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Poly[[(1,10-phenanthroline-κ^2N,N')zinc]-μ-2,5-bis(allyloxy)terephthalato-$\kappa^2O^1:O^4$]

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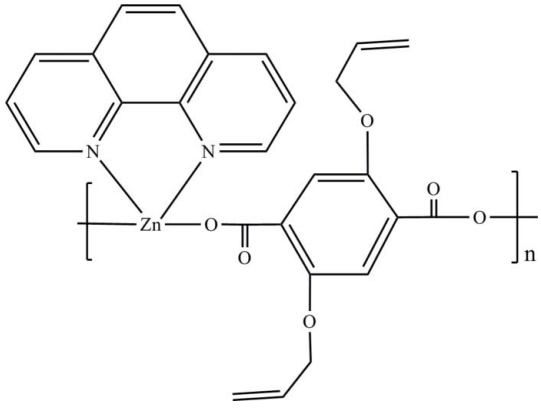
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.078; data-to-parameter ratio = 16.0.

The title compound, $[Zn(C_{14}H_{12}O_6)(C_{12}H_8N_2)]_n$, is a coordination polymer forming one-dimensional infinite zigzag chains along $[10\bar{1}]$ by interconnection of Zn^{II} atoms by 2,5-bis(allyloxy)terephthalate anions *via* the carboxylate groups. The Zn^{II} atom is located on a twofold axis and is in a distorted tetrahedral coordination formed by the two carboxylate O atoms [Zn—O = 1.9647 (12) Å] and two phenanthroline N atoms [Zn—N = 2.0949 (14) Å].

Related literature

Some other low-dimensional Zn^{II} complexes based on different organic carboxylic acids are described by Zhou *et al.* (2009). For the preparation of 2,5-bis(allyloxy)terephthalic acid, see: Kenichiro *et al.* (1998).



Experimental

Crystal data

$[Zn(C_{14}H_{12}O_6)(C_{12}H_8N_2)]$
M_r = 521.81
Monoclinic, $C2/c$
a = 21.428 (10) Å
b = 9.458 (4) Å
c = 12.897 (6) Å
β = 118.462 (5)°
V = 2297.9 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 293 K
0.25 × 0.23 × 0.22 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.768, T_{max} = 0.792
8294 measured reflections
2546 independent reflections
2325 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
Standard reflections: 0

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.078
S = 1.04
2546 reflections
159 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; 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: VN2012).

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supporting information

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Poly[[(1,10-phenanthroline-κ^2N,N')zinc]-μ-2,5-bis(allyloxy)terephthalato-$\kappa^2O^1:O^4$]

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S1. Experimental

2,5-Bis(allyloxy)terephthalic acid was prepared according to the literature (Kenichiro *et al.*, 1998). Other chemicals were used as purchased. $Zn(NO_3)_26(H_2O)$ (8.9 mg, 0.03 mmol), 1,10-phenanthroline (1.98 mg, 0.01 mmol) and 2 ,5-bis(allyloxy)terephthalic acid (2.48 mg, 0.01 mmol) were added to the 15 ml N, *N*-dimethylacetamide. After stirring at room temperature for 1 h, the solution was kept at 140 °C for 3 days. Crystallization yielded pink crystals suitable for X-ray diffraction analysis (yield 2.25 mg, 39%).

S2. Refinement

The methylene H atoms were placed in calculated positions with a C—H bond distance of 0.97 Å of the carrier atom, and the other C—H distance were placed at 0.93 Å. U_{iso}(H) was set at 1.2U_{eq} of the carrier atom. Two reflections have been omitted from the refinement as they were most probably partially affected by the beamstop.

