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catena-Poly[[dichloridozinc(II)]-μ-1-carboxylatomethyl-3-methylimidazolium-κ^2O:O']

Xia Shi,[a,b] Jie Zhang,[b] Tao-Kai Ying[a,b] and Guo-Liang Zhao[a,b]*

[a]Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, Zhejiang 321004, People's Republic of China, and [b]College of Chemistry and Life Science, Zhejiang Normal University, Jinhua 321004, Zhejiang, People's Republic of China
Correspondence e-mail: sky53@zjnu.cn

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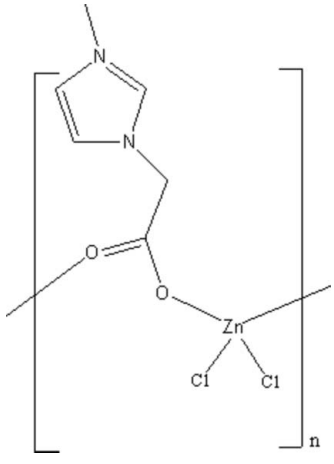
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.068; data-to-parameter ratio = 16.9.

The crystal structure of the title compound, $[ZnCl_2(C_6H_8N_2O_2)]_n$, consists of a zigzag chain in which adjacent $ZnCl_2$ groups are bridged by 1-carboxylatomethyl-3-methylimidazolium through its two O atoms. The environment around the Zn atom can be described as a *cis*-ZnO_2Cl_2 tetrahedron. The formation of the chain is strengthened by π–π stacking interactions between adjacent imidazole ring planes (π–π distance = 3.618 Å).

Related literature

For related literature, see: Shi *et al.* (2004, 2007).



Experimental

Crystal data

$[ZnCl_2(C_6H_8N_2O_2)]$
M_r = 276.43
Monoclinic, *Pc*
a = 4.8362 (4) Å
b = 10.5820 (9) Å
c = 10.1164 (7) Å
β = 102.183 (5)°
V = 506.06 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.92 mm^{-1}
T = 296 (2) K
0.35 × 0.11 × 0.05 mm

Data collection

Bruker *P*4 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.687, T_{max} = 0.864
3003 measured reflections
1994 independent reflections
1691 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.068
S = 1.01
1994 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Absolute structure: Flack (1983), with 824 Friedel pairs
Flack parameter: 0.055 (15)

Data collection: *SMART* (Bruker, 2004); cell refinement: *SMART* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *SHELXTL* (Bruker, 2002); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: RK2036).

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supplementary materials

Acta Cryst. (2007). E**63**, m2603 [**doi:10.1107/S1600536807046545**]

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Comment

It is known that the research of coordination polymers receives great interest nowadays, because they may afford new materials with useful properties, such as catalytic activity, microporosity and so on (Shi *et al.*, 2004). Recently, we have synthesized and reported cadmium polymer with 1-methyl-3-carboxymethylimidazole (Shi *et al.*, 2007). As an extension of our work in this field, we synthesized the title compound and solved its crystal structure (I).

The asymmetric unit of (I) contains one Zn atom, one 1-methyl-3-carboxymethylimidazole molecule, and two chlorine atoms (Fig. 1). The structure of (I) is a one-dimensional coordination chain in which the adjacent ($ZnCl_2$) groups are bridged by 1-methyl-3-carboxymethylimidazole through its two O atoms with the distance of 4.8362 (4)Å (*a*-translation) between two adjacent Zn atoms. There exists π-π interaction between the adjacent imidazole-ring planes (π-π distance = 3.618 Å), which strengthens the formation of the chain.

Experimental

A mixture of $ZnCl_2$ (1 mmol), ion liquid 1-methyl-3-carboxymethylimidazole hydroxide (1 mmol) and water (20 ml) was sealed in a 25 ml Teflon-lined stainless steel reactor and heated at 393 K for 48 h. A colourless solution was obtained after cooling the reaction to room temperature, colourless single crystals were obtained after three weeks.

Refinement

The H atoms bonded to C atoms were positioned geometrically (aromatic C–H = 0.93Å and aliphatic C–H = 0.97 Å, U_{iso}(H) = 1.2U_{eq}(C)). In the X-ray diffraction experiment 794 Friedel pairs were measured.

Figures

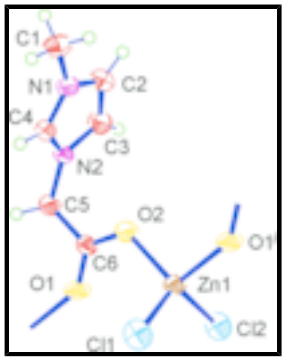

Fig. 1. A view of the molecule of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability. H atoms are presented as spheres with arbitrary radius. Symmetry code: (i) −1 + *x*, *y*, *z*;

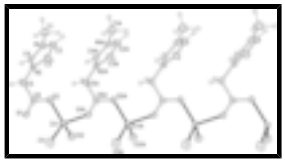

Fig. 2. The one-dimensional chain in crystal structure of (I).

