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catena-Poly[[dibromidozinc(II)]-μ-4-(3-pyridyl)-4*H*-1,2,4-triazole]

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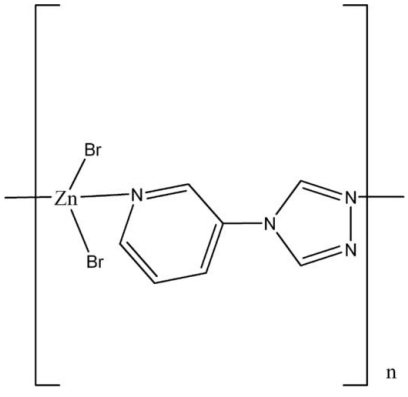
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.010 Å; R factor = 0.039; wR factor = 0.090; data-to-parameter ratio = 14.9.

The title complex, $[ZnBr_2(C_7H_6N_4)]_n$, was formed under hydrothermal conditions using the ligand 4-(3-pyridyl)-4*H*-1,2,4-triazole (*L*). The unique Zn^{II} ion is coordinated by one triazole N atom, one pyridine N atom and two Br atoms in a slightly distorted tetrahedral coordination environment. Symmetry-related Zn^{II} ions are connected by bridging *L* ligands into chains parallel to [001] in which the Zn···Zn separation is 8.643 (7) Å. In the crystal structure, weak intermolecular C—H···Br hydrogen bonds link the chains into a three-dimensional network.

Related literature

For the preparation of the ligand used to synthesize the title compound, see: Gioia *et al.* (1988). For background literature on supramolecular polymer chemistry, see: Lehn (1995); Ouahab (1997). For complexes incorporating 4-3-pyridyl-1,2,4-triazole ligands, see: Moulton & Zaworotko (2001); Pan *et al.* (2001); Prior & Rosseinsky (2001); Ma *et al.* (2001); Ding *et al.* (2006).



Experimental

Crystal data

$[ZnBr_2(C_7H_6N_4)]$
M_r = 371.35
Monoclinic, $P2_1/c$
a = 6.787 (6) Å
b = 18.769 (15) Å
c = 8.643 (7) Å
β = 101.316 (11)°
V = 1079.6 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 9.64 mm^{-1}
T = 293 K
0.18 × 0.12 × 0.06 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.522, T_{max} = 1.000
5681 measured reflections
1903 independent reflections
1510 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.090
S = 1.10
1903 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···Br1^{i}	0.93	2.92	3.711 (7)	145
C6—H6···Br2^{ii}	0.93	2.93	3.779 (8)	153

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x-1, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5068).

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supplementary materials

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catena-Poly[[dibromidozinc(II)]-μ-4-(3-pyridyl)-4*H*-1,2,4-triazole]

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Comment

Supramolecular polymer chemistry is a branch of modern science which is developing rapidly through the combination of polymer chemistry with supramolecular chemistry (Lehn, 1995; Ouahab, 1997). Recently, considerable efforts have been devoted to crystal engineering of supramolecular architecture sustained by coordination covalent bonding, hydrogen bonding or some molecular interaction and their combination. The compounds formed are of interest owing to their fascinating structural diversity and potential application in design of porous materials with novel inclusion or reactivity properties and in supramolecular devices such as sensors and indicators (Moulton & Zaworotko, 2001; Pan *et al.*, 2001; Prior & Rosseinsky, 2001; Ma *et al.*, 2001; Ding *et al.*, 2006). We report herein the crystal structure of the title complex.

A view of the coordination around the Zn^{II} ion of the title compound is shown in Fig. 1. The unique Zn^{II} ion is coordinated by one triazole nitrogen atom, one pyridine nitrogen atom and two bromine ligands in a slightly distorted tetrahedral coordination environment. Symmetry related Zn^{II} ions are connected by bridging *L* ligands to form one-dimensional chains (Fig. 2) in which the Zn···Zn separation is 8.643 (7) Å. In the crystal structure, weak intermolecular C—H···Br hydrogen bonds (Table 1) exist between *L* triazole rings and bromine atoms pairs of inversion related 1-D chains, which are further assembled through C—H···Br interactions to form a 3-D network (see Fig. 3).

