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Crystallographic report

Diiodo[tris(2-pyridyl)amine]zinc(II), $[(C_5H_4N)_3N]ZnI_2$

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The zinc(II) atom in the molecule of $[(C_5H_4N)_3N]ZnI_2$ is tetrahedrally coordinated to two nitrogen atoms of the tris(2-pyridyl)amine ligand and two iodides. The coordination moieties are connected to give a linear structure by intermolecular $\pi-\pi$ interactions between the pyridyl rings. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc complex; $\pi-\pi$ interactions; linear structure

COMMENT

X-ray structure analyses reveal that $[(C_5H_4N)_3N]ZnI_2$ (**1**) is mononuclear (Fig. 1). The zinc(II) atom is tetrahedrally coordinated to two iodides and two nitrogen atoms of the tris(2-pyridyl)amine (TPA) ligand.[1] The distortion of the coordination tetrahedron can be seen from the N–Zn–N and I–Zn–I bond angles of 88.59(19)° and 117.48(3)° respectively. It is worth noting that two of the three pyridyl rings of a TPA ligand are involved in intermolecular face-to-face $\pi-\pi$ interactions.[2] Thus, the $[(C_5H_4N)_3N]ZnI_2$ molecules are connected in a one-dimensional linear structure by the $\pi-\pi$ interactions between the parallel pyridyl rings (Fig. 2).

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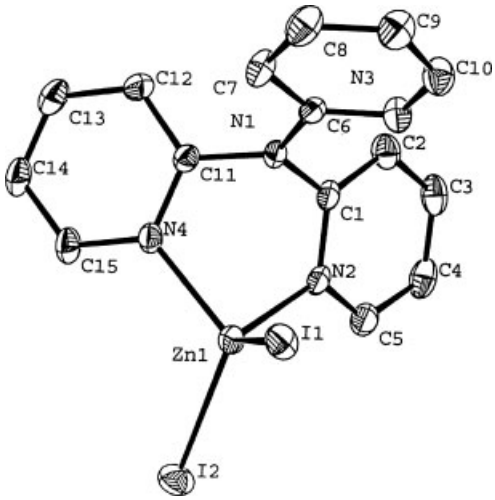

Figure 1. Molecular structure of **1**. Key geometric parameters: Zn–I1 2.5483(12), Zn–I2 2.5353(10), Zn–N1 2.063(5), Zn–N2 2.065(5) Å; N1–Zn–N2 88.59(19), N1–Zn–I2 113.03(15), N2–Zn–I2 112.02(14), N1–Zn–I1 111.27(16), N2–Zn–I1, 110.86(15), I2–Zn–I1 117.48(3)°.

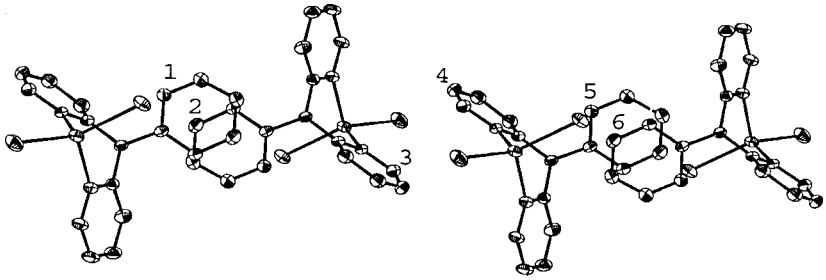

Figure 2. One-dimensional linear packing of **1**, showing weak intermolecular $\pi-\pi$ interactions between the pyridyl rings. (Distances between the pyridyl rings: 1–2, 3.89 Å; 3–4, 3.52 Å; 5–6, 3.89 Å).

EXPERIMENTAL

1 was synthesized by the reaction of $Zn(NO_3)_2 \cdot 6H_2O$, TPA, 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.

Intensity data for **1** were collected at 291 K on a Rigaku RAXIS–IV diffractometer for a colorless crystal $0.28 \times 0.20 \times 0.20\ mm^3$. $C_{15}H_{12}I_2N_4Zn$, $M = 567.46$, triclinic, $P\bar{1}$, $a = 14.970(3)$, $b = 8.6729(17)$, $c = 14.559(3)$ Å, $\alpha = 90$, $\beta = 105.22(3)$, $\gamma = 90°$, $V = 1824.0(6)$ Å^3, $Z = 4$, 3632 unique data (θ_{max} 27.52°), 2565 data with $I \geq 2\sigma(I)$, $R = 0.0451$(obs.), $wR = 0.1064$ (all data), $\rho_{max} = 0.983\ e^-$ Å^{-3}. Programs used: SHELXS-97, SHELXL-97. CCDC deposition number: 184924.

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