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catena-Poly[[bis(benzene-1,3-dicarboxylato-κ^2O,O')zinc(II)]-μ-4,4′-bipyridine-$\kappa^2N:N'$]

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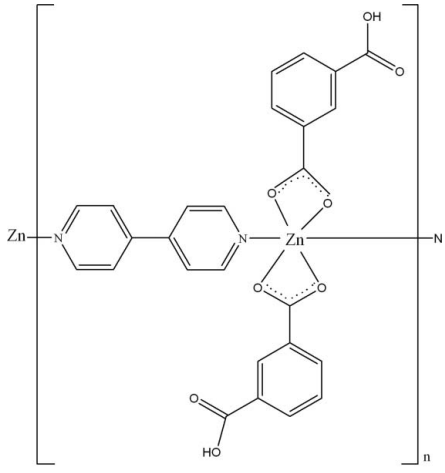
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.091; data-to-parameter ratio = 14.2.

In the title compound, $[Zn(C_8H_5O_4)_2(C_{10}H_8N_2)]_n$, the Zn^{II} atom lies on a twofold rotation axis, and is coordinated by two N atoms of two 4,4′-bipyridine ligands and two carboxylate groups, each in a chelating mode, from two isophthalate ligands. The 4,4′-bipyridine ligand, located on an inversion center, bridges the Zn^{II} atoms, forming a one-dimensional zigzag chain structure. O—H···O hydrogen bonds and π–π stacking interactions [with a shortest atom-to-atom distance of 3.41 (1) Å] are observed between the chains.

Related literature

For general background, see: Eddaoudi *et al.* (2001). For related structures, see: Chen & Liu (2002); Groeneman *et al.* (1999); Li *et al.* (2006).



Experimental

Crystal data

$[Zn(C_8H_5O_4)_2(C_{10}H_8N_2)]$
M_r = 551.79
Monoclinic, $C2/c$
a = 20.940 (3) Å
b = 9.6078 (12) Å
c = 14.7942 (19) Å
β = 125.884 (2)°
V = 2411.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 292 (2) K
0.12 × 0.09 × 0.05 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.890, T_{max} = 0.951
6569 measured reflections
2385 independent reflections
2096 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.091
S = 1.04
2385 reflections
168 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.9689 (15)	Zn1—O2	2.5953 (15)
Zn1—N1	2.0669 (16)		
O1^i—Zn1—O1	139.21 (9)	O1^i—Zn1—O2	97.19 (5)
O1—Zn1—N1	107.76 (6)	N1—Zn1—O2	86.01 (6)
O1—Zn1—N1^i	98.86 (6)	N1^i—Zn1—O2	153.80 (6)
N1—Zn1—N1^i	97.64 (9)	O2^i—Zn1—O2	102.11 (6)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O2^{ii}	0.82	1.97	2.771 (3)	165

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

We thank Mr Heng-Qing Jia of Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2062).

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supplementary materials

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catena-Poly[[bis(benzene-1,3-dicarboxylato-κ^2O,O')zinc(II)]-μ-4,4'-bipyridine-$\kappa^2N:N'$]

X.-M. Li, Y.-H. Dong, Q.-W. Wang and B. Liu

Comment

Metal-organic complexes with a variety of supramolecular architectures have attracted increasing interest because of their novel topologies and potential applications as functional materials (Eddaoudi *et al.*, 2001). Recently, a successful strategy for preparing these materials has been the assembly reaction between transition metal ions and two types of ligands, one acts as a terminal ligand and the other acts as a bridging ligand. In this respect, diverse dicarboxylates with various oriented carboxyl groups have been utilized to build coordination polymers. These ligands are able to bridge metal centers in different modes and also produce either linear or zigzag polymeric chains (Chen & Liu, 2002; Groeneman *et al.*, 1999; Li *et al.*, 2006). In this work, we use isophthalic acid as a terminal ligand and 4,4'-bipyridine (bpy) as a bridging ligand, generating a new compound, (I), under hydrothermal condition.