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Crystal data

$[ZnCl_2(C_6H_8N_2O_2)]$	F_{000} = 276
M_r = 276.43	D_x = 1.814 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 1309 reflections
a = 4.8362 (4) Å	θ = 2.8–27.7º
b = 10.5820 (9) Å	μ = 2.92 mm^{-1}
c = 10.1164 (7) Å	*T* = 296 (2) K
β = 102.183 (5)º	Prism, colourless
V = 506.06 (7) Å^3	0.35 × 0.11 × 0.05 mm
Z = 2	

Data collection

Bruker P4 diffractometer	1994 independent reflections
Radiation source: fine-focus sealed tube	1691 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 296(2) K	θ_{max} = 27.7º
ω scans	θ_{min} = 2.8º
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	*h* = −6→6
T_{min} = 0.687, T_{max} = 0.864	*k* = −13→13
3003 measured reflections	*l* = −12→12

Refinement

Refinement on F^2	Hydrogen site location: Geom
Least-squares matrix: Full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$w = 1/[\sigma^2(F_o^2) + (0.025P)^2]$, where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.068	$(\Delta/\sigma)_{max} < 0.001$
S = 1.01	$\Delta\rho_{max}$ = 0.45 e Å^{-3}
1994 reflections	$\Delta\rho_{min}$ = −0.59 e Å^{-3}
118 parameters	Extinction correction: none
Primary atom site location: Direct	Absolute structure: Flack (1983)

Secondary atom site location: Difmap Flack parameter: 0.055 (15)

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 $F^2 > 2\sigma(F^2)$ 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	0.03320 (7)	0.76339 (4)	−0.06177 (5)	0.03457 (14)
Cl1	0.0646 (3)	0.96102 (10)	−0.13316 (14)	0.0511 (3)
Cl2	−0.0059 (2)	0.61405 (10)	−0.21919 (13)	0.0468 (3)
C1	0.3986 (10)	0.8408 (5)	0.6340 (4)	0.0485 (12)
H1A	0.4590	0.9268	0.6288	0.073*
H1B	0.4907	0.8052	0.7192	0.073*
H1C	0.1974	0.8386	0.6263	0.073*
C2	0.4180 (10)	0.6411 (4)	0.5010 (5)	0.0415 (11)
H2A	0.3230	0.5893	0.5510	0.050*
C3	0.5240 (9)	0.6061 (4)	0.3952 (4)	0.0395 (11)
H3A	0.5146	0.5260	0.3566	0.047*
C4	0.6128 (8)	0.8075 (4)	0.4347 (5)	0.0339 (10)
H4A	0.6756	0.8899	0.4289	0.041*
C5	0.7844 (8)	0.7217 (4)	0.2374 (4)	0.0352 (9)
H5A	0.8972	0.6465	0.2335	0.042*
H5B	0.9111	0.7938	0.2495	0.042*
C6	0.5754 (8)	0.7356 (4)	0.1059 (4)	0.0317 (9)
N1	0.4738 (8)	0.7668 (3)	0.5229 (4)	0.0355 (9)
N2	0.6513 (7)	0.7124 (4)	0.3538 (4)	0.0305 (8)
O1	0.6675 (6)	0.7498 (3)	0.0018 (3)	0.0518 (9)
O2	0.3161 (5)	0.7312 (3)	0.1078 (3)	0.0481 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02622 (18)	0.0510 (3)	0.0276 (2)	0.0024 (3)	0.00809 (14)	0.0035 (3)
Cl1	0.0555 (6)	0.0378 (6)	0.0633 (8)	0.0024 (5)	0.0199 (6)	−0.0084 (6)
Cl2	0.0494 (6)	0.0366 (6)	0.0562 (7)	0.0000 (5)	0.0149 (5)	−0.0038 (5)
C1	0.060 (3)	0.056 (3)	0.032 (3)	0.006 (2)	0.014 (2)	−0.005 (2)
C2	0.045 (2)	0.045 (3)	0.038 (3)	−0.006 (2)	0.014 (2)	0.005 (2)
C3	0.046 (2)	0.035 (3)	0.039 (3)	−0.002 (2)	0.012 (2)	−0.0028 (19)

