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catena-Poly[[dichlorozinc(II)]-μ-1,3-di-4-pyridylpropane-κ^2N:N']

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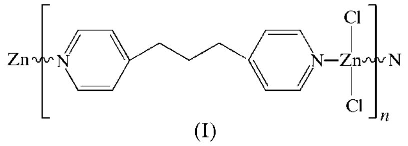
The title compound, $[\mathrm{ZnCl_2(bpp)}]_n$ (where bpp is 1,3-di-4-pyridylpropane, $C_{13}H_{14}N_2$), has been prepared by the hydrothermal reaction of $ZnCl_2$ and bpp at 433 K. The Zn, Cl and central propyl C atom lie on the mirrors of the $P2_1/m$ space group. The molecular structure shows a weave-like polymeric chain. Each Zn atom is coordinated by two N atoms and two Cl atoms in a distorted tetrahedral geometry, with the Zn—N distance being 2.055 (5) Å and the Zn—Cl distances being 2.239 (3) and 2.247 (2) Å.

Comment

A large amount of research effort has involved linear pyridyl-donor ligands, including pyrazine (Real *et al.*, 1991; Kitagawa *et al.*, 1992; Carlucci *et al.*, 1995), 4,4′-bipyridine (bipy; Blake *et al.*, 1997; Yaghi & Li, 1996; Tong *et al.*, 1998) and longer bridges (Fujita *et al.*, 1995; Withersby *et al.*, 1997). The commercially available compound 1,3-di-4-pyridylpropane (bpp) is a bipyridine-type ligand with a flexible $-CH_2CH_2CH_2-$ spacer, and a number of metal–bpp coordination polymers have been reported (Pan *et al.*, 2001; Fu *et al.*, 2001; Carlucci *et al.*, 2002). However, to our knowledge, only a few structures of Zn–bpp coordination polymers have been reported (Plater *et al.*, 2000). We report here a new zinc(II) polymeric compound, $[\mathrm{ZnCl_2(bpp)}]_n$, (I), with a weave-like polymeric chain structure, obtained *via* hydrothermal synthesis.



(I)

In the title compound, (I), each Zn atom is coordinated by two N atoms from two bpp ligands and two Cl atoms to form a distorted tetrahedral geometry, with the Zn—N distance being 2.055 (5) Å and the Zn—Cl distances being 2.239 (3) and 2.247 (2) Å. As the result of this coordination, the molecular structure shows a weave-like polymeric chain, as shown in Fig. 1. The chains have a repeat length ('wavelength') of 12.937 Å, which is approximately one half of the values of 24.6 Å in $[\mathrm{Ag(bpp)}](\mathrm{CF_3SO_3})\cdot\mathrm{EtOH}$ and 23.98 Å in $[\mathrm{Ag(bpp)}](\mathrm{NO_3})$ (Batten *et al.*, 1999). This result is due to the different coordination mode [N1—Zn—N1′ = 111.7 (3), N1—Zn1—Cl1 = 104.5 (1), N1—Zn1—Cl2 = 105.1 (1) and Cl1—Zn1—Cl2 = 126.0 (1)°] of the two-coordinate Ag^+ ions (N—Ag—N = 180°) in $[\mathrm{Ag(bpp)}](\mathrm{NO_3})$. In addition, this molecule–polymer transition is linked to the capacity of the bidentate ligand (bpp) to span two metal centres (Zn). The pyridine rings in the same bpp ligand are not coplanar [dihedral angle of two planes = 66.66 (18)°].

Experimental

A mixture of $ZnCl_2$ (0.259 g, 1.9 mmol), bpp (0.255 g, 1.3 mmol), ethanol (3 ml) and H_2O (13 ml) was sealed in a 25 ml Teflon-lined stainless-steel reactor, heated to 443 K for 60 h, and then slowly cooled to room temperature. Block-shaped colourless crystals of (I), suitable for X-ray analysis, were obtained by filtration (yield 41.8%). Analysis calculated for $C_{13}H_{14}Cl_2N_2Zn$ (%): C 46.67, H 4.22, N 8.37;

