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catena-Poly[(dichloridozinc)-μ-4,4′-bis[(1*H*-imidazol-1-yl)methyl]biphenyl-$\kappa^2N^3:N^{3'}$]

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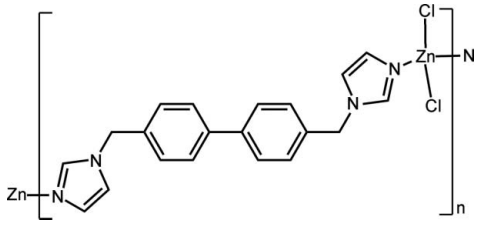
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 17.9.

In the title compound, $[ZnCl_2(C_{20}H_{18}N_4)]_n$, the Zn^{II} ion lies on a twofold rotation axis and is four-coordinated in a tetrahedral geometry defined by two Cl anions and two N atoms from two 4,4′-bis[(imidazol-1-yl)methyl]biphenyl ligands. The mid-point of the ligand is located on an inversion center, and shows a *trans* conformation. The ligands link the Zn^{II} ions, forming a chain structure along $[10\bar{1}]$.

Related literature

For the synthesis of the ligand, see: Zhu *et al.* (2002).



Experimental

Crystal data

$[ZnCl_2(C_{20}H_{18}N_4)]$ M_r = 450.67
Monoclinic, $C2/c$
a = 22.837 (5) Å
b = 5.9004 (12) Å
c = 16.012 (3) Å
β = 117.08 (3)°
V = 1921.0 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.57 mm^{-1}
T = 293 K
0.36 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.601, T_{max} = 0.765
8827 measured reflections
2204 independent reflections
1890 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
S = 1.07
2204 reflections
123 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—Cl1	2.2349 (9)	Zn1—N1	2.0224 (16)

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2529).

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supplementary materials

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catena-Poly[(dichloridozinc)-μ-4,4′-bis[(1*H*-imidazol-1-yl)methyl]biphenyl-$\kappa^2N^3:N^{3'}$]

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Comment

N-containing ligands with an arene center have been widely used as building blocks for constructing inorganic-organic supramolecular architectures. Herein, we report the title compound constructed from 4,4′-(dimethylenebiphenyl)-diimidazole and $ZnCl_2$.

In the title compound, the Zn^{II} ion lies on a twofold rotation axis and is four-coordinated in a tetrahedral environment defined by two Cl anions and two N atoms from two ligands (Fig. 1, Table 1). The mid-point of the ligand is located in an inversion center. The ligands showing a *trans* conformation link the Zn^{II} ions into a chain structure along [1 0 $\bar{1}$] (Fig. 2).

Experimental

The 4,4′-(dimethylenebiphenyl)diimidazol ligand was synthesized followed the reference method (Zhu *et al.*, 2002). $ZnCl_2$ (0.140 g, 1 mmol) and ligand (0.32 g, 1 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 (yield: 35% based on Zn).

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding atoms, with C—H = 0.93 (aromatic) and 0.97 (methylene) Å and with U_{iso}(H) = 1.2U_{eq}(C).

Computing details

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO* (Rigaku, 1998); data reduction: *CrystalClear* (Rigaku/MSC, 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: *SHELXTL* (Sheldrick, 2008).

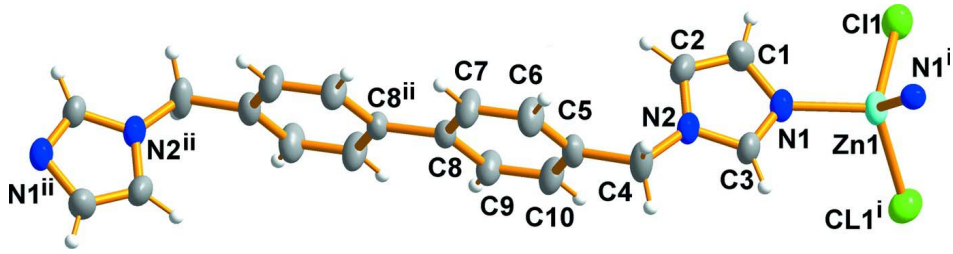

Figure 1

The asymmetric unit of the title compound, showing displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) -x, y, 1/2-z; (ii) 1/2-x, -1/2-y, -z.]

