Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[dichloridozinc(II)]-μ-[1,1′-(butane-1,4-diyl)diimidazole-$\kappa^2N^3:N^{3'}$]]

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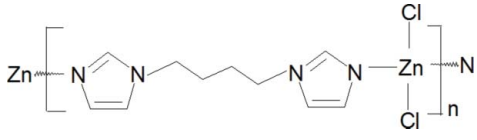
Received 24 October 2010; accepted 10 November 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.126; data-to-parameter ratio = 21.5.

The title one-dimensional coordination polymer, $[ZnCl_2(C_{10}H_{14}N_4)]_n$, was synthesized by hydrothermal methods from $ZnCl_2$ and 1,1′-(butane-1,4-diyl)diimidazole. The Zn atom is coordinated by two chloride ions and two N atoms from two symmetry-independent organic ligands and shows a distorted tetrahedral coordination geometry. The 1,1′-(butane-1,4-diyl)-diimidazole ligands are located around two sets of inversion centers and bridge Zn^{II} ions, forming a zigzag polymeric chain. C—H···Cl hydrogen bonding results in the formation of a three-dimensional supramolecular network

Related literature

For general background to this work, see: Hamada *et al.* (2004); Wang *et al.* (2006).



Experimental

Crystal data

$[ZnCl_2(C_{10}H_{14}N_4)]$ M_r = 326.52
Monoclinic, $P2_1/c$
a = 7.8583 (16) Å
b = 11.689 (2) Å
c = 15.882 (3) Å
β = 93.82 (3)°
V = 1455.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.04 mm^{-1}
T = 293 K
0.34 × 0.27 × 0.22 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.428, T_{max} = 0.731
13865 measured reflections
3309 independent reflections
2701 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.126
S = 1.01
3309 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···Cl2^{i}	0.93	2.77	3.601 (4)	149
C6—H6A···Cl1^{ii}	0.93	2.65	3.553 (3)	164

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

Data collection: *SMART* (Siemens, 1994); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; 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: *SHELXTL*.

We are grateful for financial support from the Natural Science Foundation of Fujian (2008 J0172) and the Foundation of Fujian Education Committee (JA10205).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2314).

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supplementary materials

Acta Cryst. (2010). E**66**, m1580 [**doi:10.1107/S1600536810046611**]

catena-Poly[[dichloridozinc(II)]-μ-[1,1'-(butane-1,4-diyl)diimidazole-$\kappa^2N^3:N^{3'}$]]

J. Lin, W.-L. Cai, X.-Z. Li and S.-K. Huang

Comment

The chemistry of novel metal–organic coordination complexes has attached more and more attention in recent years because of their interesting topologies and unexpected properties for potential applications . Recently, there has been increasing interest in zinc–halogen compounds because of their applications in molecular materials (Hamada *et al.* 2004; Wang *et al.*, 2006). In this communication, we have introduced 1,1'-(butane-1,4-diyl)diimidazole (bbi) as a bridging ligand which favors crystal growth of the 1-D chain-like polymer. Through a mild-temperature hydrothermal process, we have successfully synthesized the title crystalline Cl-coordinated Zn complex, $[ZnCl_2(C_{10}H_{14}N_4)]_n$, (I).

The molecular structure of (I) is shown in Fig. 1. The compound features 1-D chain-like polymer complex, in which the Zn atom is coordinated by two Cl anions and two N atoms from two bbi ligands in a distorted tetrahedral geometry, in which the Zn—Cl (2.238 (1) and 2.2567 (9) Å) and Zn—N(2.010 (2) and 2.016 (3) Å) bond lengths are in the expected ranges. Each bbi ligand in the title compound is located on an inversion center and bridges Zn^{II} ions, forming a zigzag polymeric chain with the adjacent Zn···Zn separation of 13.971 Å.

The strong C—H···Cl hydrogen bonding results in the formation of a 3-D supramolecular network, as shown in Fig. 2.

Experimental

The hydrothermal reaction of $ZnCl_2$ (0.041 g, 0.3 mmol), bbi (0.076 g, 0.4 mmol) and water (15.0 ml) was carried out at 423 K for 3 d. After cooling to room temperature at a rate of 5 K h^{-1}, block-shaped colorless crystals of the title compound suitable for X-ray analysis were obtained.

Refinement

The C-bound H atoms were positioned geometrically, with C—H = 0.93 - 0.97 Å and all refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The crystal exhibited minor twinning which was not accounted for.

Figures

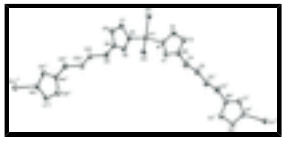

Fig. 1. View of the title coordination polymer showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level. Symmetry code: (i) -*x*, -1/2 + *y*, 1/2 - *z*; (ii) *x*, 3/2 - *y*, -1/2 + *z*.

