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## Structure Reports

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# catena-Poly[(dichloridozinc)- $\mu$ -1-[4-[(1*H*-imidazol-1-yl)methyl]benzyl]-1*H*-imidazole- $\kappa^2$ N<sup>3</sup>:N<sup>3'</sup>]

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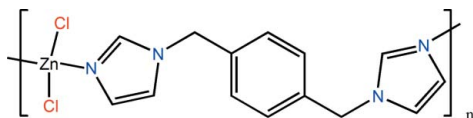
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.023;  $wR$  factor = 0.063; data-to-parameter ratio = 20.0.

The asymmetric unit of the title compound,  $[\text{ZnCl}_2(\text{C}_{14}\text{H}_{14}\text{N}_4)]_n$ , contains a  $\text{Zn}^{\text{II}}$  ion situated on a twofold rotation axis and one-half of a 1-[4-[(1*H*-imidazol-1-yl)methyl]benzyl]-1*H*-imidazole (*L*) ligand with the benzene ring situated on an inversion center. The  $\text{Zn}^{\text{II}}$  ion is coordinated by two chloride anions and two N atoms from two *L* ligands in a distorted tetrahedral geometry. The *L* ligands bridge  $\text{ZnCl}_2$  fragments into polymeric chains parallel to  $[20\bar{1}]$ .

## Related literature

 For the synthesis of the ligand, see: Yang *et al.* (2006).


## Experimental

## Crystal data

 $[\text{ZnCl}_2(\text{C}_{14}\text{H}_{14}\text{N}_4)]$ 
 $M_r = 374.56$ 

 Orthorhombic, *Pbcn*
 $a = 11.327$  (2) Å

 $b = 10.207$  (2) Å

 $c = 14.452$  (3) Å

 $V = 1670.8$  (6) Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 1.79$  mm<sup>-1</sup>
 $T = 293$  K

 $0.58 \times 0.55 \times 0.49$  mm

## Data collection

Rigaku R-AXIS RAPID diffractometer

 Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)

 $T_{\text{min}} = 0.421$ ,  $T_{\text{max}} = 0.477$ 

15231 measured reflections

1916 independent reflections

 1718 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.022$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.023$ 
 $wR(F^2) = 0.063$ 
 $S = 1.08$ 

1916 reflections

96 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.20$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.29$  e Å<sup>-3</sup>

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The present study was supported by the NSFC (grant Nos. 51143002, 21072049, 21072050, 21110402016 and 21074031), the CPDF (grant No. 201104456), the HLJNSF of Heilongjiang (grant Nos. E201118 and E201144), the Abroad Person with Ability Foundation of Heilongjiang Province (grant No. 2010td03) and the Innovation Fellowship Foundation of Heilongjiang University (grant No. Hdtd2010-11).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5275).

## References

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## supporting information

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**catena-Poly[(dichloridozinc)- $\mu$ -1-[4-[(1*H*-imidazol-1-yl)methyl]benzyl]-1*H*-imidazole- $\kappa^2$ N<sup>3</sup>:N<sup>3'</sup>]**

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**S1. Comment**

The synthesis and characterization of coordination networks based on the idea of self-assembly of specifically designed building blocks has been an area of rapid growth in recent years. Herein, we report the title compound constructed by 1-[4-[(1*H*-imidazol-1-yl)methyl]benzyl]-1*H*-imidazole and ZnCl<sub>2</sub>.

The asymmetric unit of the title compound, [ZnCl<sub>2</sub>L]<sub>n</sub> (*L* = 1-[4-[(1*H*-imidazol-1-yl)methyl]benzyl]-1*H*-imidazole, C<sub>14</sub>H<sub>14</sub>N<sub>4</sub>), contains a Zn<sup>II</sup> ion situated on a twofold rotational axis and one-half ligand *L* with the benzene ring situated on an inversion center. Each Zn<sup>II</sup> ion is coordinated by two chlorido anions and two N atoms from two ligands *L* in a distorted tetrahedral geometry (Figure 1). Ligands *L* bridge ZnCl<sub>2</sub> fragments into polymeric chains in [20-1] (Figure 2).

**S2. Experimental**

The 1-[4-[(1*H*-imidazol-1-yl)methyl]benzyl]-1*H*-imidazole was synthesized following the reference method (Yang *et al.*, 2006). Synthesis of the title compound: ligand (0.120 g, 0.5 mmol) and ZnCl<sub>2</sub> (0.080 g, 0.5 mmol) were dissolved in a mixed solution of 4 mL ethanol and 4 mL water. After stirring, the suspension was sealed in a 18 mL Teflon-lined autoclave and heated at 140 °C for 5 days. After slow cooling to room temperature, colorless block crystals were filtered and washed with distilled water (52% yield based on Zn).

