Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[(μ_5-2,6-dimethylpyridine-3,5-dicarboxylato)zinc]

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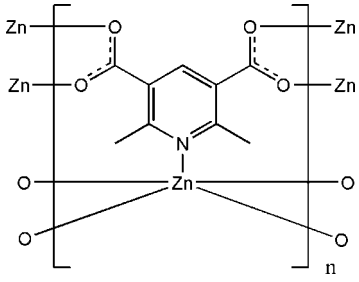
Received 18 June 2011; accepted 20 June 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.023; wR factor = 0.067; data-to-parameter ratio = 10.3.

In the polymeric title complex, $[Zn(C_9H_7NO_4)]_n$, the Zn^{II} cation is located on a twofold rotation axis and is coordinated by five 2,6-dimethylpyridine-3,5-dicarboxylate (mpdc) anions in a distorted $ZnNO_4$ trigonal–bipyramidal geometry. The mpdc anion is also located on the twofold rotation axis and bridges five Zn^{II} cations, forming the three-dimensional polymeric complex. Weak C—H$\cdots\pi$ interactions are present in the crystal structure.

Related literature

For a related structure, see: Huang *et al.* (2007). For background to metal-organic frameworks (MOFs), see: Long & Yaghi (2009); Zhao *et al.* (2003).



Experimental

Crystal data

$[Zn(C_9H_7NO_4)]$
M_r = 258.53
Monoclinic, $C2/c$
a = 8.578 (7) Å
b = 14.016 (11) Å
c = 7.382 (7) Å
β = 112.176 (17)°
V = 821.9 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.98 mm^{-1}
T = 293 K
0.30 × 0.25 × 0.16 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.469, T_{max} = 0.647
2615 measured reflections
732 independent reflections
709 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.067
S = 1.00
732 reflections
71 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	2.207 (3)	Zn1—N1^{ii}	2.089 (3)
Zn1—O2^{i}	1.977 (2)		

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

Table 2
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the pyridine ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$C\cdots Cg^{ii}$	0.96	2.67	3.573 (4)	158

Symmetry code: (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2008) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

This work was supported by Science and Technology Projects of Chongqing Municipal Education Commission (KJ100602) and Chongqing Normal University Scientific Research Foundation Project (10XLZ005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5247).

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supplementary materials

Acta Cryst. (2011). E**67**, m977 [**doi:10.1107/S1600536811024172**]

Poly[(μ_5-2,6-dimethylpyridine-3,5-dicarboxylato)zinc]

M.-X. Zhang, X. Chen and Y. Zhu

Comment

Recently, research on metal-organic frameworks (MOFs) has become of increasing interest (Long & Yaghi, 2009). However, it is still a great challenge to assemble a predicted structure because there are numerous influences that can play decisive roles on the structure and crystal packing. Fortunately, these uncertainties can be reduced by the use of well selected spacers that have the ability to aggregate metal ions into different secondary building units (Zhao *et al.*, 2003). Herein we reports an interesting five-connected zeolite-like coordination polymer based on highly-substituted pyridinedicarboxylates.

The title compound is a three-dimensional framework built from Zn cations that are linked by mpdc anions. From this arrangement cavities are formed. Zn1 is coordinated by four oxygen atoms from four different CO_2^- groups of mpdc ligands and one pyridyl nitrogen atom from another mpdc ligand. The mpdc ligand bridges five different Zn atoms and favors the construction of the structure with zeolite-like topology.The topology of the title compound is identical with the reported $[Cd(mpdc)]_n$ (Huang *et al.*, 2007), but the coordination sphere of cation, the binding mode of the carboxylate group and the synthesis condition are different.

The combination of the dramatic twists between two carboxylate groups in mpdc ligands results in the formation of the intersecting double-stranded helical chain comprised of $[Zn(CO_2)_2]_n$ (Zn atoms as nodes).

