building blocks of supermolecular frameworks [8–10]. The rigid bisimidazole ligand, 1,4-bis(2-methyl-1*H*-imidazol-1-yl)benzene, as the building unit, which features one special characteristics: the free rotation of imidazole rings can promote the flexibility of the ligand to meet the requirements of coordination geometries of metal ions for tuning the fine structure. The bisimidazole ligands not only act as bidentate ligand to coordinate two metal ions but can also be used to assemble supramolecular architectures.

The asymmetric unit of the title compound consists of one crystallographically independent Hg(II) ion, one half 1,4-bis(2-methyl-1*H*-imidazol-1-yl)benzene ligand, and two iodide anions. Each Hg(II) cation is four-coordinated with three iodide anions and one nitrogen atom from the bisimidazole ligand to form distorted tetrahedron geometry (upper part of the figure; $A = -x, 1 - y, -z$; $B = -1 - x, 1 - y, -z$; $C = 1 + x, y, z$). The bond lengths of Hg–I vary slightly in the range of $2.6351(9) \text{ \AA}$ – $3.1005(10) \text{ \AA}$, and the Hg–N distance is $2.331(9) \text{ \AA}$, both of which are in the normal range [10–12]. The involving Hg atoms bond angles of $I(1)–Hg(1)–I(2)$, $I(1)–Hg(1)–N(1)$, $I(2)–Hg(1)–I(2C)$ and $I(2)–Hg(1)–N(1)$ are $144.01(3)^\circ$, $108.4(2)^\circ$, $97.48(3)^\circ$ and $101.7(2)^\circ$, respectively. Each bisimidazole ligand linked two Hg(II) ions through N1 and N1A to generate a dinuclear secondary building unit (SBU). Each SBU is linked by two iodide anions to yield a 1D ladder-like coordination polymer chain (lower part of the figure).

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