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catena-Poly[[$(1,10\text{-phenanthroline-}\kappa^2\text{N,N'})\text{zinc}]$ - μ -furan-2,5-dicarboxylato- $\kappa^4\text{O}^2,\text{O}^2':\text{O}^5,\text{O}^5'$]

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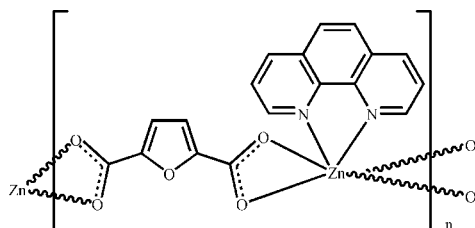
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Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$; R factor = 0.055; wR factor = 0.121; data-to-parameter ratio = 15.7.

In the title coordination polymer, $[\text{Zn}(\text{C}_6\text{H}_2\text{O}_5)(\text{C}_{12}\text{H}_8\text{N}_2)]_n$, an infinite chain is formed along $[010]$ by linking the chelated $\{\text{Zn}(\text{phen})\}$ entities (phen is 1,10-phenanthroline) with two carboxylate groups of the furan-2,5-dicarboxylate ligand. The Zn^{II} atom shows trigonal-prismatic coordination.

Related literature

For related structures, see: Li, Gao *et al.* (2012); Li, Xu *et al.* (2012).



Experimental

Crystal data

$[\text{Zn}(\text{C}_6\text{H}_2\text{O}_5)(\text{C}_{12}\text{H}_8\text{N}_2)]$

$M_r = 399.67$

Monoclinic, $P2_1/c$
 $a = 5.8725(10)\text{ \AA}$
 $b = 15.013(3)\text{ \AA}$
 $c = 19.241(8)\text{ \AA}$
 $\beta = 104.42(3)^\circ$
 $V = 1642.9(8)\text{ \AA}^3$

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.53\text{ mm}^{-1}$
 $T = 293\text{ K}$
 $0.16 \times 0.13 \times 0.12\text{ mm}$

Data collection

Rigaku R-Axis RAPID
 diffractometer
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.792$, $T_{\text{max}} = 0.838$

14467 measured reflections
 3688 independent reflections
 2166 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.066$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.121$
 $S = 1.04$
 3688 reflections
 235 parameters

156 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.37\text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.37\text{ e \AA}^{-3}$

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXL97*.

This project was sponsored by the Scientific Research Foundation for the Returned Overseas Team, Chinese Education Ministry.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5269).

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supporting information

Acta Cryst. (2012). E68, m750 [doi:10.1107/S1600536812019836]

***catena*-Poly[[*(1,10-phenanthroline- κ^2 N,N')*zinc]- μ -furan-2,5-dicarboxylato- κ^4 O²,O^{2'}:O⁵,O^{5'}]**

Ya-Feng Li, Yue Xu, Xiao-Lin Qin, Wen-Yuan Gao and Yue Gao

S1. Comment

Recently, we utilized furan-2,5-dicarboxylic acid as the ligand to construct the MOFs (Li, Gao *et al.* 2012; Li, Xu *et al.*, 2012). In this work, a chainlike compound, $[\text{Zn}(\text{C}_{12}\text{H}_8\text{N}_2)(\text{C}_6\text{H}_2\text{O}_5)]_n$ (I), is reported.

The asymmetric unit consists of one Zn cation, one furan-2,5-dicarboxylate anion and one $\text{C}_{12}\text{H}_8\text{N}_2$ (Fig. 1). The Zn cation is coordinated by four carboxylate O atoms, two nitrogen of one $\text{C}_{12}\text{H}_8\text{N}_2$, exhibiting trigonal prismatic coordination. The furan-2,5-dicarboxylate shows a $\mu_2:\eta^1,\eta^1;\eta^1,\eta^1$ coordinating mode. The dihedral angles of two furan rings *versus* $\text{C}_6\text{H}_2\text{O}_5$ ring and two furan rings, which are coordinated to the same Zn cation, are 52.06 (12)°, 62.18 (11)° and 88.27 (12)°, respectively.

