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

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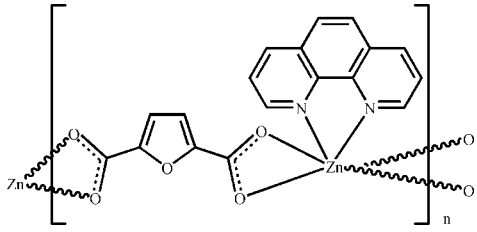
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.055; wR factor = 0.121; data-to-parameter ratio = 15.7.

In the title coordination polymer, $[Zn(C_6H_2O_5)(C_{12}H_8N_2)]_n$, an infinite chain is formed along [010] by linking the chelated {Zn(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

$[Zn(C_6H_2O_5)(C_{12}H_8N_2)]$ M_r = 399.67
Monoclinic, $P2_1/c$
a = 5.8725 (10) Å
b = 15.013 (3) Å
c = 19.241 (8) Å
β = 104.42 (3)°
V = 1642.9 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.53 mm^{-1}
T = 293 K
0.16 × 0.13 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
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_{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
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 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*.

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

References

Brandenburg, K. (2000). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Li, Y.-F., Gao, Y., Xu, Y., Qin, X. & Gao, W.-Y. (2012). *Acta Cryst.* E**68**, m445.
Li, Y.-F., Xu, Y., Qin, X.-L., Gao, W.-Y. & Gao, Y. (2012). *Acta Cryst.* E**68**, m659.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2012). E**68**, m750 [doi:10.1107/S1600536812019836]

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

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Comment

Recently, we utilized furan-2,5-dicarboxyl icacid as the ligand to constructed the MOFs (Li, Gao *et al.* 2012; Li, Xu *et al.*, 2012). In this work, a chainlike compound, $[Zn(C_{12}H_8N_2)(C_6H_2O_5)]_n$ (I), is reported.

The asymmetric unit consists of one Zn cation, one furan-2,5-dicarboxylate anion and one $C_{12}H_8N_2$ (Fig.1). The Zn cation is coordinated by four carboxylate O atoms, two nitrogen of one $C_{12}H_8N_2$, exhibiting triganol prismatic coordination. The furan-2,5-dicarboxylate shows a μ_2:η^1,η^1;η^1,η^1 coordinating mode. The dihedral angles of two furan rings *versus*. $C_6H_2O_5$ 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.

TheZn 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 $C_{12}H_8N_2$ molecules of different chains. vVan der Waals forces exist between the layers (Fig. 3).

Experimental

Furan-2,5-dicarboxylic acid (0.0156 g, 0.10 mmol), $Zn(NO_3)_2{\cdot}6H_2O$ (0.0298 g, 0.10 mmol), and $C_{12}H_8N_2$ (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-dicarboxyl acid): 1 ($Zn(NO_3)_2{\cdot}6H_2O$): 1.1 ($C_{12}H_8N_2$): 480 DMI was heated under 120°C for 2 days. Colorless blocks were collected as a single phase.

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_{iso}(H) = 1.2Ueq(C).

Computing details

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *CrystalStructure* (Rigaku/MSC, 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* (Sheldrick, 2008).

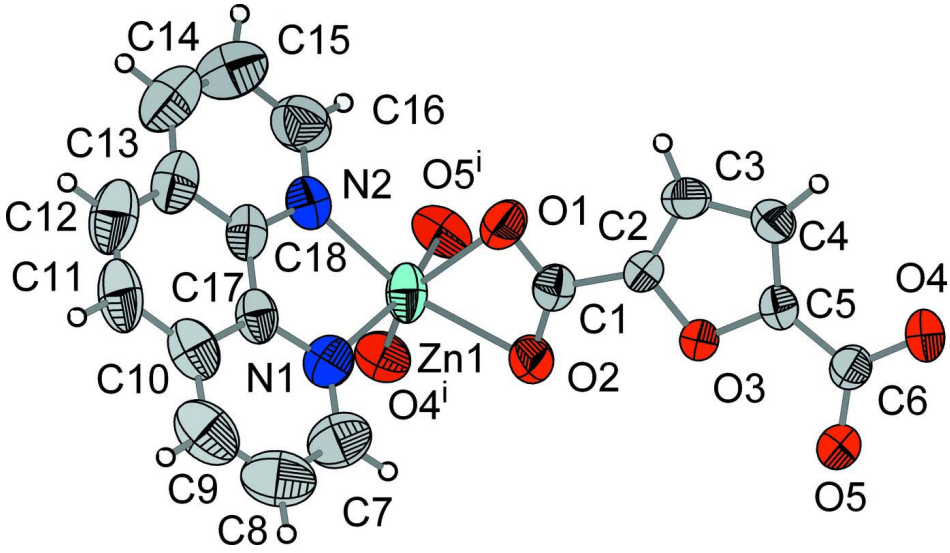

Figure 1

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*.]

