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Crystallographic report

Diiodo[tris(2-pyridyl)amine]mercury(II), $[(C_5H_4N)_3N]HgI_2$

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In mononuclear $HgI_2[(C_5H_4N)_3N]$, mercury is tetrahedrally coordinated by two nitrogen atoms of a tris(2-pyridyl)amine ligand and two iodides. The coordination moieties are connected by weak intermolecular Hg(II)···I interactions to give a one-dimensional structure. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; mercury complex; one-dimensional structure; pyridyl ligand

COMMENT

X-ray structure analyses reveal that $[(C_5H_4N)_3N]HgI_2$ (**1**) is mononuclear (Fig. 1). The mercury(II) atom is tetrahedrally coordinated to two iodides and two nitrogen atoms of the tris(2-pyridyl)amine ligand.[1] The severe distortion of the coordination geometry can be seen from the N(2)–Hg–N(3) and I(1)–Hg–I(2) bond angles of 77.63(18)° and 140.71(2)° respectively. The mercury atoms are involved in weak intermolecular secondary interactions with the symmetry-related iodide atoms resulting in a one-dimensional (1D) chain (Fig. 1) with the intermolecular Hg···I′ distances of 3.948(1) Å. Unlike the similar zinc(II) complex,[2] no $\pi-\pi$ interactions are observed between the pyridyl rings.

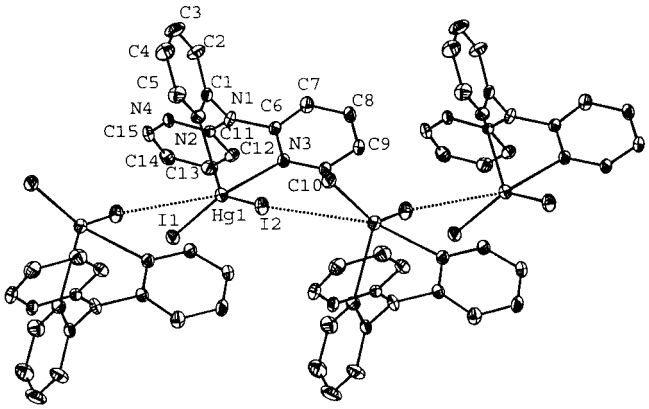

Figure 1. The 1D structure of **1**.

EXPERIMENTAL

1 was synthesized by the reaction of $Hg(NO_3)_2{\cdot}6H_2O$, tris(2-pyridyl)amine, and KI (molar ratio, 1:1:2) in methanol. The concentrated solution was left undisturbed for slow evaporation of the solvent to give colorless crystals. Anal. Found: C, 25.98; H, 1.84; N, 8.18. Calc. for $C_{15}H_{12}HgI_2N_4$: C, 25.64; H, 1.72; N, 7.97%.

Intensity data were collected at 291 K on a Rigaku RAXIS–IV diffractometer for a colorless crystal $0.20 \times 0.20 \times 0.30$ mm^3. $C_{15}H_{12}HgI_2N_4$, $M = 702.68$, monoclinic, $P2_1/c$, $a = 9.6334(19)$, $b = 8.7232(17)$, $c = 21.999(4)$ Å, $\beta = 98.92(3)°$, $V = 1826.3(6)$ Å^3, $Z = 4$, 3939 unique data (θ_{max} 27.5°), 3496 data with $I \geq 2\sigma(I)$, $R = 0.036$ (observed), $wR = 0.089$ (all data), $\rho_{max} = 0.69$ e$^-$ Å^{-3}. Programs used: *SHELXS-97, SHELXL-97*. CCDC deposition number: 184 929.

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