Experimental

All chemicals were of reagent grade and used as purchased without further purification. A mixture of $Zn(NO_3)_2.6H_2O$ (450 mg, 1.5 mmol), H_2mpdc (97.5 mg, 0.5 mmol), $(Et)_3N$ 0.07 mL and H_2O 10 mL was sealed in a 25 ml stainless steel reactor with Teflon liner and directly heated to 180 °C for 3 days, and then cooled to room temperature. The crystal samples were washed with methanol to give the title compound in about 35% yield (based on H_2mpdc ligand).

Refinement

Constraint instruction 'delu 0.001 Zn1 O1' was used in the refinement. All H atoms were placed in geometrically idealized positions (C—H = 0.93 Å) and treated as riding on their parent atoms, with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for aromatic H atom.

Figures

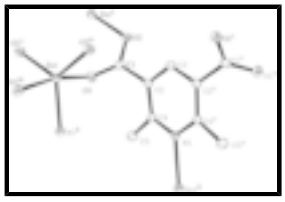

Fig. 1. The coordination environments of Zinc ions, showing 30% probability displacement ellipsoids and hydrogen atoms have been removed for clarity. Symmetry codes: (i) -*x*, -*y*, -*z*+1; (ii) -*x* + 1/2, -*y* + 1/2,-*z* + 1; (iii) -*x*, *y*, -*z*+1/2; (iv) *x*, -*y*, *z* - 1/2; (v) -*x* + 1, +*y*, -*z* + 3/2.

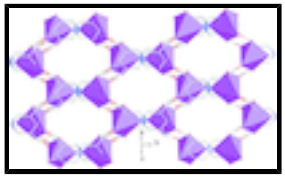

Fig. 2. The presentation of the 3-D zeolite-like architecture. Methyl groups and hydrogen atoms have been removed for clarity. Polyhedra represent the $ZnNO_4$ groups.

Poly[(μ$_5$-2,6-dimethylpyridine-3,5-dicarboxylato)zinc]

Crystal data

$[Zn(C_9H_7NO_4)]$	$F(000) = 520$
$M_r = 258.53$	$D_x = 2.089$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 535 reflections
a = 8.578 (7) Å	θ = 2.9–27.5°
b = 14.016 (11) Å	μ = 2.98 mm^{-1}
c = 7.382 (7) Å	*T* = 293 K
β = 112.176 (17)°	Prism, colorless
V = 821.9 (12) Å^3	0.30 × 0.25 × 0.16 mm
Z = 4	

Data collection

Rigaku Mercury2 diffractometer	732 independent reflections
Radiation source: fine-focus sealed tube	709 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.022$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.9°$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	*h* = −10→10
$T_{min} = 0.469$, $T_{max} = 0.647$	*k* = −14→16
2615 measured reflections	*l* = −8→8