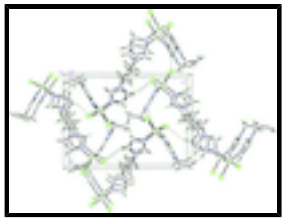

Fig. 2. Crystal packing viewed along the a axis. C-H···Cl contacts are shown with dashed lines

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Crystal data

$[ZnCl_2(C_{10}H_{14}N_4)]$	$F(000) = 664$
$M_r = 326.52$	$D_x = 1.490$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 13865 reflections
$a = 7.8583$ (16) Å	$\theta = 3.1–27.4°$
$b = 11.689$ (2) Å	$\mu = 2.04$ mm^{-1}
$c = 15.882$ (3) Å	$T = 293$ K
$\beta = 93.82$ (3)°	Block, colorless
$V = 1455.6$ (5) Å^3	0.34 × 0.27 × 0.22 mm
$Z = 4$	

Data collection

Siemens SMART CCD area-detector diffractometer	3309 independent reflections
Radiation source: fine-focus sealed tube	2701 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.036$
Detector resolution: 0 pixels mm^{-1}	$\theta_{max} = 27.4°$, $\theta_{min} = 3.1°$
φ and ω scans	$h = -10\rightarrow8$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$k = -15\rightarrow15$
$T_{min} = 0.428$, $T_{max} = 0.731$	$l = -20\rightarrow20$
13865 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.126$	H-atom parameters constrained
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0822P)^2 + 0.5697P]$ where $P = (F_o^2 + 2F_c^2)/3$
3309 reflections	$(\Delta/\sigma)_{max} = 0.001$
154 parameters	$\Delta\rho_{max} = 1.33$ e Å^{-3}

0 restraints $\Delta\rho_{min} = -0.35$ e Å^{-3}

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	0.03756 (4)	0.88757 (3)	0.221856 (19)	0.03812 (15)
Cl1	0.16460 (10)	1.03238 (7)	0.15605 (5)	0.0490 (2)
Cl2	−0.16703 (11)	0.94302 (9)	0.30450 (5)	0.0595 (3)
N1	−0.0583 (3)	0.7849 (2)	0.12834 (15)	0.0459 (6)
N2	−0.1741 (4)	0.6401 (3)	0.05838 (18)	0.0564 (7)
N3	0.2244 (3)	0.7996 (2)	0.28566 (15)	0.0414 (5)
N4	0.3570 (3)	0.6570 (2)	0.35199 (15)	0.0418 (5)
C1	−0.1396 (5)	0.6874 (3)	0.1340 (2)	0.0561 (9)
H1A	−0.1695	0.6554	0.1845	0.067*
C2	−0.0383 (5)	0.7996 (3)	0.0444 (2)	0.0604 (9)
H2A	0.0175	0.8607	0.0209	0.072*
C3	−0.1123 (6)	0.7112 (4)	0.0007 (2)	0.0692 (11)
H3A	−0.1192	0.7015	−0.0575	0.083*
C4	−0.2665 (6)	0.5326 (3)	0.0393 (3)	0.0721 (11)
H4A	−0.2590	0.4840	0.0890	0.087*
H4B	−0.2132	0.4926	−0.0055	0.087*
C5	−0.4511 (6)	0.5543 (3)	0.0128 (3)	0.0687 (11)
H5A	−0.4577	0.6072	−0.0344	0.082*
H5B	−0.5053	0.5904	0.0591	0.082*
C6	0.2058 (4)	0.7031 (3)	0.32738 (19)	0.0443 (7)
H6A	0.1011	0.6712	0.3383	0.053*
C7	0.3969 (4)	0.8154 (3)	0.2830 (2)	0.0539 (8)
H7A	0.4483	0.8769	0.2576	0.065*
C8	0.4809 (4)	0.7279 (3)	0.3232 (2)	0.0565 (9)
H8A	0.5984	0.7176	0.3299	0.068*
C9	0.3835 (4)	0.5474 (3)	0.3955 (2)	0.0487 (7)
H9A	0.4469	0.4969	0.3607	0.058*
H9B	0.2735	0.5123	0.4026	0.058*
C10	0.4794 (4)	0.5590 (3)	0.48174 (18)	0.0437 (7)
H10A	0.5842	0.6014	0.4762	0.052*
H10B	0.4102	0.6010	0.5195	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0373 (2)	0.0380 (2)	0.0379 (2)	−0.00093 (13)	−0.00600 (14)	0.00377 (12)
Cl1	0.0466 (4)	0.0420 (4)	0.0590 (5)	−0.0042 (3)	0.0084 (3)	0.0081 (3)
Cl2	0.0531 (5)	0.0777 (7)	0.0488 (4)	0.0073 (4)	0.0110 (4)	0.0122 (4)
N1	0.0504 (15)	0.0459 (14)	0.0400 (12)	−0.0080 (12)	−0.0086 (10)	0.0022 (11)
N2	0.0651 (19)	0.0498 (16)	0.0520 (15)	−0.0153 (14)	−0.0124 (14)	0.0002 (13)
N3	0.0360 (13)	0.0409 (13)	0.0460 (12)	0.0014 (10)	−0.0065 (10)	0.0084 (11)
N4	0.0400 (13)	0.0421 (14)	0.0422 (12)	0.0022 (11)	−0.0056 (10)	0.0072 (10)
C1	0.073 (2)	0.052 (2)	0.0418 (16)	−0.0170 (17)	−0.0112 (15)	0.0081 (14)
C2	0.073 (2)	0.064 (2)	0.0437 (16)	−0.0237 (19)	0.0012 (16)	0.0009 (16)
C3	0.087 (3)	0.077 (3)	0.0434 (17)	−0.028 (2)	0.0009 (18)	−0.0078 (18)
C4	0.087 (3)	0.051 (2)	0.074 (2)	−0.020 (2)	−0.022 (2)	0.0015 (19)
C5	0.081 (3)	0.057 (2)	0.065 (2)	−0.025 (2)	−0.0131 (19)	−0.0024 (18)
C6	0.0374 (15)	0.0431 (16)	0.0507 (16)	−0.0028 (13)	−0.0089 (12)	0.0069 (13)
C7	0.0449 (17)	0.057 (2)	0.0591 (19)	−0.0017 (15)	0.0001 (14)	0.0220 (16)
C8	0.0363 (16)	0.066 (2)	0.067 (2)	0.0072 (15)	0.0039 (14)	0.0189 (18)
C9	0.0534 (19)	0.0411 (17)	0.0499 (17)	0.0026 (14)	−0.0097 (14)	0.0074 (13)
C10	0.0476 (17)	0.0436 (17)	0.0393 (15)	0.0059 (13)	−0.0007 (12)	0.0060 (12)

