

Crystallographic report

A coordination polymer containing $[\text{Zn}(\text{NO}_3)(\text{H}_2\text{O})_2(\text{btp})_2]^+$ units bridged by btp ligands (btp = 2,6-bis(N' -1,2,4-triazolyl)pyridine)

Ji Young Ryu¹, Jun Yong Lee¹, Jin Soo Seo¹, Cheal Kim^{1*} and Youngmee Kim^{2**}

¹Department of Fine Chemistry, Seoul National University of Technology, Seoul 139-743, Korea

²Department of Chemistry, Ewha Womans University, Seoul 120-750, Korea

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A zinc(II) coordination polymer has been formed from $\text{Zn}(\text{NO}_3)_2$ and 2,6-bis(N' -1,2,4-triazolyl)pyridine (btp) ligands in which each zinc(II) atom is coordinated by three nitrogen donor atoms from btp and three oxygen donor atoms from a nitrate and two water molecules. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc(II); coordination polymer

*Correspondence to: Cheal Kim, Department of Fine Chemistry, Seoul National University of Technology, Seoul 139-743, Korea. E-mail: chealkim@snut.ac.kr

**Correspondence to: Youngmee Kim, Department of Chemistry, Ewha Womans University, Seoul 120-750, Korea. E-mail: ymeekim@ewha.ac.kr

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COMMENT

A zinc(II) coordination polymer is found in the cation in $[\text{Zn}(\text{NO}_3)(\text{OH}_2)_2(\text{btp})_2]\text{NO}_3$, where btp = 2,6-bis(N' -1,2,

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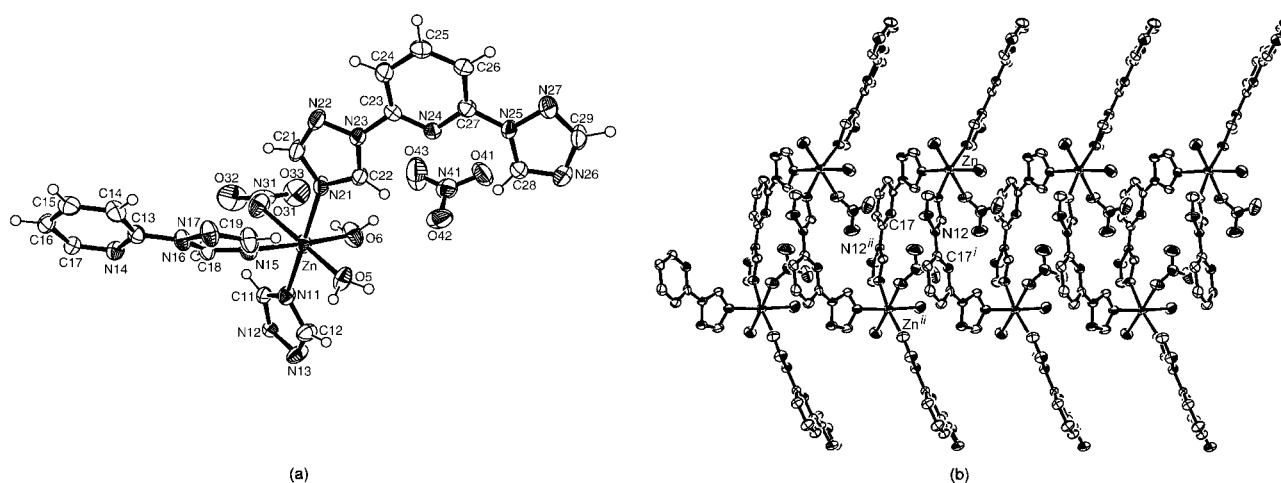


Figure 1. (a) The asymmetric unit of $[\text{Zn}(\text{NO}_3)(\text{H}_2\text{O})_2(\text{btp})_2]\text{NO}_3$. Selected bond distances and angles: Zn–N11 2.124(4), Zn–N21 2.103(4), Zn–N15 2.125(4), Zn–O5 2.033(4), Zn–O6 2.141(5), Zn–O31 2.231(4), N12–C17ⁱ 1.413(6), C17–N12ⁱⁱ 1.413(6) Å; N11–Zn–N21 171.77(18), N15–Zn–O6 174.79(18), O31–Zn–O5 175.92(17)°. Symmetry operation: (i) $-x + 1/2, y - 1/2, -z + 1$, (ii) $-x + 1/2, y + 1/2, -z + 1$. (b) The structure of a coordination polymer with hydrogen atoms omitted for clarity.

4-triazolyl)pyridine. Each zinc(II) atom is coordinated by three nitrogen donor atoms from btp and three oxygen donor atoms from a nitrate and two water molecules, so that the coordination geometry is distorted octahedral (Fig. 1a). Two btp ligands bridge two zinc(II) atoms to form a coordination polymer, as shown in Fig. 1b. A water molecule hydrogen bonds to an oxygen atom of a nitrate counteranion ($O6 \cdots O43$ 2.838(7) Å).

CRYSTALLOGRAPHY

Colorless block-type crystals were obtained from the aqua mixture solution of $Zn(NO_3)_2$ and a btp¹ ligand. Anal. Found: C, 33.27; H, 2.82; N, 34.39. Calc. for $C_{18}H_{18}N_{16}O_8Zn$: C, 33.16; H, 2.79; N, 34.36%. Intensity data were collected at 293 K on an Enraf-Nonius MACH-3 diffractometer for a colorless block $0.30 \times 0.35 \times 0.45$ mm³.

$C_{18}H_{18}N_{16}O_8Zn$, $M = 651.85$, monoclinic, $P2_1/a$, $a = 17.4996(10)$, $b = 7.3988(10)$, $c = 19.4847(10)$ Å, $\beta = 97.976(10)^\circ$, $V = 2498.4(4)$ Å³, $Z = 4$, 4881 unique data, $\theta_{\max} = 26.0^\circ$, $R = 0.055$ ($R_w = 0.135$) for $I \geq 2\sigma(I)$, $\rho_{\max} = 0.52$ e Å⁻³. Programs used: CAD-4-PC software, XCAD4, SHELXS97, SHELXL97, ORTEP-3 for Windows. CCDC deposition number: 208 842.

Acknowledgements

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REFERENCE

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