C4	0.031 (2)	0.041 (2)	0.030 (2)	−0.0055 (16)	0.007 (2)	0.002 (2)
C5	0.0240 (17)	0.051 (3)	0.032 (2)	0.0018 (18)	0.0103 (16)	0.003 (2)
C6	0.0272 (18)	0.041 (2)	0.029 (2)	0.0004 (17)	0.0096 (16)	0.0044 (18)
N1	0.035 (2)	0.045 (2)	0.027 (2)	0.0004 (16)	0.0067 (17)	0.0027 (17)
N2	0.0275 (17)	0.042 (2)	0.024 (2)	−0.0023 (16)	0.0103 (15)	0.0028 (17)
O1	0.0256 (13)	0.105 (3)	0.0262 (18)	0.0044 (15)	0.0089 (12)	0.0114 (16)
O2	0.0210 (13)	0.091 (3)	0.0336 (17)	0.0011 (14)	0.0078 (12)	0.0107 (17)

Geometric parameters (Å, °)

Zn1—O2	1.985 (3)	C3—H3A	0.9300
Zn1—O1^{i}	2.011 (3)	C4—N1	1.298 (6)
Zn1—Cl2	2.2231 (13)	C4—N2	1.335 (6)
Zn1—Cl1	2.2281 (12)	C4—H4A	0.9300
C1—N1	1.477 (6)	C5—N2	1.460 (6)
C1—H1A	0.9600	C5—C6	1.499 (6)
C1—H1B	0.9600	C5—H5A	0.9700
C1—H1C	0.9600	C5—H5B	0.9700
C2—C3	1.334 (6)	C6—O1	1.235 (5)
C2—N1	1.366 (5)	C6—O2	1.259 (5)
C2—H2A	0.9300	O1—Zn1^{ii}	2.011 (3)
C3—N2	1.388 (6)		
O2—Zn1—O1^{i}	101.74 (11)	N1—C4—H4A	125.3
O2—Zn1—Cl2	115.85 (11)	N2—C4—H4A	125.3
O1^{i}—Zn1—Cl2	103.34 (11)	N2—C5—C6	113.2 (3)
O2—Zn1—Cl1	111.06 (11)	N2—C5—H5A	108.9
O1^{i}—Zn1—Cl1	107.20 (11)	C6—C5—H5A	108.9
Cl2—Zn1—Cl1	115.87 (5)	N2—C5—H5B	108.9
N1—C1—H1A	109.5	C6—C5—H5B	108.9
N1—C1—H1B	109.5	H5A—C5—H5B	107.8
H1A—C1—H1B	109.5	O1—C6—O2	123.9 (4)
N1—C1—H1C	109.5	O1—C6—C5	118.1 (3)
H1A—C1—H1C	109.5	O2—C6—C5	118.0 (3)
H1B—C1—H1C	109.5	C4—N1—C2	108.9 (4)
C3—C2—N1	107.7 (4)	C4—N1—C1	126.4 (4)
C3—C2—H2A	126.1	C2—N1—C1	124.6 (4)
N1—C2—H2A	126.1	C4—N2—C3	107.3 (4)
C2—C3—N2	106.7 (4)	C4—N2—C5	125.9 (4)
C2—C3—H3A	126.7	C3—N2—C5	126.6 (4)
N2—C3—H3A	126.7	C6—O1—Zn1^{ii}	141.3 (3)
N1—C4—N2	109.4 (4)	C6—O2—Zn1	119.1 (3)
N1—C2—C3—N2	1.1 (5)	C2—C3—N2—C5	−176.8 (4)
N2—C5—C6—O1	176.9 (4)	C6—C5—N2—C4	−96.5 (5)
N2—C5—C6—O2	−3.7 (5)	C6—C5—N2—C3	78.6 (5)
N2—C4—N1—C2	0.2 (5)	O2—C6—O1—Zn1^{ii}	−180.0 (4)
N2—C4—N1—C1	177.2 (4)	C5—C6—O1—Zn1^{ii}	−0.6 (7)
C3—C2—N1—C4	−0.8 (5)	O1—C6—O2—Zn1	−5.6 (6)

C3—C2—N1—C1	−178.0 (4)	C5—C6—O2—Zn1	175.0 (3)
N1—C4—N2—C3	0.5 (5)	O1^{i}—Zn1—O2—C6	−178.3 (3)
N1—C4—N2—C5	176.4 (4)	Cl2—Zn1—O2—C6	70.5 (3)
C2—C3—N2—C4	−1.0 (5)	Cl1—Zn1—O2—C6	−64.5 (3)

