Crystal Structure of One-dimensional $[\text{ZnCl}_2(\text{N}_2\text{C}_{13}\text{H}_{14})]_n$ ($\text{N}_2\text{C}_{13}\text{H}_{14}$ = 1,3-bis(4-pyridyl)propane)

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The ligand ($\text{N}_2\text{C}_{13}\text{H}_{14}$) bridges Zn(II) atoms to form a one-dimensional chain compound, and two chloro ligands are also coordinated to Zn(II) atoms. The coordination geometry of the Zn atom is distorted tetrahedral with a Cl-Zn-Cl angle of $125.69(3)^\circ$. The crystal packing is consolidated by both intra- and inter-chain C-H...Cl interactions.

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The crystal engineering of networked coordination polymers is of great current interest due to their potential properties for ion exchange, gas storage, molecular sensing, and catalysis.^{1,2} Many efforts have been devoted to investigating new synthetic strategies using novel rigid or flexible spacer ligands.^{3,4} In our previous attempt to investigate the design and control of the

self-assembly of coordination polymers with flexible bridging ligands, we synthesized different dimensional structures from different zinc salts with the flexible ligand 1,3-bis(4-pyridyl)propane.⁵ In this study, we employed zinc chloride to continuously examine the counter-anion effect in combination with the same ligand. We report here on the crystal structure of a coordination polymer, $[\text{ZnCl}_2(\text{N}_2\text{C}_{13}\text{H}_{14})]_n$ ($\text{N}_2\text{C}_{13}\text{H}_{14}$ = 1,3-bis(4-pyridyl)propane).

All chemicals used were of analytical reagent grade, and were used directly without further purification. Colorless crystals were obtained from a direct diffusion technique in which an aqueous solution of ZnCl_2 was carefully layered by a methanol solution of $\text{N}_2\text{C}_{13}\text{H}_{14}$. The X-ray diffraction data for the title compound were collected on a Bruker SMART AXS diffractometer equipped with a monochromator in the Mo K_α (λ = 0.71073 Å) incident beam. A colorless crystal was mounted on a glass fiber. The crystal and experimental data are given in Table 1. The CCD data were integrated and scaled by using the Bruker-SAINT software package, and the structure was solved by the direct method and refined by using SHELXTL V6.14. The atomic coordinates for non-hydrogen atoms are listed in Table 2, and the selected bond distances and angles are listed in Table 3. All hydrogen atoms were placed at the calculated positions.

Table 1 Crystal data and experimental data

Formula:	$\text{C}_{13}\text{H}_{14}\text{Cl}_2\text{N}_2\text{Zn}$
Formula weight:	334.53
Temperature:	273(2)K
Crystal size:	$0.25 \times 0.20 \times 0.10$ mm ³
Crystal color:	colorless
Crystal description:	block
Crystal system:	Monoclinic
Space group:	$P2_1/m$ $Z = 2$
a =	5.2254(4) Å
b =	12.9296(10) Å
c =	10.5169(8) Å
β =	94.1890(10)°
V =	708.65(9) Å ³
Calculated density:	1.568 Mg/m ³
Radiation:	0.71073 Å (Mo K_α)
$2\theta_{\text{max}}$:	56.26°
R =	0.0314 [1725 reflections, $I > 2\sigma(I)$]
wR =	0.0854
Goodness-of-fit	= 1.149
$(\Delta/\sigma)_{\text{max}}$ final cycle	= 0.001
$(\Delta\rho)_{\text{min, max}}$	= -0.459, 0.598 e Å ⁻³
No. of reflections collected	= 7732
No. of reflections used	= 1572
No. of parameters	= 88
Diffractometer:	Bruker SMART
Monochromator:	graphite
Structure determination:	Bruker SHELXTL
Refinement:	full-matrix least-squares on F^2
Structural information was deposited at the Cambridge Crystallographic Data Center (CCDC 285350).	

Table 2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	$U(\text{eq})$
Zn(1)	4588(1)	7500	7208(1)	46(1)
Cl(2)	7498(1)	7500	8883(1)	53(1)
Cl(1)	5459(1)	7500	5160(1)	62(1)
N(1)	2456(2)	6188(1)	7411(1)	44(1)
C(1)	529(3)	5936(1)	6560(2)	52(1)
C(2)	-1027(4)	5086(1)	6693(2)	52(1)
C(3)	-570(3)	4435(1)	7737(2)	45(1)
C(4)	1441(4)	4700(1)	8608(2)	52(1)
C(5)	2879(3)	5569(1)	8424(2)	50(1)
C(6)	-2125(3)	3477(1)	7920(2)	51(1)
C(7)	-625(4)	2500	7644(2)	46(1)

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Table 3 Selected bond lengths [Å] and angles [°]

Zn(1)-N(1)	2.0485(13)	Zn(1)-Cl(1)	2.2334(6)
Zn(1)-Cl(2)	2.2412(6)		
N(1)-Zn(1)-N(1)#1	111.75(7)	N(1)-Zn(1)-Cl(1)	104.54(4)
N(1)-Zn(1)-Cl(2)	105.13(4)	Cl(1)-Zn(1)-Cl(2)	125.69(3)

Symmetry transformations used to generate equivalent atoms:

#1: $-x, -y + 3/2, z$, #2: $x, -y + 1/2, z$

Fig. 1 Structural chemical diagram.

Fig. 2 Structure of one-dimensional chain, $[ZnCl_2(N_2C_{13}H_{14})]_n$ along with the labeling atoms.

Fig. 3 Crystal structure including intra- and intermolecular non-covalent interactions.

The molecular structure was drawn by Ortep-3 for the Windows program. A chemical diagram is shown in Fig. 1, and the structure is shown in Fig. 2.

The ligand ($N_2C_{13}H_{14}$) bridges Zn(II) atoms to form a one-dimensional chain compound, and two chloro ligands are also coordinated to Zn(II) atoms (Fig. 2). The asymmetric unit of the title compound contains half of the formula ($Zn(N_2C_{13}H_{14})Cl_2$). The whole chain is generated by two crystallographic mirror planes: one resides through Cl1-Zn1-Cl2, and the other through H7A-C7-H7B. The Zn-N distance is 2.0485(13) Å, and the Zn-Cl distances are 2.2334(6) and 2.2412(6) Å which are typical for Zn complexes. The Zn atom is coordinated by two nitrogen atoms from the ligands and two chloro ligands, and the coordination geometry of the Zn atom is distorted tetrahedral with N-Zn-N and Cl-Zn-Cl angles of 111.75(7)° and 125.69(3)°, respectively (Table 3). Crystal packing in the title compound is consolidated by both intra- and inter-chain C-H...Cl non-covalent interactions⁶ (Fig. 3). The intra-chain interaction is between C5-H5 and Cl2 with a distance of 2.87(1) Å, and the inter-chain interactions are between C4-H4 and Cl2 of the neighbor chain (2.989(1) Å) and between C6-H6A and Cl1 of the neighbor chain (3.031(1) Å).

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