Experimental

The ligand *L* was prepared according to the previously reported literature methods (Gioia, *et al.*, 1988). A mixture of $ZnBr_2$ (22.5 mg, 0.1 mmol), *L* (14.6 mg, 0.1 mmol) and water (10 ml) was stirred for 5 h and filtered. The filtrate was kept in a $CaCl_2$ desiccator. Suitable single crystals for X-ray diffraction study were obtained after a few days, yield 23% (based on Zn(II) salts). Anal. Calc. for $C_7H_6Br_2N_4Zn$: C, 22.64%; H, 1.63%; N, 15.09%. Found: C, 22.75%; H, 1.87%; N, 15.14%. FT—IR (KBr): 3115 (w), 3050 (w), 2940(w), 1540(*s*), 1473(*m*), 1395(*m*), 1368(w), 1244(w), 1199(*s*), 1075(*s*), 1030(*s*), 978(w), 945(w), 869(*s*), 684(w), 640 (*s*), 489(*m*), 425 (w) cm_{-1}.

Refinement

H atoms were positioned geometrically and were allowed to ride on their parent C atoms with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

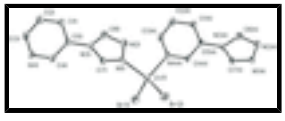

Fig. 1. A view of the coordination around the Zn^{II} ion of the title 1-D compound [symmetry code: (A) *x*, *y*, *z* - 1].

Fig. 2. One-dimensional structure of the title compound

Fig. 3. Part of the crystal structure of the title compound showing hydrogen bonds as dashed lines.

catena-Poly[[dibromidozinc(II)]-μ-4-(3-pyridyl)- 4_H_-1,2,4-triazole]

Crystal data

$[ZnBr_2(C_7H_6N_4)]$	$F(000) = 704$
$M_r = 371.35$	$D_x = 2.285$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1387 reflections
$a = 6.787$ (6) Å	$\theta = 2.6$–$24.1°$
$b = 18.769$ (15) Å	$\mu = 9.64$ mm^{-1}
$c = 8.643$ (7) Å	$T = 293$ K
$\beta = 101.316$ (11)°	Block, colorless
$V = 1079.6$ (15) Å^3	0.18 × 0.12 × 0.06 mm
$Z = 4$	

Data collection

Bruker APEXII diffractometer	1903 independent reflections
Radiation source: fine-focus sealed tube	1510 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.041$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -7 \rightarrow 8$
$T_{min} = 0.522$, $T_{max} = 1.000$	$k = -22 \rightarrow 22$
5681 measured reflections	$l = -10 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.090$	$w = 1/[\sigma^2(F_o^2) + (0.0105P)^2 + 4.1488P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
1903 reflections	$\Delta\rho_{max} = 0.65$ e Å^{-3}
128 parameters	$\Delta\rho_{min} = -0.60$ e Å^{-3}

0 restraints

Primary atom site location: structure-invariant direct methods

Extinction correction: *SHELXL97* (Sheldrick, 2008)

Extinction coefficient: 0.00010 (0)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.39470 (11)	0.63872 (4)	0.68138 (8)	0.0337 (2)
Br1	0.61578 (12)	0.54147 (4)	0.76801 (9)	0.0506 (3)
Br2	0.54852 (11)	0.74575 (4)	0.62834 (9)	0.0469 (2)
N1	0.2184 (8)	0.6476 (3)	0.8432 (5)	0.0334 (12)
N2	0.0687 (8)	0.6990 (3)	0.8251 (6)	0.0435 (14)
N3	0.0872 (8)	0.6435 (3)	1.0539 (5)	0.0324 (12)
N4	0.1730 (8)	0.6178 (3)	1.4833 (5)	0.0339 (12)
C1	−0.1373 (10)	0.5977 (4)	1.2212 (8)	0.0419 (17)
H1	−0.2388	0.5907	1.1332	0.050*
C2	−0.1642 (11)	0.5823 (4)	1.3737 (8)	0.0513 (19)
H2	−0.2868	0.5653	1.3907	0.062*
C3	−0.0079 (10)	0.5926 (4)	1.4974 (8)	0.0415 (17)
H3	−0.0279	0.5815	1.5980	0.050*
C4	0.2014 (10)	0.6340 (3)	1.3381 (7)	0.0373 (15)
H4	0.3248	0.6520	1.3251	0.045*
C5	0.0513 (10)	0.6243 (3)	1.2085 (7)	0.0333 (15)
C6	−0.0101 (11)	0.6954 (4)	0.9528 (8)	0.0451 (17)
H6	−0.1155	0.7235	0.9722	0.054*
C7	0.2253 (9)	0.6162 (3)	0.9792 (7)	0.0322 (14)
H7	0.3142	0.5799	1.0188	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0344 (4)	0.0455 (5)	0.0238 (4)	−0.0007 (3)	0.0122 (3)	0.0026 (3)
Br1	0.0527 (5)	0.0476 (4)	0.0534 (5)	0.0094 (4)	0.0153 (4)	0.0096 (3)
Br2	0.0419 (4)	0.0489 (4)	0.0529 (5)	−0.0042 (3)	0.0168 (3)	0.0093 (3)
N1	0.033 (3)	0.047 (3)	0.021 (2)	0.002 (3)	0.007 (2)	0.003 (2)
N2	0.042 (4)	0.055 (4)	0.036 (3)	0.011 (3)	0.015 (3)	0.012 (3)
N3	0.033 (3)	0.045 (3)	0.022 (2)	0.000 (2)	0.010 (2)	0.002 (2)