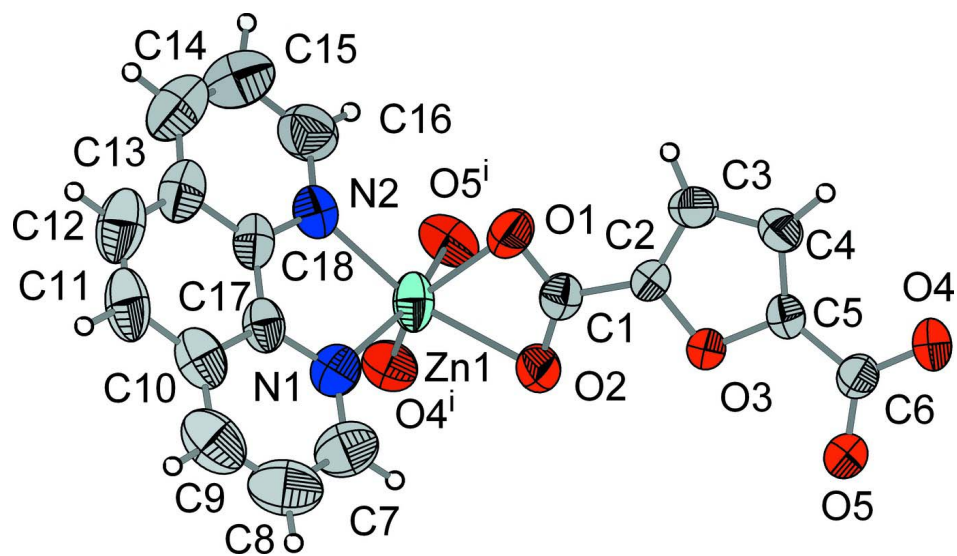
The Zn cations are linked by two carboxylate of furan-2,5-dicarboxylate to give rise to an infinite chain (Fig. 2). The adjacent chains are piled up along [100] through π - π interactions between $\text{C}_{12}\text{H}_8\text{N}_2$ molecules of different chains. van der Waals forces exist between the layers (Fig. 3).

S2. Experimental

Furan-2,5-dicarboxylic acid (0.0156 g, 0.10 mmol), $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.0298 g, 0.10 mmol), and $\text{C}_{12}\text{H}_8\text{N}_2$ (0.0198, 0.11 mmol) were dissolved in DMF (5 ml, 48 mmol) under stirring. The mixture with molar ratio of 1 (furan-2,5-dicarboxylic acid): 1 ($\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$): 1.1 ($\text{C}_{12}\text{H}_8\text{N}_2$): 480 DMI was heated under 120°C for 2 days. Colorless blocks were collected as a single phase.