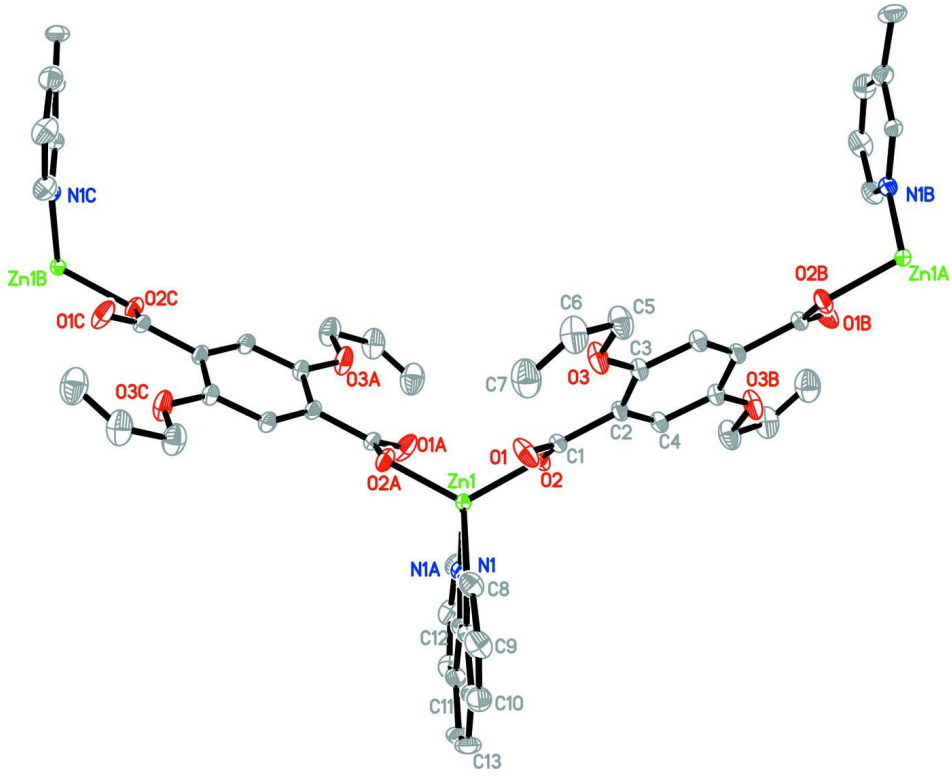

Figure 1

Atom numbering scheme for the title compound with displacement ellipsoids shown at the 30% probability level. [symmetry codes: A, 2 - *x*, *y*, 1.5 - *z*; B, 1.5 - *x*, 0.5 - *y*,1 - *z*; C, 1/2 + *x*, 0.5 - *y*, 1/2 + *z*]

Poly[[(1,10-phenanthroline-κ^2N,N')zinc]-μ-2,5- bis(allyloxy)terephthalato-κ^2O^1:O^4]

Crystal data

$[Zn(C_{14}H_{12}O_6)(C_{12}H_8N_2)]$
M_r = 521.81
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 21.428 (10) Å
b = 9.458 (4) Å
c = 12.897 (6) Å
β = 118.462 (5)°
V = 2297.9 (18) Å^3
Z = 4
F(000) = 1072
D_x = 1.508 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 80 reflections
θ = 2.4–27.2°
μ = 1.12 mm^{-1}
T = 293 K
Block, pink
0.25 × 0.23 × 0.22 mm

Data collection

Bruker P4
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
T_{min} = 0.768, T_{max} = 0.792
8294 measured reflections
2546 independent reflections
2325 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.5°, θ_{min} = 3.9°
h = −27→27
k = −12→7
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.078$
$S = 1.04$
2546 reflections
159 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
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.943P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	1.0000	0.52903 (2)	0.7500	0.02792 (10)
O1	0.89786 (8)	0.40767 (17)	0.77262 (12)	0.0557 (4)
O2	0.91910 (6)	0.43004 (14)	0.62292 (11)	0.0391 (3)
O3	0.80413 (7)	0.19659 (16)	0.73891 (11)	0.0514 (4)
N1	0.97095 (7)	0.69874 (13)	0.82237 (11)	0.0301 (3)
C1	0.88075 (8)	0.38949 (16)	0.66788 (14)	0.0336 (3)
C2	0.81280 (8)	0.31540 (16)	0.58400 (14)	0.0312 (3)
C3	0.77669 (8)	0.22152 (18)	0.62095 (14)	0.0337 (3)
C4	0.78541 (8)	0.34259 (17)	0.46410 (15)	0.0345 (3)
H4	0.8092	0.4055	0.4398	0.041*
C5	0.76293 (11)	0.1225 (3)	0.78059 (18)	0.0574 (5)
H5A	0.7644	0.0218	0.7674	0.069*
H5B	0.7139	0.1533	0.7381	0.069*
C6	0.79184 (12)	0.1506 (3)	0.90851 (19)	0.0650 (6)
H6	0.7738	0.0967	0.9484	0.078*
C7	0.83955 (14)	0.2426 (3)	0.9693 (2)	0.0753 (7)
H7A	0.8592	0.2989	0.9331	0.090*
H7B	0.8545	0.2528	1.0494	0.090*
C8	0.94114 (9)	0.6966 (2)	0.89252 (16)	0.0409 (4)
H8	0.9341	0.6100	0.9195	0.049*
C9	0.92019 (11)	0.8196 (2)	0.92674 (18)	0.0503 (5)
H9	0.8989	0.8143	0.9748	0.060*
C10	0.93107 (11)	0.9478 (2)	0.88954 (18)	0.0482 (5)
H10	0.9163	1.0302	0.9108	0.058*
C11	0.96472 (10)	0.95499 (17)	0.81881 (15)	0.0390 (4)