N4	0.041 (3)	0.042 (3)	0.023 (3)	−0.001 (3)	0.015 (2)	0.002 (2)
C1	0.038 (4)	0.057 (4)	0.031 (3)	−0.006 (3)	0.009 (3)	−0.002 (3)
C2	0.044 (5)	0.067 (5)	0.045 (4)	−0.014 (4)	0.014 (4)	0.002 (4)
C3	0.044 (4)	0.054 (4)	0.029 (3)	−0.010 (3)	0.013 (3)	0.006 (3)
C4	0.041 (4)	0.047 (4)	0.029 (3)	−0.002 (3)	0.019 (3)	0.002 (3)
C5	0.042 (4)	0.039 (3)	0.021 (3)	−0.002 (3)	0.013 (3)	−0.003 (3)
C6	0.041 (4)	0.052 (4)	0.046 (4)	0.011 (3)	0.019 (3)	0.006 (3)
C7	0.036 (4)	0.038 (3)	0.023 (3)	0.003 (3)	0.008 (3)	0.000 (3)

Geometric parameters (Å, °)

Zn1—N1	2.018 (5)	N4—Zn1^{ii}	2.083 (5)
Zn1—N4^{i}	2.083 (5)	C1—C2	1.396 (9)
Zn1—Br2	2.3502 (18)	C1—C5	1.397 (9)
Zn1—Br1	2.3880 (17)	C1—H1	0.9300
N1—C7	1.308 (7)	C2—C3	1.364 (9)
N1—N2	1.388 (7)	C2—H2	0.9300
N2—C6	1.319 (8)	C3—H3	0.9300
N3—C7	1.339 (8)	C4—C5	1.370 (9)
N3—C6	1.386 (8)	C4—H4	0.9300
N3—C5	1.450 (7)	C6—H6	0.9300
N4—C4	1.341 (7)	C7—H7	0.9300
N4—C3	1.343 (8)		
N1—Zn1—N4^{i}	98.9 (2)	C3—C2—C1	119.0 (6)
N1—Zn1—Br2	114.26 (15)	C3—C2—H2	120.5
N4^{i}—Zn1—Br2	106.11 (14)	C1—C2—H2	120.5
N1—Zn1—Br1	105.51 (15)	N4—C3—C2	124.2 (6)
N4^{i}—Zn1—Br1	114.96 (15)	N4—C3—H3	117.9
Br2—Zn1—Br1	116.02 (7)	C2—C3—H3	117.9
C7—N1—N2	108.1 (5)	N4—C4—C5	120.9 (6)
C7—N1—Zn1	131.6 (4)	N4—C4—H4	119.5
N2—N1—Zn1	120.0 (4)	C5—C4—H4	119.5
C6—N2—N1	106.1 (5)	C4—C5—C1	121.9 (6)
C7—N3—C6	104.9 (5)	C4—C5—N3	119.2 (6)
C7—N3—C5	127.6 (5)	C1—C5—N3	118.9 (5)
C6—N3—C5	127.6 (5)	N2—C6—N3	110.0 (6)
C4—N4—C3	117.8 (6)	N2—C6—H6	125.0
C4—N4—Zn1^{ii}	120.9 (4)	N3—C6—H6	125.0
C3—N4—Zn1^{ii}	121.1 (4)	N1—C7—N3	110.9 (6)
C2—C1—C5	116.1 (6)	N1—C7—H7	124.6
C2—C1—H1	122.0	N3—C7—H7	124.6
C5—C1—H1	122.0		
N4^{i}—Zn1—N1—C7	127.0 (6)	N4—C4—C5—N3	179.0 (5)
Br2—Zn1—N1—C7	−120.8 (5)	C2—C1—C5—C4	0.6 (10)
Br1—Zn1—N1—C7	7.9 (6)	C2—C1—C5—N3	−178.1 (6)
N4^{i}—Zn1—N1—N2	−59.6 (5)	C7—N3—C5—C4	61.5 (9)
Br2—Zn1—N1—N2	52.7 (5)	C6—N3—C5—C4	−116.6 (7)