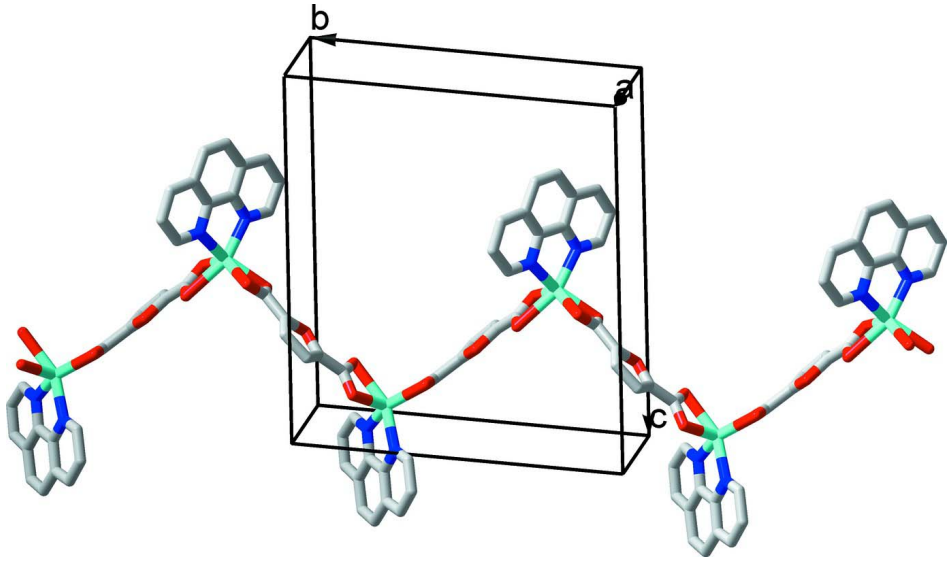

Figure 2

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.

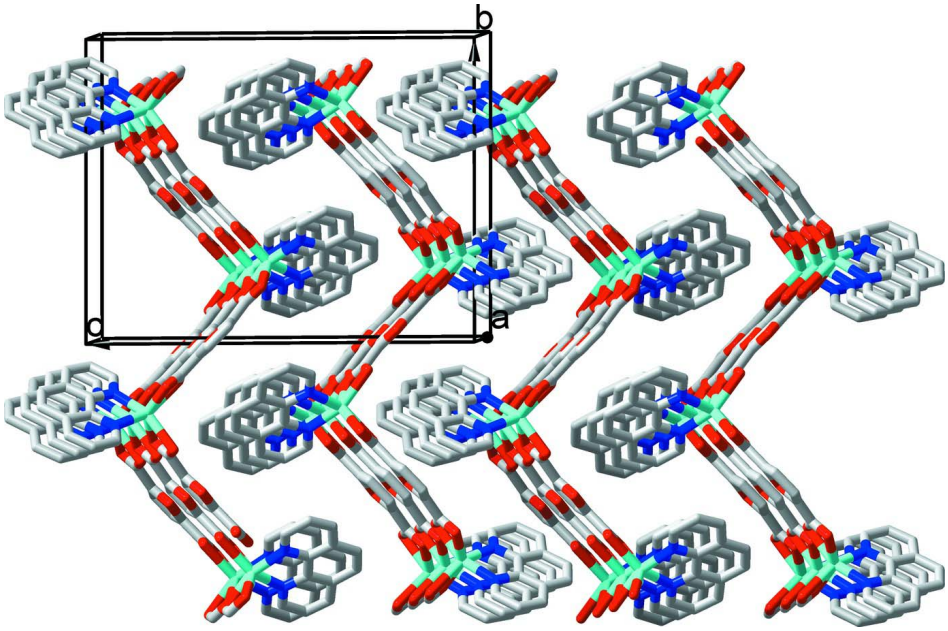

Figure 3

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.

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Crystal data

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$M_r = 399.67$
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) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.616$ 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 × 0.13 × 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 $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$
$h = -7 \rightarrow 7$
$k = -19 \rightarrow 19$
$l = -24 \rightarrow 24$

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 methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 1.7497P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ 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	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, º)

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.