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.023$	Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.067$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.6817P]$ where $P = (F_o^2 + 2F_c^2)/3$
732 reflections	$(\Delta/\sigma)_{max} < 0.001$
71 parameters	$\Delta\rho_{max} = 0.50$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.59$ 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	0.0000	0.08158 (2)	0.2500	0.01616 (18)
N1	0.5000	0.26938 (18)	0.7500	0.0137 (5)
O1	0.0625 (2)	0.09690 (11)	0.5672 (2)	0.0189 (4)
O2	0.20746 (19)	−0.00679 (11)	0.7999 (2)	0.0192 (4)
C1	0.1949 (3)	0.06763 (15)	0.6979 (3)	0.0147 (5)
C2	0.3560 (3)	0.12188 (16)	0.7360 (3)	0.0147 (5)
C3	0.5000	0.0730 (2)	0.7500	0.0168 (7)
H3	0.5000	0.0066	0.7500	0.020*
C4	0.3618 (3)	0.22210 (15)	0.7464 (3)	0.0137 (5)
C5	0.2202 (3)	0.28064 (16)	0.7589 (4)	0.0195 (5)
H5A	0.2644	0.3278	0.8596	0.029*
H5B	0.1434	0.2399	0.7893	0.029*
H5C	0.1621	0.3117	0.6358	0.029*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0108 (2)	0.0106 (3)	0.0269 (3)	0.000	0.00690 (17)	0.000
N1	0.0128 (13)	0.0115 (13)	0.0166 (12)	0.000	0.0054 (10)	0.000
O1	0.0143 (8)	0.0178 (8)	0.0228 (7)	0.0007 (7)	0.0050 (7)	0.0013 (6)
O2	0.0146 (8)	0.0135 (8)	0.0277 (8)	−0.0012 (6)	0.0061 (6)	0.0048 (6)
C1	0.0143 (12)	0.0124 (11)	0.0202 (11)	−0.0012 (9)	0.0095 (9)	−0.0039 (8)
C2	0.0145 (11)	0.0121 (12)	0.0175 (10)	−0.0004 (9)	0.0058 (9)	0.0007 (8)
C3	0.0161 (17)	0.0107 (16)	0.0226 (17)	0.000	0.0064 (14)	0.000
C4	0.0111 (11)	0.0133 (11)	0.0165 (10)	−0.0011 (8)	0.0049 (8)	−0.0001 (8)

C5	0.0160 (11)	0.0150 (12)	0.0302 (12)	0.0005 (9)	0.0118 (10)	−0.0021 (9)

Geometric parameters (Å, °)

Zn1—O1	2.207 (3)	O2—Zn1^{iii}	1.977 (2)
Zn1—O1^{i}	2.207 (3)	C1—C2	1.507 (3)
Zn1—O2^{ii}	1.977 (2)	C2—C3	1.382 (3)
Zn1—O2^{iii}	1.977 (2)	C2—C4	1.407 (3)
Zn1—N1^{iv}	2.089 (3)	C3—C2^{v}	1.382 (3)
N1—C4	1.349 (3)	C3—H3	0.9300
N1—C4^{v}	1.349 (3)	C4—C5	1.497 (3)
N1—Zn1^{iv}	2.089 (3)	C5—H5A	0.9600
O1—C1	1.250 (3)	C5—H5B	0.9600
O2—C1	1.267 (3)	C5—H5C	0.9600
O2^{iii}—Zn1—O2^{ii}	115.94 (11)	O2—C1—C2	116.0 (2)
O2^{iii}—Zn1—N1^{iv}	122.03 (5)	C3—C2—C4	118.6 (2)
O2^{ii}—Zn1—N1^{iv}	122.03 (5)	C3—C2—C1	119.6 (2)
O2^{iii}—Zn1—O1	95.17 (6)	C4—C2—C1	121.69 (19)
O2^{ii}—Zn1—O1	90.75 (6)	C2^{v}—C3—C2	120.5 (3)
N1^{iv}—Zn1—O1	84.42 (4)	C2^{v}—C3—H3	119.7
O2^{iii}—Zn1—O1^{i}	90.75 (6)	C2—C3—H3	119.7
O2^{ii}—Zn1—O1^{i}	95.17 (6)	N1—C4—C2	120.30 (19)
N1^{iv}—Zn1—O1^{i}	84.42 (4)	N1—C4—C5	117.2 (2)
O1—Zn1—O1^{i}	168.83 (9)	C2—C4—C5	122.51 (19)
C4—N1—C4^{v}	121.2 (3)	C4—C5—H5A	109.5
C4—N1—Zn1^{iv}	119.41 (13)	C4—C5—H5B	109.5
C4^{v}—N1—Zn1^{iv}	119.41 (13)	H5A—C5—H5B	109.5
C1—O1—Zn1	124.94 (16)	C4—C5—H5C	109.5
C1—O2—Zn1^{iii}	117.23 (15)	H5A—C5—H5C	109.5
O1—C1—O2	125.3 (2)	H5B—C5—H5C	109.5
O1—C1—C2	118.7 (2)		
O2^{iii}—Zn1—O1—C1	120.17 (19)	O2—C1—C2—C4	−137.8 (2)
O2^{ii}—Zn1—O1—C1	4.03 (18)	C4—C2—C3—C2^{v}	−3.21 (13)
N1^{iv}—Zn1—O1—C1	−118.08 (18)	C1—C2—C3—C2^{v}	173.1 (2)
O1^{i}—Zn1—O1—C1	−118.08 (18)	C4^{v}—N1—C4—C2	−3.33 (14)
Zn1—O1—C1—O2	−103.1 (2)	Zn1^{iv}—N1—C4—C2	176.67 (14)
Zn1—O1—C1—C2	74.7 (2)	C4^{v}—N1—C4—C5	175.2 (2)
Zn1^{iii}—O2—C1—O1	−0.8 (3)	Zn1^{iv}—N1—C4—C5	−4.8 (2)
Zn1^{iii}—O2—C1—C2	−178.63 (14)	C3—C2—C4—N1	6.6 (3)
O1—C1—C2—C3	−131.9 (2)	C1—C2—C4—N1	−169.61 (17)
O2—C1—C2—C3	46.1 (3)	C3—C2—C4—C5	−171.85 (17)
O1—C1—C2—C4	44.2 (3)	C1—C2—C4—C5	11.9 (3)