Br1—Zn1—N1—N2	−178.7 (4)	C7—N3—C5—C1	−119.8 (7)
C7—N1—N2—C6	−0.7 (7)	C6—N3—C5—C1	62.1 (9)
Zn1—N1—N2—C6	−175.6 (4)	N1—N2—C6—N3	0.8 (8)
C5—C1—C2—C3	−1.1 (10)	C7—N3—C6—N2	−0.6 (7)
C4—N4—C3—C2	0.1 (10)	C5—N3—C6—N2	177.8 (6)
Zn1^{ii}—N4—C3—C2	175.4 (6)	N2—N1—C7—N3	0.3 (7)
C1—C2—C3—N4	0.8 (11)	Zn1—N1—C7—N3	174.4 (4)
C3—N4—C4—C5	−0.7 (9)	C6—N3—C7—N1	0.2 (7)
Zn1^{ii}—N4—C4—C5	−176.0 (5)	C5—N3—C7—N1	−178.3 (6)
N4—C4—C5—C1	0.4 (10)		

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) *x*, *y*, *z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···Br1^{iii}	0.93	2.92	3.711 (7)	145
C6—H6···Br2^{iv}	0.93	2.93	3.779 (8)	153

Symmetry codes: (iii) −*x*+1, −*y*+1, −*z*+2; (iv) *x*−1, −*y*+3/2, *z*+1/2.

Fig. 1

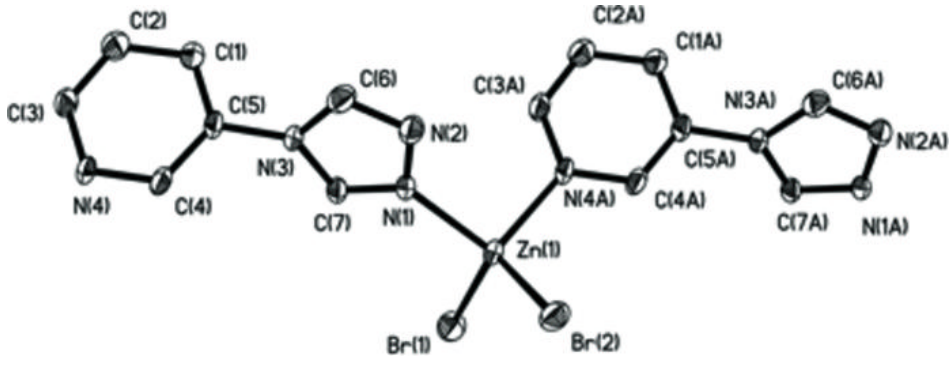
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Fig. 2

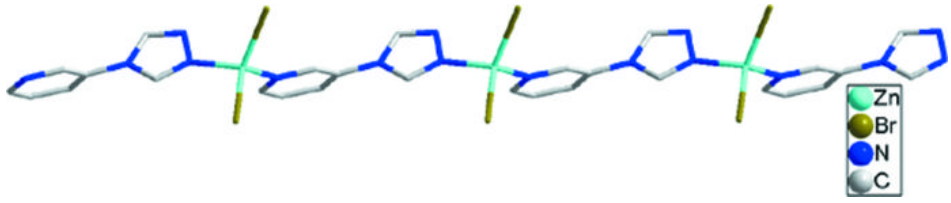

Fig. 3