**S3. Refinement**

C-bound H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic); C—H = 0.97 Å (methylene), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

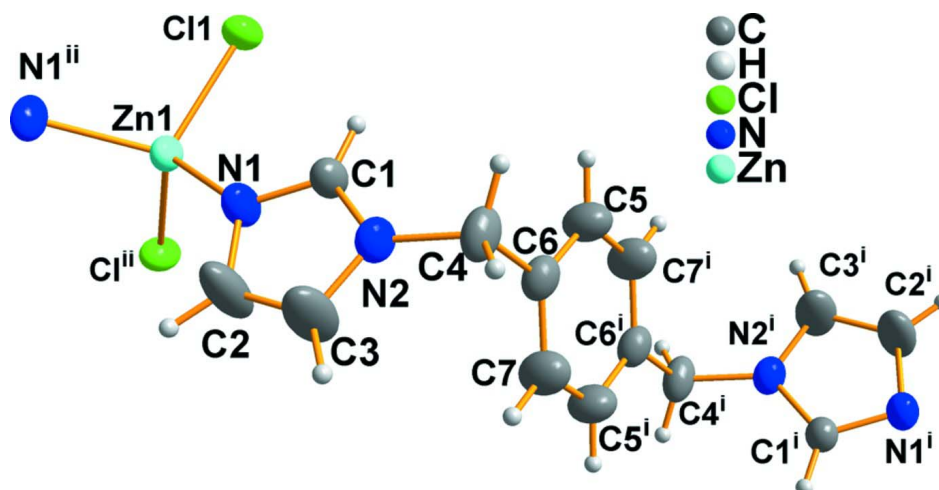


Figure 1

The molecular structure of the title compound, showing the atomic numbering and displacement ellipsoids at the 50% probability level [symmetry codes: (i) 1-x, -y, 1-z; (ii) 2-x, y, 0.5-z].

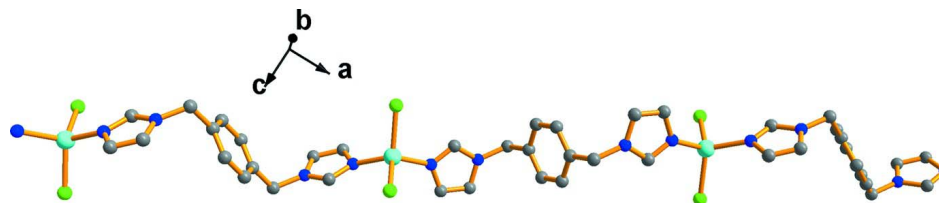


Figure 2

A portion of the polymeric chain in the title compound. H atoms omitted for clarity.

**catena-Poly[(dichloridozinc)- $\mu$ -1-{4-[(1*H*-imidazol-1-yl)methyl]benzyl}-1*H*-imidazole- $\kappa^2$ N<sup>3</sup>:N<sup>3'</sup>}]**

*Crystal data*

[ZnCl<sub>2</sub>(C<sub>14</sub>H<sub>14</sub>N<sub>4</sub>)]

$M_r = 374.56$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 11.327(2) \text{ \AA}$

$b = 10.207(2) \text{ \AA}$

$c = 14.452(3) \text{ \AA}$

$V = 1670.8(6) \text{ \AA}^3$

$Z = 4$

$F(000) = 760$

$D_x = 1.489 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 13075 reflections

$\theta = 3.0\text{--}27.5^\circ$

$\mu = 1.79 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

$0.58 \times 0.55 \times 0.49 \text{ mm}$

*Data collection*

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  scan

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.421$ ,  $T_{\max} = 0.477$

15231 measured reflections

1916 independent reflections

1718 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.0^\circ$

$h = -14 \rightarrow 14$

$k = -13 \rightarrow 13$

$l = -18 \rightarrow 16$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.023$   
 $wR(F^2) = 0.063$   
 $S = 1.08$   
 1916 reflections  
 96 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.4633P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.20 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.29 \text{ e } \text{Å}^{-3}$

Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{Å}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.83519 (13)	0.15817 (15)	0.39823 (10)	0.0350 (3)
H1	0.8723	0.1028	0.4402	0.042*
C2	0.7938 (2)	0.2662 (3)	0.27631 (15)	0.0754 (8)
H2	0.7976	0.3004	0.2168	0.090*
C3	0.7085 (2)	0.2926 (3)	0.33876 (15)	0.0733 (7)
H3	0.6436	0.3472	0.3304	0.088*
C4	0.66639 (15)	0.21680 (18)	0.50158 (12)	0.0458 (4)
H4A	0.6237	0.2983	0.5099	0.055*
H4B	0.7195	0.2065	0.5537	0.055*
C5	0.59983 (16)	-0.0048 (2)	0.55434 (14)	0.0540 (5)
H5	0.6667	-0.0088	0.5916	0.065*
C6	0.57941 (13)	0.10417 (16)	0.50083 (11)	0.0396 (4)
C7	0.47871 (17)	0.1088 (2)	0.44701 (16)	0.0556 (5)
H7	0.4635	0.1826	0.4112	0.067*
Cl1	1.08205 (3)	-0.03773 (4)	0.36609 (3)	0.04045 (11)
N1	0.87372 (11)	0.18141 (14)	0.31401 (9)	0.0391 (3)
N2	0.73601 (11)	0.22419 (13)	0.41575 (9)	0.0374 (3)
Zn1	1.0000	0.07951 (2)	0.2500	0.03065 (9)