Selected bond lengths and angles for (I) are given in Table 1. In compound (I), the Zn^{II} atom lying on a twofold rotation axis is six-coordinated by two N atoms from two bpy ligands, and two carboxylate groups, each in a chelating mode, from two isophthalate ligands (Fig. 1). The bpy ligand located on an inversion center bridges the Zn^{II} atoms, forming a one-dimensional zigzag chain structure. It is noteworthy that there exist π-π interactions, with the shortest atom-to-atom distance of 3.41 (1) Å, and O—H···O hydrogen bonds (Table 2, Fig. 2) between the isophthalate ligands in the neighboring chains, which lead to a three-dimensional supramolecular network.

Experimental

Compound (I) was prepared from a mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (0.119 g, 0.4 mmol), isophthalic acid (0.134 g, 0.8 mmol), bpy (0.070 g, 0.4 mmol) and H_2O (18 ml) in a 30 ml Teflon-lined autoclave under autogenous pressure at 423 K for 7 d. After cooling to room temperature, colorless crystals suitable for X-ray structure analysis were obtained. Analysis, calculated for $C_{26}H_{18}N_2O_8Zn$: C 64.7, H 2.7, N 5.8%; found: C 64.5, H 2.6, N 5.7%.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H= 0.93Å and U_{iso}(H) = 1.2U_{eq}(C) and with O—H = 0.82Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

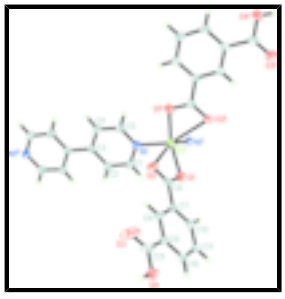

Fig. 1. The asymmetric unit of (I), together with symmetry-related atoms to complete the Zn coordination. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $1-x, y, 3/2-z$, (ii) $1/2-x, -1/2-y, 1-z$.]

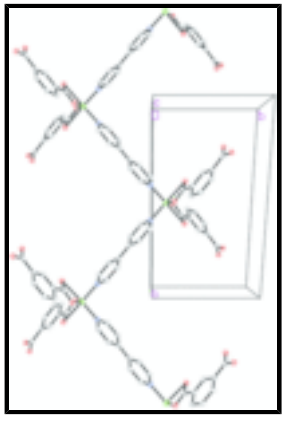

Fig. 2. View of the chain structure in (I).

catena-Poly[[bis(benzene-1,3-dicarboxylato-κ^2O,O')zinc(II)]- μ-4,4'-bipyridine-$\kappa^2N:N'$]

Crystal data

$[Zn(C_8H_5O_4)_2(C_{10}H_8N_2)]$	F_{000} = 1128
M_r = 551.79	D_x = 1.520 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2132 reflections
a = 20.940 (3) Å	θ = 2.4–26.1º
b = 9.6078 (12) Å	μ = 1.07 mm^{-1}
c = 14.7942 (19) Å	*T* = 292 (2) K
β = 125.884 (2)º	Block, colorless
V = 2411.4 (6) Å^3	0.12 × 0.09 × 0.05 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2385 independent reflections
Radiation source: fine-focus sealed tube	2096 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 292(2) K	θ_{max} = 26.1º
φ and ω scans	θ_{min} = 2.4º