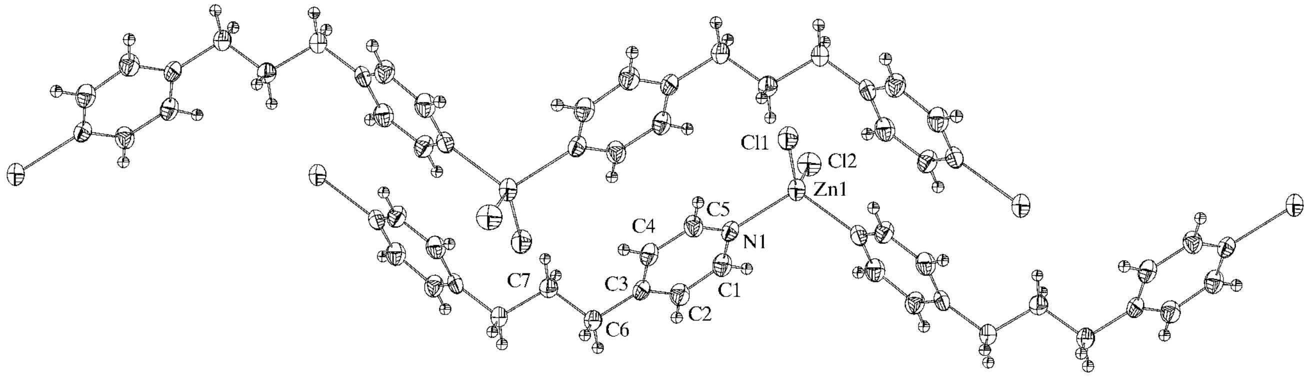


Figure 1
A view of the repeat unit of (I). Displacement ellipsoids are plotted at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

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found: C 46.46, H 3.84, N 8.35; IR spectroscopic analysis (KBr disc, ν, cm^{-1}): 1620 (*s*), 1433 (*s*), 1221 (*m*), 1072 (*m*), 1032 (*s*), 823 (*s*), 621 (*m*), 519 (*s*).

Crystal data

$[ZnCl_2(C_{13}H_{14}N_2)]$
$M_r = 334.53$
Monoclinic, $P2_1/m$
$a = 5.2254$ (4) Å
$b = 12.9371$ (9) Å
$c = 10.5425$ (6) Å
$\beta = 94.247$ (3)°
$V = 710.73$ (8) Å^3
$Z = 2$
$D_x = 1.563$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1292 reflections
$\theta = 1.9$–25.0°
$\mu = 2.09$ mm^{-1}
$T = 293$ (2) K
Block, colourless
$0.80 \times 0.26 \times 0.20$ mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.486$, $T_{max} = 0.659$
2313 measured reflections
1311 independent reflections
1091 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0°$
$h = -5 \rightarrow 6$
$k = -15 \rightarrow 15$
$l = -12 \rightarrow 4$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.153$
$S = 1.08$
1311 reflections
88 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 3.0106P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.055 (5)	C2—C3	1.386 (9)
Zn1—Cl2	2.239 (3)	C3—C4	1.381 (9)
Zn1—Cl1	2.247 (2)	C3—C6	1.505 (8)
N1—C5	1.330 (8)	C4—C5	1.369 (9)
N1—C1	1.337 (8)	C6—C7	1.518 (7)
C1—C2	1.373 (9)		
N1^{i}—Zn1—N1	111.7 (3)	C1—C2—C3	120.3 (6)
N1—Zn1—Cl2	104.45 (14)	C4—C3—C2	116.6 (6)
N1—Zn1—Cl1	105.09 (14)	C4—C3—C6	122.5 (6)
Cl2—Zn1—Cl1	125.95 (10)	C2—C3—C6	120.9 (6)
C5—N1—C1	116.8 (5)	C5—C4—C3	119.7 (6)
C5—N1—Zn1	122.2 (4)	N1—C5—C4	123.9 (6)
C1—N1—Zn1	121.0 (4)	C3—C6—C7	112.1 (5)
N1—C1—C2	122.8 (6)	C6—C7—C6^{ii}	112.6 (7)

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

All H atoms were located theoretically and refined as riding atoms, with C—H distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1996); data reduction: *XPREP* in *SHELXTL* (Siemens, 1996); program(s) used to solve structure: *SHELXTL* (Siemens, 1996); program(s) used to refine structure: *SHELXTL* (Siemens, 1996); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1639). Services for accessing these data are described at the back of the journal.

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