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

Fig. 1

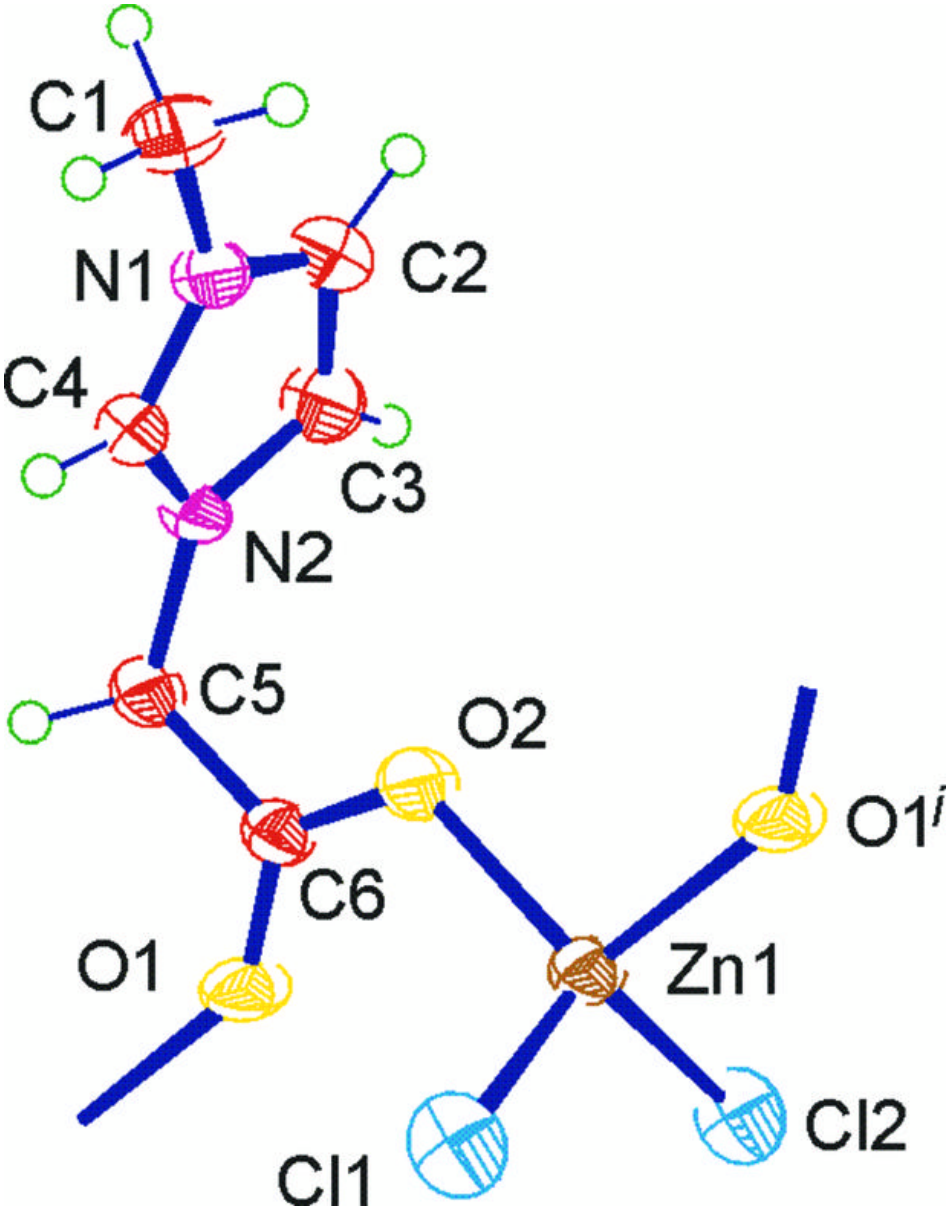
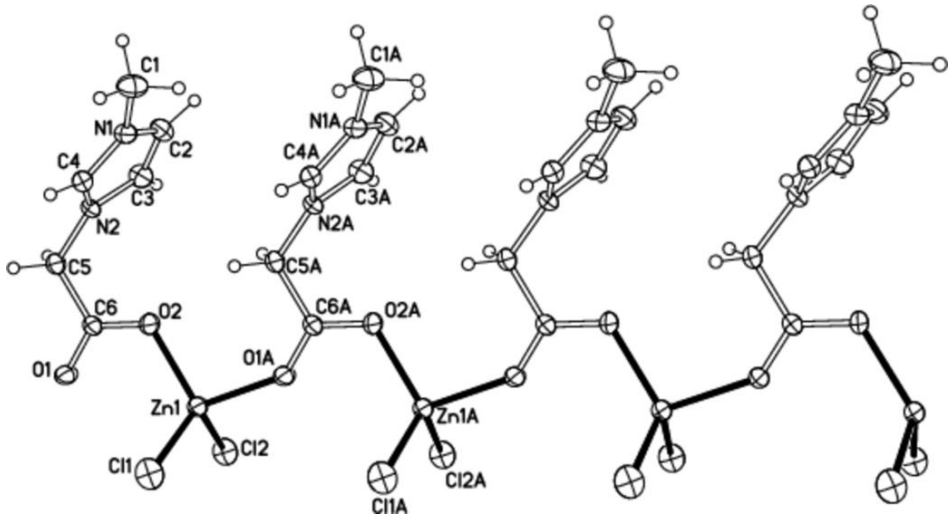


Fig. 2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C2
C4
C3
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C5
C6
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O1
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