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

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the pyridine ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5C···Cg^{iv}	0.96	2.67	3.573 (4)	158.

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

Fig. 1

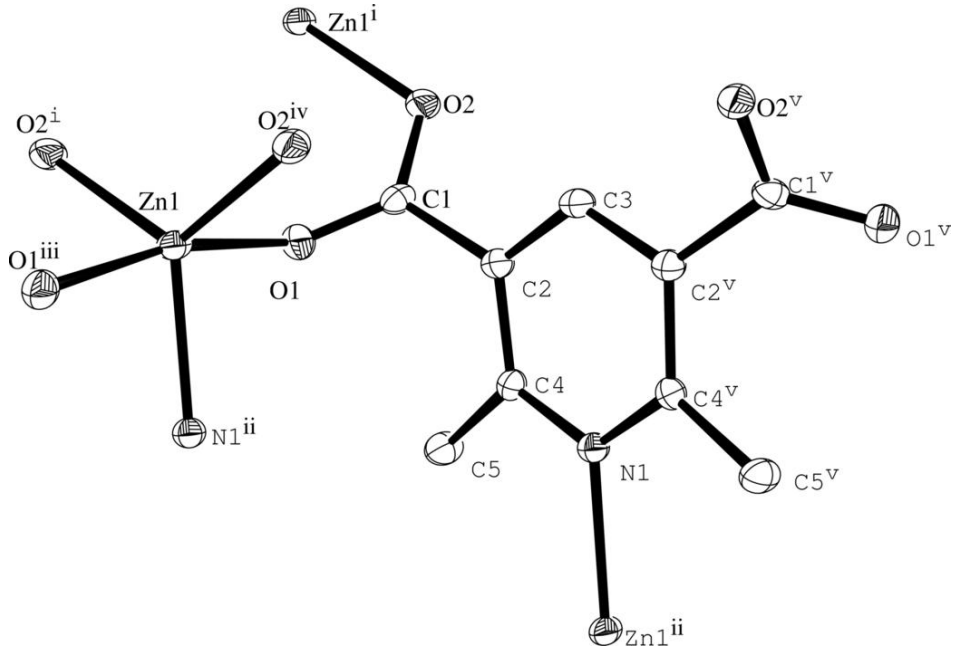
Zn1i
O2
O2i
O2iv
O2v
Zn1
C1
C3
C1v
O1v
O1iii
O1
C2
C2v
C4
C4v
N1ii
C5
N1
C5v
Zn1ii

Fig. 2