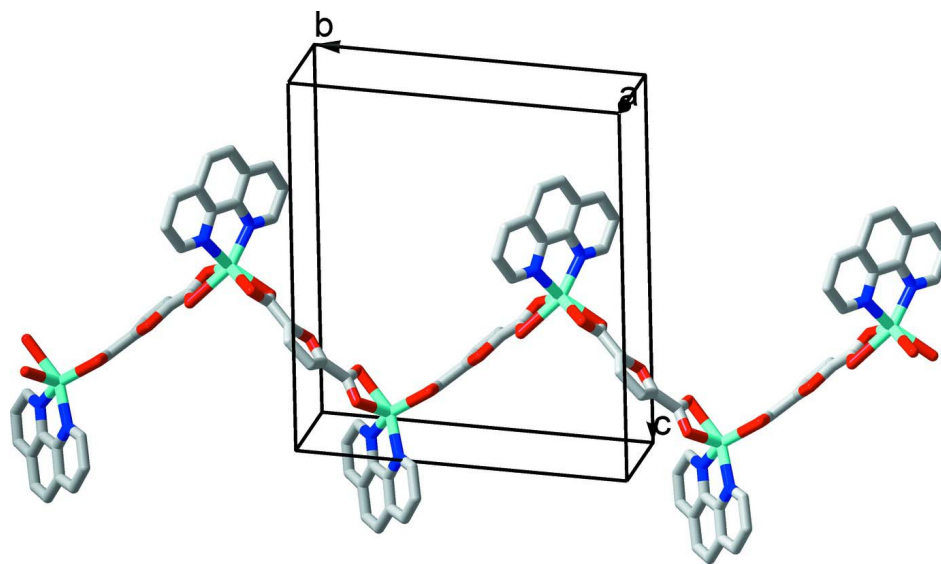
S3. Refinement

The carbon H-atoms were placed in calculated positions (C—H (furan ring and phen ring) = 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

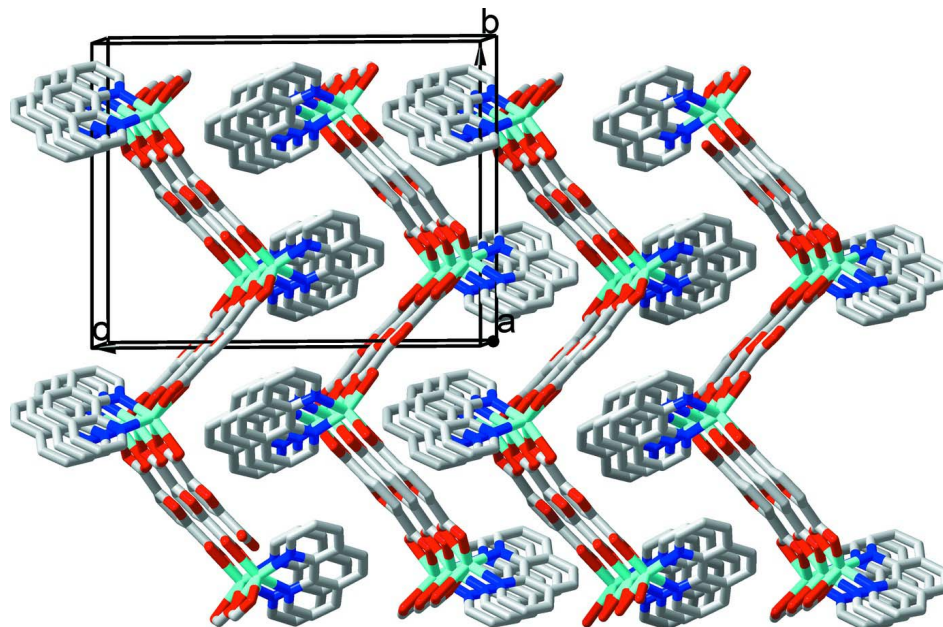
**Figure 1**

The unit cell of (I), showing the atomic labelling scheme and displacement ellipsoids at the 50% probability level.

[Symmetry codes: (i) $1 - x, -0.5 + y, 0.5 - z.$]

**Figure 2**

The stick plot of (I), displaying the infinite chain along $[010]$ direction formed by linking the Zn with two carboxyls of furan-2,5-dicarboxylate.

**Figure 3**

The ball-stick packing diagram of (I). The adjacent chains are piled up along [100] through π - π interactions between $C_{12}H_8N_2$ molecules of different chains.

catena-Poly[[**(1,10-phenanthroline- κ^2N,N')zinc**]- μ -furan-2,5-dicarboxylato- $\kappa^4O^2,O^2':O^5,O^5'$]

Crystal data

[Zn(C₆H₂O₅)(C₁₂H₈N₂)]

$M_r = 399.67$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 5.8725$ (10) Å

$b = 15.013$ (3) Å

$c = 19.241$ (8) Å

$\beta = 104.42$ (3)°

$V = 1642.9$ (8) Å³

$Z = 4$

$F(000) = 808$

$D_x = 1.616$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2000 reflections

$\theta = 3.5$ – 27.5 °

$\mu = 1.53$ mm⁻¹

$T = 293$ K

Block, colorless

$0.16 \times 0.13 \times 0.12$ mm

Data collection

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.00 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.792$, $T_{\max} = 0.838$