Geometric parameters (Å, °)

Zn1—N3	2.010 (2)	C3—H3A	0.9300
Zn1—N1	2.016 (3)	C4—C5	1.505 (6)
Zn1—Cl2	2.2381 (11)	C4—H4A	0.9700
Zn1—Cl1	2.2567 (9)	C4—H4B	0.9700
N1—C1	1.312 (4)	C5—C5^{i}	1.525 (7)
N1—C2	1.363 (4)	C5—H5A	0.9700
N2—C1	1.334 (4)	C5—H5B	0.9700
N2—C3	1.352 (5)	C6—H6A	0.9300
N2—C4	1.472 (5)	C7—C8	1.354 (5)
N3—C6	1.322 (4)	C7—H7A	0.9300
N3—C7	1.371 (4)	C8—H8A	0.9300
N4—C6	1.339 (4)	C9—C10	1.524 (4)
N4—C8	1.380 (4)	C9—H9A	0.9700
N4—C9	1.464 (4)	C9—H9B	0.9700
C1—H1A	0.9300	C10—C10^{ii}	1.522 (6)
C2—C3	1.353 (5)	C10—H10A	0.9700
C2—H2A	0.9300	C10—H10B	0.9700
N3—Zn1—N1	106.94 (11)	N2—C4—H4B	109.3
N3—Zn1—Cl2	112.43 (8)	C5—C4—H4B	109.3
N1—Zn1—Cl2	110.90 (8)	H4A—C4—H4B	108.0
N3—Zn1—Cl1	106.64 (8)	C4—C5—C5^{i}	113.2 (5)
N1—Zn1—Cl1	105.09 (8)	C4—C5—H5A	108.9
Cl2—Zn1—Cl1	114.31 (4)	C5^{i}—C5—H5A	108.9
C1—N1—C2	105.3 (3)	C4—C5—H5B	108.9

