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Crystallographic report

Bis(tripyridyldiamine)zinc(II) tetrabromozincate(II) hydrate

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The zinc(II) atom in the complex cation of $[Zn(tpda)_2][ZnBr_4]\cdot H_2O$ is octahedrally coordinated, whereas the zinc(II) atom in the anion is tetrahedrally coordinated. The cations and the anions are connected by hydrogen bonds, affording a two-dimensional network. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc complex; 2D network; tripyridyldiamine

COMMENT

The zinc(II) atom in the complex cation of $[Zn(tpda)_2][ZnBr_4]\cdot H_2O$ (**1**; tpda = tripyridyldiamine) is octahedrally coordinated to six pyridyl nitrogen atoms. The Zn–N bond lengths of 2.135(5)–2.163(5) Å lie in the normal range.[1] In the anion, zinc(II) is tetrahedrally coordinated to four bromine atoms. The lattice water molecules, the bromine atoms, and all the tpda amino groups, are involved in multiple hydrogen bonds, affording a two-dimensional (2D) network (Fig. 1).

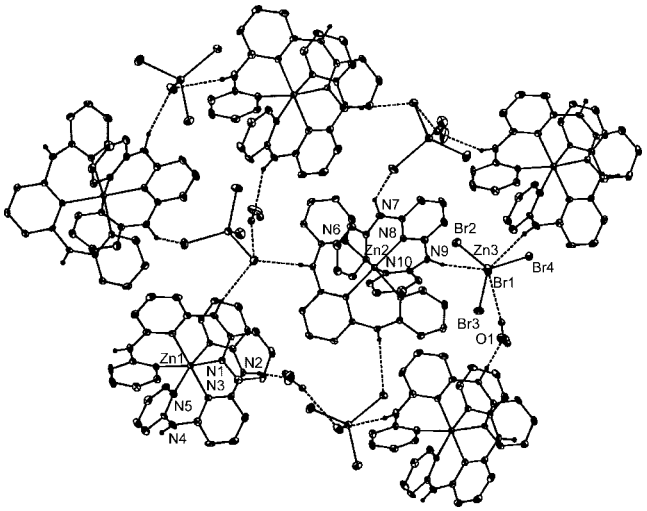

Figure 1. The 2D network of **1**. For clarity, hydrogen atoms are omitted.

EXPERIMENTAL

1 was synthesized by the reaction of $Zn(NO_3)_2\cdot 6H_2O$, tripyridyldiamine[2] and KBr (molar ratio, 1 : 1 : 2) in methanol. The concentrated solution was diffused by diethyl ether to give light yellow crystals.

Data were collected at 293 K on a CCD area detector. $C_{30}H_{28}Br_4N_{10}OZn_2$, $M = 995.00$, tetragonal, $P\text{-}4\ 21\ c$, $a = 21.805(4)$, $c = 14.391(4)$ Å, $V = 6842(2)$ Å^3, $Z = 8$, $R = 0.041$, (4145 data with $I \geq 2\sigma(I)$; $\theta_{max} = 25.0°$), $wR = 0.074$ (all 6028 data). Programs used: SHELXL-97 and ORTEP. CCDC deposition number: 236494.

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