14467 measured reflections

3688 independent reflections

2166 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.066$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 3.5$ °

$h = -7 \rightarrow 7$

$k = -19 \rightarrow 19$

$l = -24 \rightarrow 24$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.055$ $wR(F^2) = 0.121$ $S = 1.04$

3688 reflections

235 parameters

156 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 1.7497P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.37 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$ *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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.35240 (10)	0.25875 (4)	0.08732 (3)	0.0611 (2)
O1	0.6391 (5)	0.3452 (2)	0.11677 (17)	0.0704 (9)
O2	0.3330 (5)	0.3794 (2)	0.15596 (16)	0.0662 (9)
O3	0.5760 (4)	0.51458 (17)	0.23919 (13)	0.0448 (6)
O4	0.8463 (5)	0.6748 (2)	0.36985 (15)	0.0636 (8)
O5	0.4722 (5)	0.6501 (2)	0.32328 (16)	0.0686 (9)
N1	0.1045 (7)	0.3030 (3)	-0.00407 (19)	0.0614 (9)
N2	0.4670 (6)	0.1904 (3)	0.00778 (18)	0.0606 (10)
C1	0.5395 (7)	0.3928 (3)	0.1538 (2)	0.0503 (10)
C2	0.6835 (6)	0.4618 (3)	0.1988 (2)	0.0437 (9)
C3	0.9155 (7)	0.4798 (3)	0.2139 (2)	0.0565 (11)
H3	1.0259	0.4532	0.1933	0.068*
C4	0.9582 (7)	0.5469 (3)	0.2670 (2)	0.0544 (11)
H4	1.1028	0.5724	0.2886	0.065*
C5	0.7492 (6)	0.5669 (3)	0.28057 (19)	0.0444 (9)
C6	0.6828 (7)	0.6332 (3)	0.3271 (2)	0.0484 (10)
C7	-0.0749 (10)	0.3570 (4)	-0.0079 (3)	0.0833 (16)
H7	-0.0992	0.3816	0.0340	0.100*
C8	-0.2319 (10)	0.3783 (4)	-0.0746 (4)	0.0997 (19)
H8	-0.3571	0.4170	-0.0767	0.120*
C9	-0.1958 (10)	0.3409 (4)	-0.1357 (3)	0.0943 (19)
H9	-0.2991	0.3539	-0.1797	0.113*
C10	-0.0086 (9)	0.2843 (4)	-0.1334 (3)	0.0711 (14)
C11	0.0446 (11)	0.2424 (4)	-0.1952 (2)	0.0849 (17)
H11	-0.0532	0.2524	-0.2405	0.102*

