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catena-Poly[[dibromozinc(**II**)]-μ-1,2-bis-(4-pyridyl)ethane], a one-dimensional coordination polymer

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.056
wR factor = 0.146
Data-to-parameter ratio = 15.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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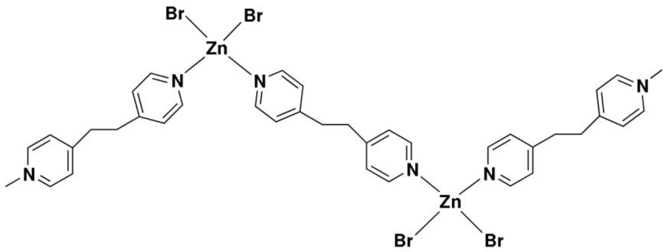
In the title compound, $[ZnBr_2(N_2C_{12}H_{12})]_n$, the 1,2-bis(4-pyridyl)ethane ligand bridges Zn^{II} ions to form a one-dimensional chain. The distorted tetrahedral Zn coordination is completed by two bromide ions. The crystal packing is consolidated by both intra- and interchain C—H$\cdots$Br interactions.

Comment

The crystal engineering of networked coordination polymers is of great current interest due to their potential properties in ion exchange, gas storage, molecular sensing and catalysis (Batten & Robson, 1998; Barnett & Champness, 2003). Many studies have been devoted to the investigation of new synthetic strategies, with the use of novel rigid or flexible spacer ligands (Hong *et al.*, 2004; Wager *et al.*, 2002; Blake *et al.*, 1997). In a previous attempt to investigate the design and control of the self–assembly of coordination polymers with flexible bridging ligands, we synthesized a one-dimensional chain polymeric compound by the reaction of zinc chloride with the flexible ligand 1,2-bis(4-pyridyl)ethane (Hong *et al.*, 2005). In this study, we have employed another zinc salt, zinc bromide, in order to examine the effect of the counter-anion in combination with the same ligand. We report here the crystal structure of the resulting coordination polymer *catena*-poly[[dibromozinc(II)]-μ-1,2-bis(4-pyridyl)ethane], (I).



(I)

The asymmetric unit of (I) (Fig. 1) contains a Zn^{2+} ion, two Br^- anions and two half molecules of the 1,2-bis(4-pyrid-

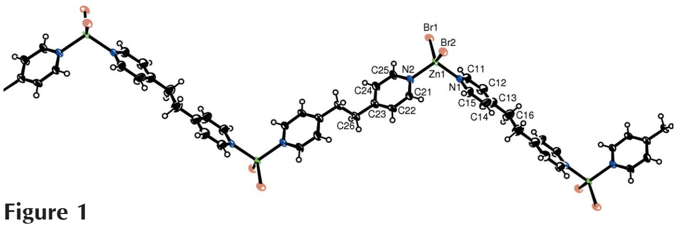


Figure 1
View of (I), showing part of a one-dimensional chain with the asymmetric-unit atoms labelled (50% displacement ellipsoids for the non-H atoms).

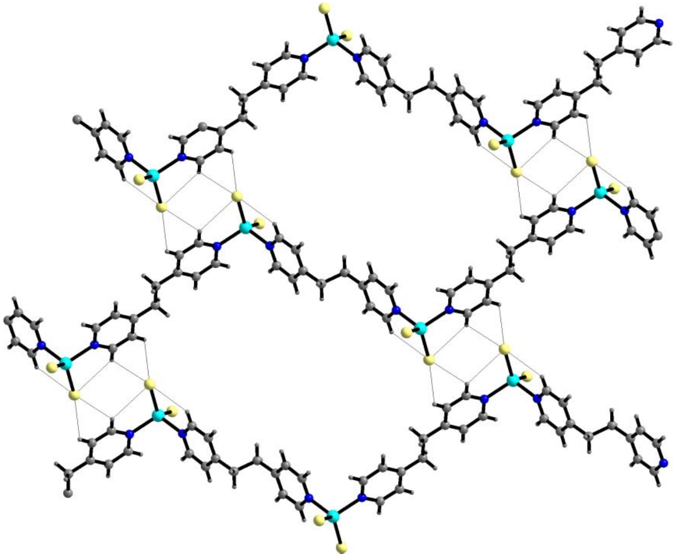


Figure 2
View of (I), showing C—H···Br interactions as dashed lines. Atom colour codes: Zn light blue, Br yellow, N blue, and C amd H dark grey.

yl)ethane ligand. Both complete ligand molecules are generated by inversion symmetry. This results in the ligands bridging Zn^{II} ions to form a one-dimensional zigzag chain compound; two bromo ligands are also coordinated to Zn^{II} ions (Fig. 1). The coordination geometry about Zn is distorted tetrahedral (Table 1), with the Br—Zn—Br angle significantly larger than the nominal value of 109.5°.

The crystal packing in (I) is consolidated by both intramolecular and intermolecular C—H···Br interactions (Janaik & Scharmann, 2003) (Fig. 2 and Table 2).

Experimental

Colourless crystals of (I) were prepared from an aqueous solution (4 ml) of $ZnBr_2{\cdot}2H_2O$ (52.8 mg, 0.2 mmol) which was carefully layered with a methanol solution (4 ml) of 1,2-bis(4-pyridyl)ethane (148.9 mg, 0.8 mmol).

Crystal data

$[ZnBr_2(C_{12}H_{12}N_2)]$
$M_r = 409.43$
Triclinic, $P\overline{1}$
$a = 5.5931\ (6)$ Å
$b = 8.8605\ (10)$ Å
$c = 14.0427\ (15)$ Å
$\alpha = 90.206\ (2)^\circ$
$\beta = 96.662\ (2)^\circ$
$\gamma = 96.181\ (2)^\circ$
$V = 687.11\ (13)$ Å^3
$Z = 2$
$D_x = 1.979$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3010 reflections
$\theta = 2.3$–28.1°
$\mu = 7.58$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.25 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: none
3602 measured reflections
2389 independent reflections
2197 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.132$
$\theta_{\rm max} = 25.0^\circ$
$h = -6 \rightarrow 5$
$k = -10 \rightarrow 10$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.146$
$S = 1.06$
2389 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1126P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 1.23$ e Å^{-3}
$\Delta\rho_{\rm min} = -2.29$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.044 (4)

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.040 (4)	Zn1—Br1	2.3634 (7)
Zn1—N1	2.045 (4)	Zn1—Br2	2.3778 (7)
N2—Zn1—N1	109.84 (17)	N2—Zn1—Br2	105.00 (12)
N2—Zn1—Br1	106.40 (12)	N1—Zn1—Br2	105.11 (12)
N1—Zn1—Br1	107.15 (12)	Br1—Zn1—Br2	122.99 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C25—H25···Br1	0.93	2.96	3.581 (6)	126
C11—H11···Br1	0.93	3.03	3.641 (6)	125
C11—H11···Br1^{i}	0.93	2.98	3.628 (6)	128
C12—H12···Br1^{i}	0.93	3.05	3.650 (6)	124

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

H atoms were placed in calculated positions, with C—H distances of 0.93 (pyridyl) and 0.97 Å (methylene). They were included in the refinement in the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The location of the highest electron-density peak is (0.4866, 0.7877, 0.0785) and the deepest hole is at (0.2221, 0.4728, 0.3604).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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