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.890, T_{max} = 0.951

6569 measured reflections

h = −25→24

k = −11→11

l = −18→17

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.033

$wR(F^2)$ = 0.091

S = 1.04

2385 reflections

168 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.39 e Å^{-3}

$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.12559 (3)	0.7500	0.03382 (14)
C2	0.32554 (15)	−0.1920 (3)	0.64815 (19)	0.0543 (6)
H2A	0.3122	−0.2483	0.6859	0.065*
O2	0.39232 (9)	0.29538 (15)	0.71869 (12)	0.0433 (4)
O1	0.49428 (9)	0.19702 (15)	0.86982 (13)	0.0461 (4)
C5	0.36932 (14)	−0.0250 (2)	0.54810 (19)	0.0533 (6)
H5A	0.3839	0.0327	0.5125	0.064*
O4	0.25572 (10)	0.67575 (18)	0.91871 (14)	0.0606 (5)
H4	0.2165	0.7250	0.8809	0.091*
O3	0.22568 (15)	0.6223 (2)	0.75308 (18)	0.1004 (9)
N1	0.40947 (9)	−0.01606 (16)	0.65816 (14)	0.0362 (4)
C3	0.28368 (11)	−0.20154 (19)	0.53335 (16)	0.0338 (4)
C10	0.38715 (12)	0.5013 (2)	1.02708 (18)	0.0437 (5)
H10A	0.3772	0.5512	1.0714	0.052*
C13	0.26886 (15)	0.6106 (2)	0.8536 (2)	0.0487 (6)
C6	0.43472 (12)	0.27635 (19)	0.82190 (17)	0.0357 (4)
C12	0.46543 (13)	0.3362 (2)	1.00919 (18)	0.0423 (5)
H12A	0.5082	0.2756	1.0425	0.051*
C7	0.41740 (12)	0.35150 (19)	0.89450 (17)	0.0339 (4)
C8	0.35402 (12)	0.4413 (2)	0.84621 (17)	0.0381 (5)
H8A	0.3213	0.4514	0.7691	0.046*
C9	0.33852 (12)	0.5171 (2)	0.91158 (18)	0.0396 (5)
C11	0.44993 (14)	0.4114 (3)	1.07490 (19)	0.0494 (6)
H11A	0.4825	0.4005	1.1520	0.059*
C4	0.30732 (15)	−0.1149 (2)	0.4840 (2)	0.0531 (6)
H4A	0.2813	−0.1172	0.4071	0.064*

C1	0.38671 (15)	−0.0992 (3)	0.70599 (19)	0.0542 (6)
H1A	0.4137	−0.0944	0.7830	0.065*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0357 (2)	0.0348 (2)	0.0313 (2)	0.000	0.01984 (17)	0.000
C2	0.0657 (15)	0.0592 (14)	0.0373 (12)	−0.0254 (12)	0.0298 (12)	−0.0015 (11)
O2	0.0557 (9)	0.0459 (8)	0.0385 (8)	−0.0018 (7)	0.0334 (8)	−0.0011 (6)
O1	0.0466 (9)	0.0489 (8)	0.0476 (9)	0.0067 (7)	0.0303 (8)	−0.0040 (7)
C5	0.0570 (14)	0.0655 (15)	0.0377 (12)	−0.0221 (12)	0.0278 (12)	−0.0006 (11)
O4	0.0575 (10)	0.0744 (11)	0.0521 (11)	0.0161 (9)	0.0334 (9)	−0.0125 (9)
O3	0.126 (2)	0.138 (2)	0.0536 (13)	0.0874 (16)	0.0614 (14)	0.0386 (13)
N1	0.0377 (9)	0.0369 (8)	0.0344 (9)	−0.0025 (7)	0.0214 (8)	−0.0009 (7)
C3	0.0372 (10)	0.0340 (10)	0.0331 (10)	−0.0006 (8)	0.0223 (9)	−0.0016 (8)
C10	0.0488 (12)	0.0509 (12)	0.0411 (12)	−0.0074 (10)	0.0317 (11)	−0.0121 (10)
C13	0.0633 (16)	0.0489 (13)	0.0509 (15)	0.0122 (11)	0.0430 (14)	0.0060 (10)
C6	0.0414 (11)	0.0325 (9)	0.0422 (12)	−0.0063 (8)	0.0295 (10)	−0.0051 (8)
C12	0.0412 (12)	0.0483 (11)	0.0391 (12)	0.0013 (9)	0.0245 (11)	−0.0001 (10)
C7	0.0370 (11)	0.0344 (10)	0.0360 (11)	−0.0056 (8)	0.0246 (10)	−0.0030 (8)
C8	0.0442 (11)	0.0422 (11)	0.0341 (11)	−0.0004 (9)	0.0265 (10)	−0.0002 (9)
C9	0.0460 (12)	0.0400 (11)	0.0423 (12)	−0.0028 (9)	0.0312 (11)	−0.0027 (9)
C11	0.0483 (13)	0.0661 (14)	0.0313 (11)	−0.0030 (11)	0.0218 (11)	−0.0053 (10)
C4	0.0581 (15)	0.0672 (15)	0.0321 (12)	−0.0238 (12)	0.0253 (12)	−0.0059 (10)
C1	0.0599 (15)	0.0638 (15)	0.0282 (11)	−0.0242 (12)	0.0199 (11)	−0.0054 (10)