C1—N1—Zn1	128.8 (2)	$C5^{i}$—C5—H5B	108.9
C2—N1—Zn1	125.7 (2)	H5A—C5—H5B	107.8
C1—N2—C3	107.1 (3)	N3—C6—N4	111.4 (3)
C1—N2—C4	127.4 (3)	N3—C6—H6A	124.3
C3—N2—C4	125.5 (3)	N4—C6—H6A	124.3
C6—N3—C7	105.8 (2)	C8—C7—N3	109.6 (3)
C6—N3—Zn1	126.0 (2)	C8—C7—H7A	125.2
C7—N3—Zn1	127.3 (2)	N3—C7—H7A	125.2
C6—N4—C8	107.1 (3)	C7—C8—N4	106.1 (3)
C6—N4—C9	125.8 (3)	C7—C8—H8A	126.9
C8—N4—C9	127.0 (3)	N4—C8—H8A	126.9
N1—C1—N2	111.7 (3)	N4—C9—C10	113.1 (3)
N1—C1—H1A	124.2	N4—C9—H9A	109.0
N2—C1—H1A	124.2	C10—C9—H9A	109.0
C3—C2—N1	109.4 (3)	N4—C9—H9B	109.0
C3—C2—H2A	125.3	C10—C9—H9B	109.0
N1—C2—H2A	125.3	H9A—C9—H9B	107.8
N2—C3—C2	106.5 (3)	$C10^{ii}$—C10—C9	110.0 (3)
N2—C3—H3A	126.8	$C10^{ii}$—C10—H10A	109.7
C2—C3—H3A	126.8	C9—C10—H10A	109.7
N2—C4—C5	111.5 (3)	$C10^{ii}$—C10—H10B	109.7
N2—C4—H4A	109.3	C9—C10—H10B	109.7
C5—C4—H4A	109.3	H10A—C10—H10B	108.2
N3—Zn1—N1—C1	64.7 (3)	C1—N2—C3—C2	1.2 (5)
Cl2—Zn1—N1—C1	−58.2 (3)	C4—N2—C3—C2	179.5 (4)
Cl1—Zn1—N1—C1	177.8 (3)	N1—C2—C3—N2	−1.7 (5)
N3—Zn1—N1—C2	−109.5 (3)	C1—N2—C4—C5	97.3 (5)
Cl2—Zn1—N1—C2	127.6 (3)	C3—N2—C4—C5	−80.7 (5)
Cl1—Zn1—N1—C2	3.6 (3)	N2—C4—C5—$C5^{i}$	176.4 (4)
N1—Zn1—N3—C6	−62.4 (3)	C7—N3—C6—N4	0.4 (4)
Cl2—Zn1—N3—C6	59.6 (3)	Zn1—N3—C6—N4	170.4 (2)
Cl1—Zn1—N3—C6	−174.4 (2)	C8—N4—C6—N3	−0.8 (4)
N1—Zn1—N3—C7	105.5 (3)	C9—N4—C6—N3	−176.6 (3)
Cl2—Zn1—N3—C7	−132.6 (3)	C6—N3—C7—C8	0.1 (4)
Cl1—Zn1—N3—C7	−6.6 (3)	Zn1—N3—C7—C8	−169.7 (2)
C2—N1—C1—N2	−0.7 (4)	N3—C7—C8—N4	−0.6 (4)
Zn1—N1—C1—N2	−175.9 (2)	C6—N4—C8—C7	0.9 (4)
C3—N2—C1—N1	−0.3 (5)	C9—N4—C8—C7	176.6 (3)
C4—N2—C1—N1	−178.6 (4)	C6—N4—C9—C10	−120.0 (3)
C1—N1—C2—C3	1.5 (5)	C8—N4—C9—C10	65.1 (4)
Zn1—N1—C2—C3	176.8 (3)	N4—C9—C10—$C10^{ii}$	−173.2 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3A···$Cl2^{iii}$	0.93	2.77	3.601 (4)	149

C6—H6A···Cl1^{iv}	0.93	2.65	3.553 (3)	164

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

Fig. 1

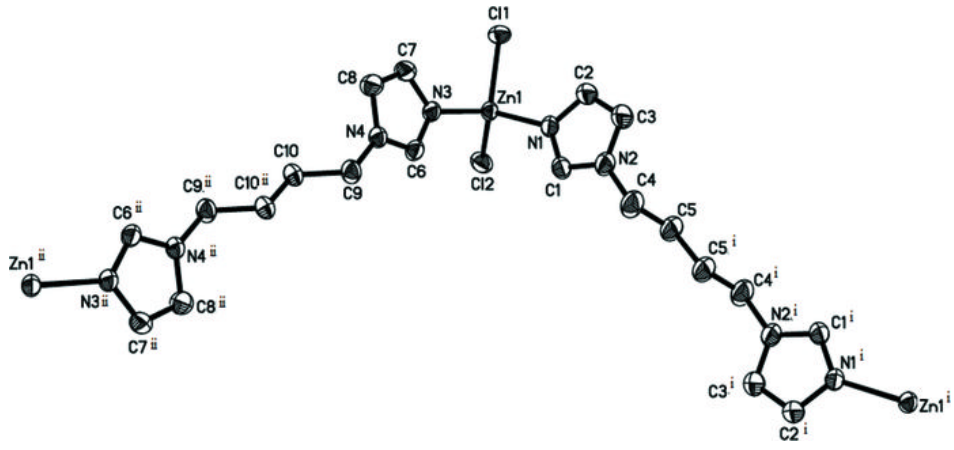

Fig. 2