C12	0.2292 (12)	0.1902 (4)	-0.1882 (3)	0.0942 (18)
H12	0.2631	0.1667	-0.2293	0.113*
C13	0.3771 (10)	0.1689 (4)	-0.1206 (3)	0.0757 (14)
C14	0.5738 (13)	0.1132 (5)	-0.1103 (4)	0.107 (2)
H14	0.6125	0.0874	-0.1497	0.129*
C15	0.7072 (12)	0.0968 (5)	-0.0442 (4)	0.112 (2)
H15	0.8534	0.0666	-0.0303	0.135*
C16	0.6508 (9)	0.1371 (4)	0.0144 (3)	0.0880 (17)
H16	0.7459	0.1262	0.0601	0.106*
C17	0.1378 (7)	0.2662 (3)	-0.0654 (2)	0.0542 (11)
C18	0.3306 (8)	0.2074 (3)	-0.0590 (2)	0.0574 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0831 (4)	0.0578 (3)	0.0401 (3)	-0.0158 (3)	0.0106 (2)	-0.0017 (2)
O1	0.0689 (19)	0.066 (2)	0.082 (2)	-0.0051 (16)	0.0292 (17)	-0.0279 (17)
O2	0.0538 (18)	0.079 (2)	0.068 (2)	-0.0167 (15)	0.0205 (15)	-0.0220 (16)
O3	0.0420 (14)	0.0468 (16)	0.0452 (14)	-0.0007 (11)	0.0099 (11)	-0.0086 (12)
O4	0.0610 (18)	0.064 (2)	0.0605 (18)	-0.0104 (15)	0.0055 (14)	-0.0212 (15)
O5	0.0543 (18)	0.082 (2)	0.0668 (19)	0.0076 (16)	0.0109 (15)	-0.0272 (17)
N1	0.071 (2)	0.061 (2)	0.054 (2)	0.0000 (19)	0.0195 (18)	0.0055 (18)
N2	0.062 (2)	0.063 (2)	0.053 (2)	-0.0052 (19)	0.0054 (18)	-0.0020 (18)
C1	0.056 (2)	0.048 (2)	0.045 (2)	0.0009 (19)	0.0110 (19)	-0.0012 (18)
C2	0.046 (2)	0.043 (2)	0.044 (2)	0.0021 (16)	0.0130 (17)	-0.0064 (17)
C3	0.045 (2)	0.058 (3)	0.068 (3)	0.0036 (19)	0.018 (2)	-0.004 (2)
C4	0.042 (2)	0.055 (3)	0.063 (3)	-0.0041 (18)	0.008 (2)	-0.007 (2)
C5	0.045 (2)	0.042 (2)	0.043 (2)	-0.0048 (17)	0.0061 (17)	-0.0030 (16)
C6	0.052 (2)	0.047 (2)	0.045 (2)	0.0031 (18)	0.0118 (19)	-0.0031 (17)
C7	0.092 (4)	0.085 (4)	0.083 (4)	0.008 (3)	0.040 (3)	0.012 (3)
C8	0.083 (4)	0.101 (5)	0.117 (5)	0.020 (3)	0.028 (4)	0.033 (4)
C9	0.082 (4)	0.109 (5)	0.080 (4)	-0.005 (3)	-0.002 (3)	0.031 (3)
C10	0.075 (3)	0.073 (3)	0.057 (3)	-0.015 (3)	0.002 (2)	0.016 (2)
C11	0.113 (4)	0.096 (4)	0.037 (2)	-0.030 (3)	0.002 (3)	0.001 (3)
C12	0.141 (5)	0.094 (4)	0.051 (3)	-0.019 (4)	0.030 (3)	-0.010 (3)
C13	0.101 (4)	0.064 (3)	0.065 (3)	-0.014 (3)	0.027 (3)	-0.012 (2)
C14	0.137 (5)	0.091 (4)	0.108 (5)	0.007 (4)	0.056 (4)	-0.022 (4)
C15	0.110 (5)	0.107 (5)	0.129 (5)	0.028 (4)	0.046 (4)	-0.001 (4)
C16	0.076 (3)	0.086 (4)	0.096 (4)	0.009 (3)	0.009 (3)	0.003 (3)
C17	0.065 (3)	0.057 (3)	0.039 (2)	-0.014 (2)	0.0092 (19)	0.0027 (18)
C18	0.072 (3)	0.056 (3)	0.045 (2)	-0.016 (2)	0.015 (2)	-0.0059 (19)

Geometric parameters (Å, °)

Zn1—O4 ⁱ	2.027 (3)	C5—C6	1.455 (5)
Zn1—N2	2.089 (4)	C7—C8	1.418 (7)
Zn1—O1	2.090 (3)	C7—H7	0.9300
Zn1—N1	2.092 (4)	C8—C9	1.367 (8)