C12	0.98315 (8)	0.82583 (15)	0.78693 (13)	0.0290 (3)
C13	0.98266 (11)	1.0847 (2)	0.78170 (17)	0.0508 (5)
H13	0.9700	1.1703	0.8020	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02088 (14)	0.02229 (15)	0.03263 (15)	0.000	0.00630 (10)	0.000
O1	0.0577 (8)	0.0624 (9)	0.0399 (7)	−0.0299 (7)	0.0174 (6)	−0.0169 (6)
O2	0.0269 (5)	0.0430 (6)	0.0418 (6)	−0.0118 (5)	0.0118 (5)	−0.0097 (5)
O3	0.0367 (7)	0.0751 (10)	0.0331 (6)	−0.0212 (6)	0.0091 (5)	0.0021 (6)
N1	0.0270 (6)	0.0291 (6)	0.0329 (6)	−0.0017 (5)	0.0132 (5)	−0.0011 (5)
C1	0.0248 (7)	0.0271 (8)	0.0398 (8)	−0.0029 (6)	0.0081 (6)	−0.0056 (6)
C2	0.0214 (7)	0.0311 (8)	0.0365 (8)	−0.0030 (5)	0.0101 (6)	−0.0066 (6)
C3	0.0246 (7)	0.0370 (8)	0.0344 (8)	−0.0036 (6)	0.0099 (6)	−0.0026 (6)
C4	0.0252 (7)	0.0353 (8)	0.0393 (8)	−0.0064 (6)	0.0124 (6)	−0.0027 (6)
C5	0.0450 (11)	0.0793 (15)	0.0469 (11)	−0.0162 (10)	0.0210 (9)	0.0023 (10)
C6	0.0535 (12)	0.0975 (19)	0.0473 (11)	−0.0056 (12)	0.0266 (10)	0.0018 (12)
C7	0.0639 (15)	0.103 (2)	0.0546 (13)	−0.0002 (14)	0.0251 (12)	−0.0175 (14)
C8	0.0395 (9)	0.0452 (10)	0.0427 (9)	−0.0084 (7)	0.0235 (8)	−0.0055 (7)
C9	0.0469 (10)	0.0625 (13)	0.0518 (11)	−0.0080 (9)	0.0320 (9)	−0.0180 (9)
C10	0.0451 (10)	0.0499 (11)	0.0482 (10)	0.0069 (8)	0.0211 (9)	−0.0151 (8)
C11	0.0418 (9)	0.0318 (9)	0.0348 (8)	0.0056 (7)	0.0113 (7)	−0.0054 (6)
C12	0.0271 (7)	0.0263 (7)	0.0275 (7)	0.0009 (5)	0.0082 (6)	−0.0016 (5)
C13	0.0718 (14)	0.0241 (8)	0.0441 (10)	0.0068 (8)	0.0175 (9)	−0.0022 (7)

Geometric parameters (Å, º)

Zn1—O2	1.9647 (12)	C5—H5A	0.9700
Zn1—O2^{i}	1.9647 (12)	C5—H5B	0.9700
Zn1—N1	2.0949 (14)	C6—C7	1.285 (4)
Zn1—N1^{i}	2.0950 (14)	C6—H6	0.9300
O1—C1	1.232 (2)	C7—H7A	0.9300
O2—C1	1.270 (2)	C7—H7B	0.9300
O3—C3	1.365 (2)	C8—C9	1.392 (3)
O3—C5	1.418 (2)	C8—H8	0.9300
N1—C8	1.333 (2)	C9—C10	1.365 (3)
N1—C12	1.355 (2)	C9—H9	0.9300
C1—C2	1.510 (2)	C10—C11	1.408 (3)
C2—C4	1.392 (2)	C10—H10	0.9300
C2—C3	1.402 (2)	C11—C12	1.404 (2)
C3—C4^{ii}	1.397 (2)	C11—C13	1.434 (3)
C4—C3^{ii}	1.397 (2)	C12—C12^{i}	1.444 (3)
C4—H4	0.9300	C13—C13^{i}	1.342 (4)
C5—C6	1.484 (3)	C13—H13	0.9300
O2—Zn1—O2^{i}	123.08 (8)	C6—C5—H5B	109.9
O2—Zn1—N1	113.91 (6)	H5A—C5—H5B	108.3