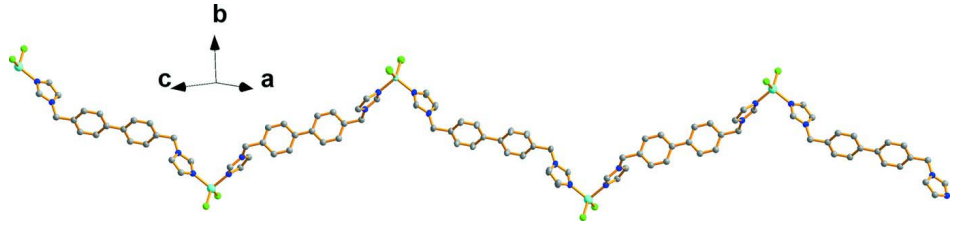

Figure 2

A partial packing view, showing the chain structure along [1 0 $\bar{1}$].

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Crystal data

$[ZnCl_2(C_{20}H_{18}N_4)]$
M_r = 450.67
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 22.837 (5) Å
b = 5.9004 (12) Å
c = 16.012 (3) Å
β = 117.08 (3)°
V = 1921.0 (9) Å^3
Z = 4
F(000) = 920
D_x = 1.558 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 7615 reflections
θ = 3.6–27.5°
μ = 1.57 mm^{-1}
T = 293 K
Block, colorless
0.36 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.601, T_{max} = 0.765
8827 measured reflections
2204 independent reflections
1890 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 3.6°
h = −29→26
k = −7→7
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
S = 1.07
2204 reflections
123 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

$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.6927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.02165 (11)	0.3388 (4)	0.10470 (15)	0.0471 (5)
H1	−0.0130	0.4089	0.0544	0.057*
C2	0.05856 (10)	0.1682 (4)	0.09746 (15)	0.0456 (5)
H2	0.0543	0.1002	0.0426	0.055*
C3	0.09174 (10)	0.2535 (3)	0.24453 (14)	0.0392 (4)
H3	0.1152	0.2508	0.3096	0.047*
C4	0.15012 (12)	−0.0734 (4)	0.21863 (17)	0.0494 (5)
H4A	0.1281	−0.2080	0.2249	0.059*
H4B	0.1856	−0.0379	0.2800	0.059*
C5	0.17867 (10)	−0.1230 (3)	0.15169 (14)	0.0389 (4)
C6	0.16437 (12)	−0.3221 (4)	0.10166 (18)	0.0502 (5)
H6	0.1358	−0.4253	0.1077	0.060*
C7	0.19175 (12)	−0.3717 (4)	0.04240 (18)	0.0499 (5)
H7	0.1810	−0.5075	0.0093	0.060*
C8	0.23486 (8)	−0.2230 (3)	0.03141 (12)	0.0317 (4)
C9	0.24832 (10)	−0.0205 (4)	0.08169 (15)	0.0440 (5)
H9	0.2766	0.0840	0.0756	0.053*
C10	0.22065 (11)	0.0283 (4)	0.14005 (16)	0.0482 (5)
H10	0.2303	0.1653	0.1722	0.058*
Cl1	−0.07645 (3)	0.79888 (10)	0.12779 (4)	0.05314 (16)
N1	0.04281 (8)	0.3932 (3)	0.19687 (12)	0.0385 (4)
N2	0.10332 (8)	0.1157 (3)	0.18714 (12)	0.0366 (3)
Zn1	0.0000	0.61108 (5)	0.2500	0.03718 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0445 (10)	0.0614 (13)	0.0393 (11)	0.0076 (10)	0.0223 (9)	0.0016 (9)
C2	0.0460 (10)	0.0579 (12)	0.0390 (10)	−0.0028 (10)	0.0247 (9)	−0.0125 (9)
C3	0.0477 (10)	0.0418 (10)	0.0378 (10)	0.0014 (9)	0.0280 (8)	−0.0045 (8)
C4	0.0707 (14)	0.0445 (11)	0.0551 (13)	0.0143 (10)	0.0479 (11)	0.0067 (9)
C5	0.0459 (10)	0.0392 (10)	0.0435 (10)	0.0063 (8)	0.0307 (9)	0.0010 (8)