Zn1—O2	2.261 (3)	C8—H8	0.9300
Zn1—O5 ⁱ	2.408 (3)	C9—C10	1.381 (8)
O1—C1	1.252 (5)	C9—H9	0.9300
O2—C1	1.240 (5)	C10—C17	1.401 (6)
O3—C2	1.369 (4)	C10—C11	1.447 (7)
O3—C5	1.372 (4)	C11—C12	1.317 (8)
O4—C6	1.263 (4)	C11—H11	0.9300
O5—C6	1.246 (4)	C12—C13	1.410 (7)
N1—C7	1.316 (6)	C12—H12	0.9300
N1—C17	1.361 (5)	C13—C14	1.399 (8)
N2—C16	1.324 (6)	C13—C18	1.405 (6)
N2—C18	1.358 (5)	C14—C15	1.341 (9)
C1—C2	1.475 (5)	C14—H14	0.9300
C2—C3	1.347 (5)	C15—C16	1.390 (8)
C3—C4	1.413 (6)	C15—H15	0.9487
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.351 (5)	C17—C18	1.416 (6)
C4—H4	0.9300		
O4 ⁱ —Zn1—N2	108.37 (14)	C4—C3—H3	126.7
O4 ⁱ —Zn1—O1	141.51 (13)	C5—C4—C3	107.0 (4)
N2—Zn1—O1	96.85 (13)	C5—C4—H4	126.5
O4 ⁱ —Zn1—N1	100.88 (13)	C3—C4—H4	126.5
N2—Zn1—N1	79.86 (15)	C4—C5—O3	109.8 (3)
O1—Zn1—N1	112.06 (14)	C4—C5—C6	131.8 (4)
O4 ⁱ —Zn1—O2	98.21 (12)	O3—C5—C6	118.4 (3)
N2—Zn1—O2	153.40 (13)	O5—C6—O4	121.3 (4)
O1—Zn1—O2	59.89 (11)	O5—C6—C5	121.1 (4)
N1—Zn1—O2	96.36 (14)	O4—C6—C5	117.5 (3)
O4 ⁱ —Zn1—O5 ⁱ	58.36 (10)	O5—C6—Zn1 ⁱⁱ	69.4 (2)
N2—Zn1—O5 ⁱ	91.83 (13)	O4—C6—Zn1 ⁱⁱ	51.9 (2)
O1—Zn1—O5 ⁱ	93.13 (12)	C5—C6—Zn1 ⁱⁱ	169.1 (3)
N1—Zn1—O5 ⁱ	154.14 (13)	N1—C7—C8	121.4 (5)
O2—Zn1—O5 ⁱ	101.54 (12)	N1—C7—H7	119.3
O4 ⁱ —Zn1—C1	121.27 (13)	C8—C7—H7	119.3
N2—Zn1—C1	126.34 (14)	C9—C8—C7	118.8 (6)
O1—Zn1—C1	30.16 (12)	C9—C8—H8	120.6
N1—Zn1—C1	107.51 (14)	C7—C8—H8	120.6
O2—Zn1—C1	29.78 (11)	C8—C9—C10	121.1 (5)
O5 ⁱ —Zn1—C1	97.18 (12)	C8—C9—H9	119.4
O4 ⁱ —Zn1—C6 ⁱ	29.39 (11)	C10—C9—H9	119.4
N2—Zn1—C6 ⁱ	101.69 (14)	C9—C10—C17	116.6 (5)
O1—Zn1—C6 ⁱ	118.33 (13)	C9—C10—C11	125.1 (5)
N1—Zn1—C6 ⁱ	128.86 (14)	C17—C10—C11	118.3 (5)
O2—Zn1—C6 ⁱ	101.04 (13)	C12—C11—C10	121.1 (5)
O5 ⁱ —Zn1—C6 ⁱ	28.98 (10)	C12—C11—H11	119.4
C1—Zn1—C6 ⁱ	111.29 (13)	C10—C11—H11	119.4
C1—O1—Zn1	92.8 (2)	C11—C12—C13	122.1 (6)

