

Sung Jin Hong,<sup>a</sup> Jung Hwan Lee,<sup>a</sup>  
 Eun Yong Lee,<sup>a</sup> Cheal Kim,<sup>a\*</sup>  
 Youngmee Kim<sup>b\*</sup> and  
 Sung-Jin Kim<sup>b</sup>

<sup>a</sup>Department of Fine Chemistry, Seoul Nation University of Technology, Seoul 139-743, South Korea, and <sup>b</sup>Division of Nano Sciences, Ewha Womans University, Seoul 120-750, South Korea

Correspondence e-mail: chealkim@snut.ac.kr, ymeekim@ewha.ac.kr

#### Key indicators

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$   
 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>.

## catena-Poly[[dibromozinc(II)]- $\mu$ -1,2-bis-(4-pyridyl)ethane], a one-dimensional coordination polymer

In the title compound,  $[\text{ZnBr}_2(\text{N}_2\text{C}_{12}\text{H}_{12})]_n$ , the 1,2-bis(4-pyridyl)ethane ligand bridges  $\text{Zn}^{\text{II}}$  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  $\text{C}-\text{H} \cdots \text{Br}$  interactions.

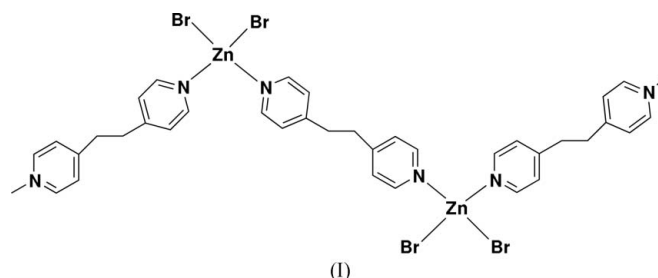
#### Comment

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)]- $\mu$ -1,2-bis(4-pyridyl)ethane], (I).

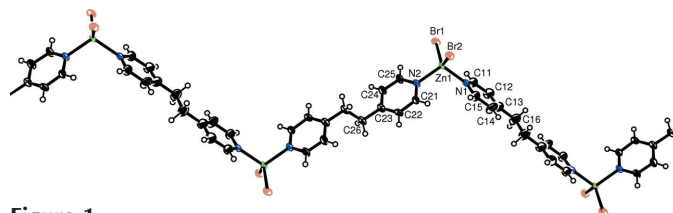
Received 28 June 2005

Accepted 8 July 2005

Online 13 July 2005

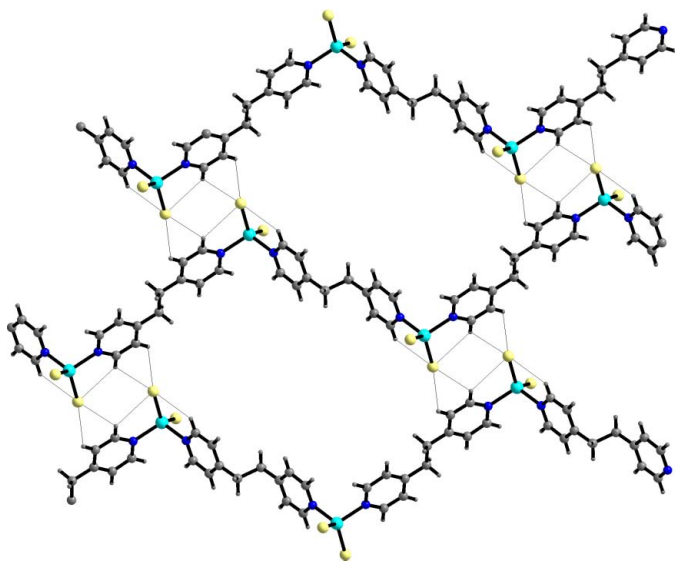


The asymmetric unit of (I) (Fig. 1) contains a  $\text{Zn}^{2+}$  ion, two  $\text{Br}^-$  anions and two half molecules of the 1,2-bis(4-pyridyl)



**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 and H dark grey.

yl)ethane ligand. Both complete ligand molecules are generated by inversion symmetry. This results in the ligands bridging Zn<sup>II</sup> ions to form a one-dimensional zigzag chain compound; two bromo ligands are also coordinated to Zn<sup>II</sup> 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<sub>2</sub>·2H<sub>2</sub>O (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 <sub>2</sub> (C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> )]	<i>Z</i> = 2
<i>M<sub>r</sub></i> = 409.43	<i>D<sub>x</sub></i> = 1.979 Mg m <sup>-3</sup>
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> α radiation
<i>a</i> = 5.5931 (6) Å	Cell parameters from 3010 reflections
<i>b</i> = 8.8605 (10) Å	<i>θ</i> = 2.3–28.1°
<i>c</i> = 14.0427 (15) Å	<i>μ</i> = 7.58 mm <sup>-1</sup>
<i>α</i> = 90.206 (2)°	<i>T</i> = 293 (2) K
<i>β</i> = 96.662 (2)°	Block, colourless
<i>γ</i> = 96.181 (2)°	0.25 × 0.25 × 0.20 mm
<i>V</i> = 687.11 (13) Å <sup>3</sup>	

### Data collection

Bruker SMART CCD diffractometer	2197 reflections with <i>I</i> > 2σ( <i>I</i> )
φ and ω scans	<i>R</i> <sub>int</sub> = 0.132
Absorption correction: none	<i>θ</i> <sub>max</sub> = 25.0°
3602 measured reflections	<i>h</i> = -6 → 5
2389 independent reflections	<i>k</i> = -10 → 10
	<i>l</i> = -16 → 16

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.1126P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.056$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.146$	(Δ/σ) <sub>max</sub> < 0.001
<i>S</i> = 1.06	Δρ <sub>max</sub> = 1.23 e Å <sup>-3</sup>
2389 reflections	Δρ <sub>min</sub> = -2.29 e Å <sup>-3</sup>
155 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	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, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
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 <sup>i</sup>	0.93	2.98	3.628 (6)	128
C12—H12...Br1 <sup>i</sup>	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*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(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*.

Financial support from the Korean Science & Engineering Foundation [ABRL R14-2003-014-01-001-0 and R01-2005-000-10490-0(2005)] and the Korea Research Foundation (2002-070-C00053) is gratefully acknowledged.

## References

- Barnett, S. A. & Champness, N. R. (2003). *Coord. Chem. Rev.* **246**, 145–168.
- Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.
- Blake, A. J., Champness, N. R., Chung, S. S. M., Li, W.-S. & Schröder, M. (1997). *Chem. Commun.* pp. 1005–1006.
- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Hong, S. J., Lee, J. Y., Kim, C., Lee, D.-H., Kim, S.-J. & Kim, Y., (2005). *Anal. Sci.* **21**, x65–x66.
- Hong, S. J., Ryu, J. Y., Lee, J. Y., Kim, C., Kim, S.-J. & Kim, Y. (2004). *Dalton Trans.* pp. 2697–2700.
- Janaik, C. & Scharmann, T. G. (2003). *Polyhedron*, **22**, 1123–1133.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Wager, B. D., McManus, G. J., Moulton, B. & Zaworotko, M. J. (2002). *Chem. Commun.* pp. 2176–2177.