C6	0.0615 (13)	0.0434 (10)	0.0690 (15)	−0.0130 (10)	0.0500 (12)	−0.0104 (10)
C7	0.0638 (13)	0.0412 (11)	0.0669 (14)	−0.0164 (10)	0.0491 (12)	−0.0197 (10)
C8	0.0333 (8)	0.0326 (9)	0.0358 (9)	−0.0002 (7)	0.0214 (7)	−0.0040 (7)
C9	0.0530 (11)	0.0374 (10)	0.0573 (13)	−0.0125 (9)	0.0388 (10)	−0.0123 (9)
C10	0.0639 (13)	0.0397 (10)	0.0576 (13)	−0.0078 (10)	0.0422 (11)	−0.0151 (10)
Cl1	0.0633 (3)	0.0527 (3)	0.0479 (3)	0.0107 (3)	0.0292 (3)	0.0057 (2)
N1	0.0449 (9)	0.0399 (8)	0.0424 (9)	0.0015 (7)	0.0302 (7)	−0.0015 (7)
N2	0.0424 (8)	0.0382 (8)	0.0400 (8)	0.0005 (7)	0.0281 (7)	−0.0036 (6)
Zn1	0.0457 (2)	0.03405 (18)	0.0461 (2)	0.000	0.03332 (15)	0.000

Geometric parameters (Å, º)

C1—C2	1.352 (3)	C5—C10	1.383 (3)
C1—N1	1.366 (3)	C6—C7	1.385 (3)
C1—H1	0.9300	C6—H6	0.9300
C2—N2	1.366 (3)	C7—C8	1.389 (3)
C2—H2	0.9300	C7—H7	0.9300
C3—N1	1.317 (3)	C8—C9	1.395 (3)
C3—N2	1.340 (2)	C8—C8^{i}	1.491 (3)
C3—H3	0.9300	C9—C10	1.376 (3)
C4—N2	1.467 (3)	C9—H9	0.9300
C4—C5	1.515 (3)	C10—H10	0.9300
C4—H4A	0.9700	Zn1—Cl1	2.2349 (9)
C4—H4B	0.9700	Zn1—N1	2.0224 (16)
C5—C6	1.375 (3)		
C2—C1—N1	109.87 (19)	C8—C7—H7	119.3
C2—C1—H1	125.1	C7—C8—C9	116.80 (16)
N1—C1—H1	125.1	C7—C8—C8^{i}	121.6 (2)
C1—C2—N2	106.02 (18)	C9—C8—C8^{i}	121.6 (2)
C1—C2—H2	127.0	C10—C9—C8	121.50 (18)
N2—C2—H2	127.0	C10—C9—H9	119.3
N1—C3—N2	111.25 (18)	C8—C9—H9	119.3
N1—C3—H3	124.4	C9—C10—C5	121.18 (19)
N2—C3—H3	124.4	C9—C10—H10	119.4
N2—C4—C5	112.62 (17)	C5—C10—H10	119.4
N2—C4—H4A	109.1	C3—N1—C1	105.60 (16)
C5—C4—H4A	109.1	C3—N1—Zn1	126.82 (14)
N2—C4—H4B	109.1	C1—N1—Zn1	127.08 (14)
C5—C4—H4B	109.1	C3—N2—C2	107.25 (16)
H4A—C4—H4B	107.8	C3—N2—C4	124.48 (18)
C6—C5—C10	117.91 (18)	C2—N2—C4	127.82 (17)
C6—C5—C4	120.83 (18)	N1—Zn1—N1^{ii}	101.05 (9)
C10—C5—C4	121.25 (18)	N1—Zn1—Cl1^{ii}	110.42 (5)
C5—C6—C7	121.24 (19)	N1^{ii}—Zn1—Cl1^{ii}	106.35 (5)
C5—C6—H6	119.4	N1—Zn1—Cl1	106.35 (5)
C7—C6—H6	119.4	N1^{ii}—Zn1—Cl1	110.42 (5)

C6—C7—C8	121.37 (18)	Cl1^{ii}—Zn1—Cl1	120.56 (4)
C6—C7—H7	119.3		

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