C1—O2—Zn1	85.3 (2)	C11—C12—H12	119.0
C2—O3—C5	106.3 (3)	C13—C12—H12	119.0
C6—O4—Zn1 ⁱⁱ	98.7 (2)	C14—C13—C18	116.9 (5)
C6—O5—Zn1 ⁱⁱ	81.6 (2)	C14—C13—C12	124.3 (6)
C7—N1—C17	119.2 (4)	C18—C13—C12	118.7 (5)
C7—N1—Zn1	128.5 (4)	C15—C14—C13	120.8 (6)
C17—N1—Zn1	112.3 (3)	C15—C14—H14	119.6
C16—N2—C18	118.7 (4)	C13—C14—H14	119.6
C16—N2—Zn1	129.0 (4)	C14—C15—C16	119.2 (6)
C18—N2—Zn1	112.3 (3)	C14—C15—H15	129.0
O2—C1—O1	121.8 (4)	C16—C15—H15	111.2
O2—C1—C2	121.1 (4)	N2—C16—C15	122.5 (6)
O1—C1—C2	117.0 (4)	N2—C16—H16	118.7
O2—C1—Zn1	64.9 (2)	C15—C16—H16	118.7
O1—C1—Zn1	57.0 (2)	N1—C17—C10	122.9 (4)
C2—C1—Zn1	170.2 (3)	N1—C17—C18	117.5 (4)
C3—C2—O3	110.2 (3)	C10—C17—C18	119.6 (4)
C3—C2—C1	132.0 (4)	N2—C18—C13	121.8 (5)
O3—C2—C1	117.5 (3)	N2—C18—C17	118.0 (4)
C2—C3—C4	106.7 (4)	C13—C18—C17	120.1 (4)
C2—C3—H3	126.7		
O4 ⁱ —Zn1—O1—C1	-59.7 (3)	O2—C1—C2—C3	168.7 (4)
N2—Zn1—O1—C1	168.9 (3)	O1—C1—C2—C3	-7.3 (7)
N1—Zn1—O1—C1	87.1 (3)	O2—C1—C2—O3	-4.5 (6)
O2—Zn1—O1—C1	2.6 (2)	O1—C1—C2—O3	179.6 (4)
O5 ⁱ —Zn1—O1—C1	-98.9 (3)	O3—C2—C3—C4	0.5 (5)
C6 ⁱ —Zn1—O1—C1	-83.9 (3)	C1—C2—C3—C4	-173.0 (4)
O4 ⁱ —Zn1—O2—C1	143.5 (2)	C2—C3—C4—C5	-0.9 (5)
N2—Zn1—O2—C1	-34.5 (4)	C3—C4—C5—O3	0.9 (5)
O1—Zn1—O2—C1	-2.6 (2)	C3—C4—C5—C6	-176.6 (4)
N1—Zn1—O2—C1	-114.5 (3)	C2—O3—C5—C4	-0.6 (4)
O5 ⁱ —Zn1—O2—C1	84.3 (3)	C2—O3—C5—C6	177.3 (3)
C6 ⁱ —Zn1—O2—C1	113.8 (3)	Zn1 ⁱⁱ —O5—C6—O4	1.0 (4)
O4 ⁱ —Zn1—N1—C7	71.3 (4)	Zn1 ⁱⁱ —O5—C6—C5	-176.7 (4)
N2—Zn1—N1—C7	178.3 (4)	Zn1 ⁱⁱ —O4—C6—O5	-1.2 (5)
O1—Zn1—N1—C7	-88.4 (4)	Zn1 ⁱⁱ —O4—C6—C5	176.6 (3)
O2—Zn1—N1—C7	-28.3 (4)	C4—C5—C6—O5	168.5 (4)
O5 ⁱ —Zn1—N1—C7	105.4 (5)	O3—C5—C6—O5	-8.9 (6)
C1—Zn1—N1—C7	-56.6 (4)	C4—C5—C6—O4	-9.3 (7)
C6 ⁱ —Zn1—N1—C7	81.4 (5)	O3—C5—C6—O4	173.3 (3)
O4 ⁱ —Zn1—N1—C17	-106.0 (3)	C4—C5—C6—Zn1 ⁱⁱ	4.8 (19)
N2—Zn1—N1—C17	1.0 (3)	O3—C5—C6—Zn1 ⁱⁱ	-172.5 (13)
O1—Zn1—N1—C17	94.3 (3)	C17—N1—C7—C8	-0.8 (7)
O2—Zn1—N1—C17	154.4 (3)	Zn1—N1—C7—C8	-178.0 (4)
O5 ⁱ —Zn1—N1—C17	-71.9 (4)	N1—C7—C8—C9	0.7 (9)
C1—Zn1—N1—C17	126.1 (3)	C7—C8—C9—C10	-0.9 (9)
C6 ⁱ —Zn1—N1—C17	-95.9 (3)	C8—C9—C10—C17	1.2 (8)