Geometric parameters (Å, °)

Zn1—O1^{i}	1.9689 (15)	C3—C4	1.377 (3)
Zn1—O1	1.9689 (15)	C3—C3^{ii}	1.483 (4)
Zn1—N1	2.0669 (16)	C10—C11	1.373 (3)
Zn1—N1^{i}	2.0669 (16)	C10—C9	1.393 (3)
Zn1—O2	2.5953 (15)	C10—H10A	0.9300
C2—C1	1.372 (3)	C13—C9	1.485 (3)
C2—C3	1.384 (3)	C6—C7	1.504 (3)
C2—H2A	0.9300	C12—C7	1.383 (3)
O2—C6	1.251 (2)	C12—C11	1.394 (3)
O1—C6	1.266 (2)	C12—H12A	0.9300
C5—N1	1.327 (3)	C7—C8	1.380 (3)
C5—C4	1.374 (3)	C8—C9	1.392 (3)
C5—H5A	0.9300	C8—H8A	0.9300
O4—C13	1.307 (3)	C11—H11A	0.9300
O4—H4	0.8200	C4—H4A	0.9300
O3—C13	1.210 (3)	C1—H1A	0.9300
N1—C1	1.327 (3)		
O1^{i}—Zn1—O1	139.21 (9)	O3—C13—O4	122.2 (2)
O1^{i}—Zn1—N1	98.86 (6)	O3—C13—C9	122.7 (2)
O1—Zn1—N1	107.76 (6)	O4—C13—C9	115.1 (2)

$O1^{i}$—Zn1—$N1^{i}$	107.76 (6)	O2—C6—O1	122.22 (18)
O1—Zn1—$N1^{i}$	98.86 (6)	O2—C6—C7	120.39 (18)
N1—Zn1—$N1^{i}$	97.64 (9)	O1—C6—C7	117.37 (18)
O1—Zn1—O2	55.71 (5)	C7—C12—C11	120.1 (2)
$O1^{i}$—Zn1—O2	97.19 (5)	C7—C12—H12A	119.9
N1—Zn1—O2	86.01 (6)	C11—C12—H12A	119.9
$N1^{i}$—Zn1—O2	153.80 (6)	C8—C7—C12	119.26 (18)
$O2^{i}$—Zn1—O2	102.11 (6)	C8—C7—C6	119.45 (18)
C1—C2—C3	119.8 (2)	C12—C7—C6	121.25 (19)
C1—C2—H2A	120.1	C7—C8—C9	120.82 (19)
C3—C2—H2A	120.1	C7—C8—H8A	119.6
C6—O1—Zn1	105.40 (13)	C9—C8—H8A	119.6
N1—C5—C4	123.4 (2)	C8—C9—C10	119.66 (19)
N1—C5—H5A	118.3	C8—C9—C13	117.70 (19)
C4—C5—H5A	118.3	C10—C9—C13	122.63 (19)
C13—O4—H4	109.5	C10—C11—C12	120.7 (2)
C5—N1—C1	116.62 (18)	C10—C11—H11A	119.6
C5—N1—Zn1	121.76 (14)	C12—C11—H11A	119.6
C1—N1—Zn1	121.57 (14)	C5—C4—C3	120.1 (2)
C4—C3—C2	116.42 (19)	C5—C4—H4A	119.9
$C4—C3—C3^{ii}$	121.6 (2)	C3—C4—H4A	119.9
$C2—C3—C3^{ii}$	122.0 (2)	N1—C1—C2	123.7 (2)
C11—C10—C9	119.43 (19)	N1—C1—H1A	118.2
C11—C10—H10A	120.3	C2—C1—H1A	118.2
C9—C10—H10A	120.3		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
$O4—H4···O2^{iii}$	0.82	1.97	2.771 (3)	165