O2^{i}—Zn1—N1	108.96 (6)	C7—C6—C5	126.0 (2)
O2—Zn1—N1^{i}	108.96 (6)	C7—C6—H6	117.0
O2^{i}—Zn1—N1^{i}	113.91 (6)	C5—C6—H6	117.0
N1—Zn1—N1^{i}	79.98 (8)	C6—C7—H7A	120.0
C1—O2—Zn1	105.59 (11)	C6—C7—H7B	120.0
C3—O3—C5	119.50 (14)	H7A—C7—H7B	120.0
C8—N1—C12	118.32 (14)	N1—C8—C9	122.23 (17)
C8—N1—Zn1	129.09 (11)	N1—C8—H8	118.9
C12—N1—Zn1	112.55 (10)	C9—C8—H8	118.9
O1—C1—O2	122.65 (14)	C10—C9—C8	119.77 (16)
O1—C1—C2	122.14 (15)	C10—C9—H9	120.1
O2—C1—C2	115.21 (14)	C8—C9—H9	120.1
C4—C2—C3	119.07 (14)	C9—C10—C11	119.75 (16)
C4—C2—C1	117.55 (14)	C9—C10—H10	120.1
C3—C2—C1	123.39 (15)	C11—C10—H10	120.1
O3—C3—C4^{ii}	122.92 (15)	C12—C11—C10	116.75 (16)
O3—C3—C2	118.29 (14)	C12—C11—C13	119.27 (17)
C4^{ii}—C3—C2	118.79 (15)	C10—C11—C13	123.96 (16)
C2—C4—C3^{ii}	122.14 (15)	N1—C12—C11	123.14 (14)
C2—C4—H4	118.9	N1—C12—C12^{i}	117.39 (8)
C3^{ii}—C4—H4	118.9	C11—C12—C12^{i}	119.47 (10)
O3—C5—C6	109.10 (18)	C13^{i}—C13—C11	121.18 (11)
O3—C5—H5A	109.9	C13^{i}—C13—H13	119.4
C6—C5—H5A	109.9	C11—C13—H13	119.4
O3—C5—H5B	109.9		

O2^{i}—Zn1—O2—C1	78.15 (10)	C3—C2—C4—C3^{ii}	−0.5 (3)
N1—Zn1—O2—C1	−57.33 (12)	C1—C2—C4—C3^{ii}	179.32 (15)
N1^{i}—Zn1—O2—C1	−144.52 (10)	C3—O3—C5—C6	−160.82 (19)
O2—Zn1—N1—C8	72.39 (16)	O3—C5—C6—C7	9.4 (4)
O2^{i}—Zn1—N1—C8	−69.20 (15)	C12—N1—C8—C9	2.2 (3)
N1^{i}—Zn1—N1—C8	178.81 (18)	Zn1—N1—C8—C9	−175.24 (14)
O2—Zn1—N1—C12	−105.20 (11)	N1—C8—C9—C10	−1.0 (3)
O2^{i}—Zn1—N1—C12	113.21 (11)	C8—C9—C10—C11	−1.3 (3)
N1^{i}—Zn1—N1—C12	1.21 (7)	C9—C10—C11—C12	2.2 (3)
Zn1—O2—C1—O1	−3.4 (2)	C9—C10—C11—C13	−175.80 (19)
Zn1—O2—C1—C2	177.38 (10)	C8—N1—C12—C11	−1.2 (2)
O1—C1—C2—C4	157.66 (17)	Zn1—N1—C12—C11	176.68 (12)
O2—C1—C2—C4	−23.1 (2)	C8—N1—C12—C12^{i}	178.70 (17)
O1—C1—C2—C3	−22.5 (2)	Zn1—N1—C12—C12^{i}	−3.4 (2)
O2—C1—C2—C3	156.76 (15)	C10—C11—C12—N1	−1.0 (2)
C5—O3—C3—C4^{ii}	−11.2 (3)	C13—C11—C12—N1	177.11 (15)
C5—O3—C3—C2	169.03 (18)	C10—C11—C12—C12^{i}	179.11 (18)
C4—C2—C3—O3	−179.70 (15)	C13—C11—C12—C12^{i}	−2.8 (3)
C1—C2—C3—O3	0.5 (2)	C12—C11—C13—C13^{i}	−0.7 (3)

C4—C2—C3—C4^{ii}	0.5 (3)	C10—C11—C13—C13^{i}	177.2 (2)
C1—C2—C3—C4^{ii}	−179.32 (14)		

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