O4 ⁱ —Zn1—N2—C16	-84.1 (4)	C8—C9—C10—C11	-179.5 (5)
O1—Zn1—N2—C16	66.4 (4)	C9—C10—C11—C12	179.0 (6)
N1—Zn1—N2—C16	177.7 (4)	C17—C10—C11—C12	-1.7 (8)
O2—Zn1—N2—C16	93.7 (5)	C10—C11—C12—C13	3.3 (9)
O5 ⁱ —Zn1—N2—C16	-27.0 (4)	C11—C12—C13—C14	179.4 (6)
C1—Zn1—N2—C16	73.3 (5)	C11—C12—C13—C18	-2.5 (9)
C6 ⁱ —Zn1—N2—C16	-54.5 (4)	C18—C13—C14—C15	1.2 (9)
O4 ⁱ —Zn1—N2—C18	97.8 (3)	C12—C13—C14—C15	179.4 (6)
O1—Zn1—N2—C18	-111.7 (3)	C13—C14—C15—C16	-1.2 (11)
N1—Zn1—N2—C18	-0.4 (3)	C18—N2—C16—C15	-1.1 (8)
O2—Zn1—N2—C18	-84.3 (4)	Zn1—N2—C16—C15	-179.1 (5)
O5 ⁱ —Zn1—N2—C18	154.9 (3)	C14—C15—C16—N2	1.2 (10)
C1—Zn1—N2—C18	-104.8 (3)	C7—N1—C17—C10	1.2 (7)
C6 ⁱ —Zn1—N2—C18	127.5 (3)	Zn1—N1—C17—C10	178.8 (3)
Zn1—O2—C1—O1	4.5 (4)	C7—N1—C17—C18	-179.0 (4)
Zn1—O2—C1—C2	-171.2 (4)	Zn1—N1—C17—C18	-1.4 (5)
Zn1—O1—C1—O2	-4.9 (4)	C9—C10—C17—N1	-1.4 (7)
Zn1—O1—C1—C2	171.0 (3)	C11—C10—C17—N1	179.2 (4)
O4 ⁱ —Zn1—C1—O2	-43.5 (3)	C9—C10—C17—C18	178.9 (4)
N2—Zn1—C1—O2	161.7 (2)	C11—C10—C17—C18	-0.5 (6)
O1—Zn1—C1—O2	175.4 (4)	C16—N2—C18—C13	1.2 (7)
N1—Zn1—C1—O2	71.5 (3)	Zn1—N2—C18—C13	179.5 (3)
O5 ⁱ —Zn1—C1—O2	-100.7 (2)	C16—N2—C18—C17	-178.5 (4)
C6 ⁱ —Zn1—C1—O2	-74.5 (3)	Zn1—N2—C18—C17	-0.2 (5)
O4 ⁱ —Zn1—C1—O1	141.0 (2)	C14—C13—C18—N2	-1.2 (7)
N2—Zn1—C1—O1	-13.8 (3)	C12—C13—C18—N2	-179.5 (5)
N1—Zn1—C1—O1	-103.9 (3)	C14—C13—C18—C17	178.5 (5)
O2—Zn1—C1—O1	-175.4 (4)	C12—C13—C18—C17	0.2 (7)
O5 ⁱ —Zn1—C1—O1	83.8 (3)	N1—C17—C18—N2	1.1 (6)
C6 ⁱ —Zn1—C1—O1	110.1 (3)	C10—C17—C18—N2	-179.1 (4)
C5—O3—C2—C3	0.0 (4)	N1—C17—C18—C13	-178.6 (4)
C5—O3—C2—C1	174.6 (3)	C10—C17—C18—C13	1.2 (6)

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