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

Fig. 1

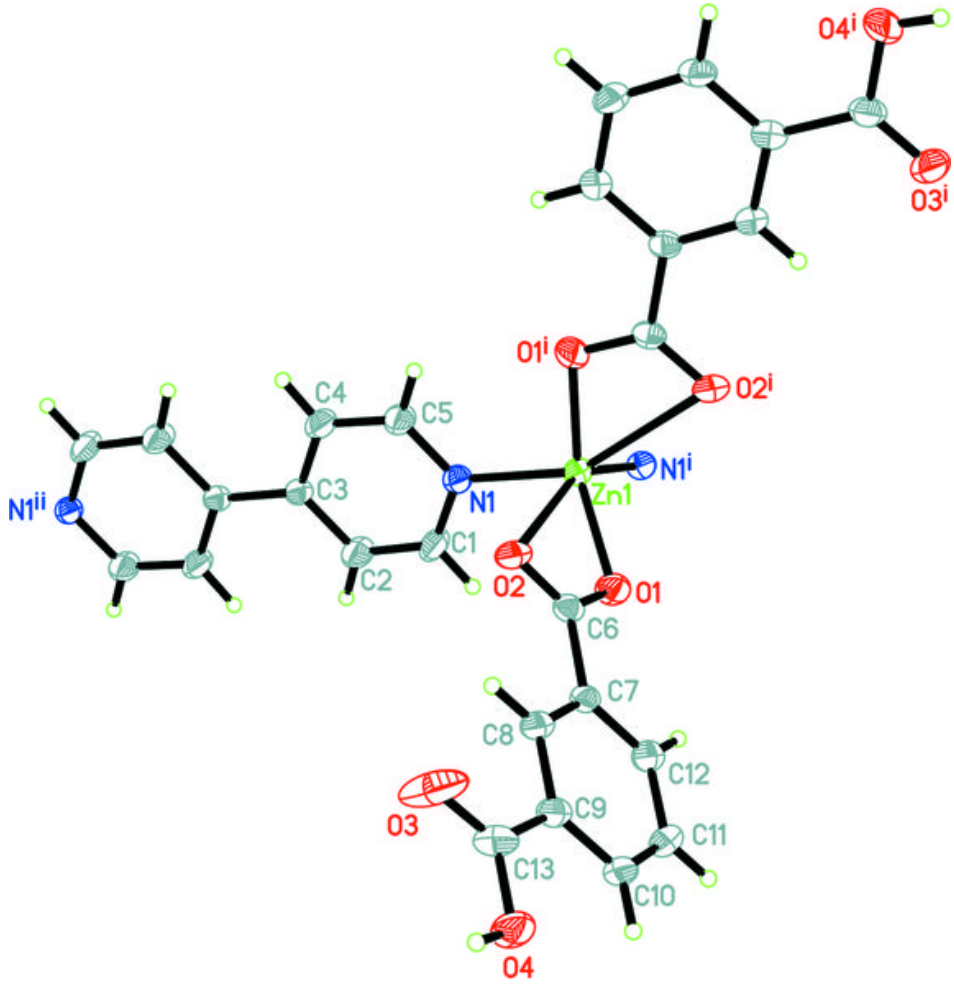
O4i
O3i
O1i
O2i
C4
C5
N1i
C3
N1ii
N1
Zn1
C1
C2
O2
O1
C6
C7
C8
C12
O3
C9
C11
C13
C10
O4

Fig. 2