Atomic displacement parameters ( $\text{Å}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0346 (7)	0.0395 (8)	0.0308 (7)	0.0067 (6)	0.0040 (6)	0.0015 (6)
C2	0.0835 (16)	0.0979 (19)	0.0448 (10)	0.0500 (14)	0.0178 (10)	0.0316 (11)
C3	0.0737 (14)	0.0870 (16)	0.0592 (12)	0.0511 (13)	0.0165 (10)	0.0251 (11)

C4	0.0439 (9)	0.0499 (10)	0.0437 (9)	-0.0023 (7)	0.0163 (7)	-0.0125 (8)
C5	0.0408 (9)	0.0609 (12)	0.0603 (11)	-0.0004 (8)	-0.0097 (8)	0.0075 (10)
C6	0.0346 (8)	0.0439 (9)	0.0402 (8)	0.0035 (6)	0.0096 (6)	-0.0074 (7)
C7	0.0489 (10)	0.0507 (11)	0.0674 (13)	0.0018 (8)	-0.0055 (9)	0.0146 (10)
Cl1	0.0367 (2)	0.0478 (2)	0.0369 (2)	0.00320 (16)	-0.00610 (14)	0.00531 (16)
N1	0.0407 (7)	0.0447 (8)	0.0319 (6)	0.0120 (6)	0.0078 (5)	0.0048 (6)
N2	0.0360 (6)	0.0390 (7)	0.0371 (7)	0.0064 (5)	0.0079 (5)	-0.0017 (5)
Zn1	0.02814 (14)	0.03731 (15)	0.02650 (14)	0.000	0.00440 (8)	0.000

*Geometric parameters (Å, °)*

C1—N1	1.3146 (19)	C4—H4B	0.9700
C1—N2	1.3343 (19)	C5—C6	1.375 (3)
C1—H1	0.9300	C5—C7 <sup>i</sup>	1.384 (3)
C2—C3	1.350 (3)	C5—H5	0.9300
C2—N1	1.365 (2)	C6—C7	1.381 (3)
C2—H2	0.9300	C7—C5 <sup>i</sup>	1.384 (3)
C3—N2	1.350 (2)	C7—H7	0.9300
C3—H3	0.9300	Cl1—Zn1	2.2606 (5)
C4—N2	1.4718 (19)	N1—Zn1	1.9959 (13)
C4—C6	1.514 (2)	Zn1—N1 <sup>ii</sup>	1.9959 (13)
C4—H4A	0.9700	Zn1—Cl1 <sup>ii</sup>	2.2606 (5)
N1—C1—N2	111.35 (14)	C5—C6—C7	118.89 (16)
N1—C1—H1	124.3	C5—C6—C4	120.07 (16)
N2—C1—H1	124.3	C7—C6—C4	121.04 (17)
C3—C2—N1	109.55 (17)	C6—C7—C5 <sup>i</sup>	120.84 (19)
C3—C2—H2	125.2	C6—C7—H7	119.6
N1—C2—H2	125.2	C5 <sup>i</sup> —C7—H7	119.6
C2—C3—N2	106.38 (16)	C1—N1—C2	105.29 (14)
C2—C3—H3	126.8	C1—N1—Zn1	124.96 (11)
N2—C3—H3	126.8	C2—N1—Zn1	128.33 (12)
N2—C4—C6	112.43 (13)	C1—N2—C3	107.42 (14)
N2—C4—H4A	109.1	C1—N2—C4	125.82 (14)
C6—C4—H4A	109.1	C3—N2—C4	126.67 (15)
N2—C4—H4B	109.1	N1 <sup>ii</sup> —Zn1—N1	117.19 (8)
C6—C4—H4B	109.1	N1 <sup>ii</sup> —Zn1—Cl1 <sup>ii</sup>	103.09 (4)
H4A—C4—H4B	107.8	N1—Zn1—Cl1 <sup>ii</sup>	108.98 (4)
C6—C5—C7 <sup>i</sup>	120.26 (17)	N1 <sup>ii</sup> —Zn1—Cl1	108.98 (4)
C6—C5—H5	119.9	N1—Zn1—Cl1	103.09 (4)
C7 <sup>i</sup> —C5—H5	119.9	Cl1 <sup>ii</sup> —Zn1—Cl1	116.08 (3)

Symmetry codes: (i)  $-x+1, -y, -z+1$ ; (ii)  $-x+2, y, -z+1/2$ .