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catena-Poly[[(1,10-phenanthroline)zinc]-*μ*-3-[3-(carboxylatomethoxy)phenyl]-acrylato]

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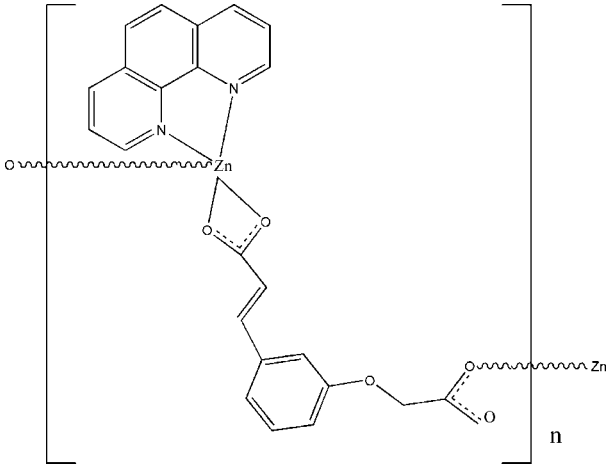
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.070; data-to-parameter ratio = 12.2.

The asymmetric unit of the title compound, $[Zn(C_{11}H_8O_5)(C_{12}H_8N_2)]_n$, is composed of a Zn^{II} ion and 3-[3-(carboxylatomethoxy)phenyl]acrylate and 1,10-phenanthroline ligands. The Zn^{II} ion adopts a distorted square-pyramidal ZnN_2O_3 coordination. The bridging mode of the dianion leads to the formation of zigzag chains parallel to [010]. Intermolecular π–π stacking interactions [centroid–centroid distance of 3.5716 (12) Å] lead to the formation of a two-dimensional network parallel to (001).

Related literature

For background to inorganic-organic hybrid materials, see: Fujita *et al.* (1994) and for their applications and topological structures, see: Comotti *et al.* (2008); Hong *et al.* (2006); Moulton & Zaworotko (2001); Swiegers & Malefeste (2000); Kaes *et al.* (2000).



Experimental

Crystal data

$[Zn(C_{11}H_8O_5)(C_{12}H_8N_2)]$
M_r = 465.75
Monoclinic, $P2_1/c$
a = 10.2744 (4) Å
b = 14.9979 (6) Å
c = 15.9060 (6) Å
β = 127.347 (2)°
V = 1948.51 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.30 mm^{-1}
T = 296 K
0.46 × 0.42 × 0.26 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.56, T_{max} = 0.71
26006 measured reflections
3430 independent reflections
2980 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.070
S = 1.02
3430 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2464).

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supplementary materials

Acta Cryst. (2012). E**68**, m882 [doi:10.1107/S1600536812024610]

catena-Poly[[(1,10-phenanthroline)zinc]-μ-3-[3-(carboxylatomethoxy)phenyl]-acrylato]

Ling Chen

Comment

In recent decades, inorganic-organic hybrid materials such as coordination complexes have attracted plenty of attention (Fujita *et al.* (1994)) due to the fact that they might have potential applications as functional solid materials in adsorption, catalysis, and ion exchange (Comotti *et al.* (2008), Hong *et al.* (2006)), at the same time that they usually present intriguing topological structures (Moulton *et al.*(2001), Swiegers *et al.*(2000),Kaes *et al.*(2000)). Herein we report one such inorganic-organic hybrid compound, [Zn *L* (phen), where *L* is 3-carboxymethoxy phenyl acrylate ($C_{11}H_8O_5$) and phen is 1,10-phenanthroline($C_{12}H_8N_2$)].

As shown in Figure 1, the strucure contains one Zn^{II} ion coordinated by two N atoms from a chelating phen and two O atoms from a chelating carboxylato group from one *L* ligand, defining the base of a distorted square pyramidal coordination; the apical site is occupied by a third O from the reamining carboxylato group of another *L* ligand which thus behaves in a $\mu_2\kappa^3$ bridging chelating mode, forming a one-dimensional zigzag chain which extends along the *b* axis (Figure 2).

In this structure, the benzene ring from a *L* ligand and an adjacent six-membered heterocycle ring of phen are nearly parallel (dihedral angle: 4.83 (10)°), affording a face-to-face intermolecular π-π stacking with an intercentroid distance of 3.5716 (12) Å. Intermolecular π-π stacking interactions lead to the formation of a two-dimensional network (Figure 3).

Experimental

A mixture of $ZnCl_2$(0.136 g,1 mmol),3-carboxymethoxy phenycl acrylic acid(0.2220 g,1 mmol) and 1,10-phenanthroline(0.0991 g,0.5 mmol) was dissolved in a 20 mL EtOH/H_2O(*v*/*v*,1:9). Then, the pH value was adjusted to 7 through the use of a 2 mol/*L* NaOH solution. The mixture was then sealed in a 25 mL stainless steel reactor and heated to 433 K for 3 days. Then the reactant mixture was cooled to room temperature at the rate of 5 degrees per hour. Evaporation of the resulting solution for a few days afforded colorless crystals of title compound.

Refinement

The carbon-bound H-atoms were positioned geometrically and included in the refinement using a riding model [C—H 0.93 Å U_{iso}(H) = 1.2U_{eq}(C)].

Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

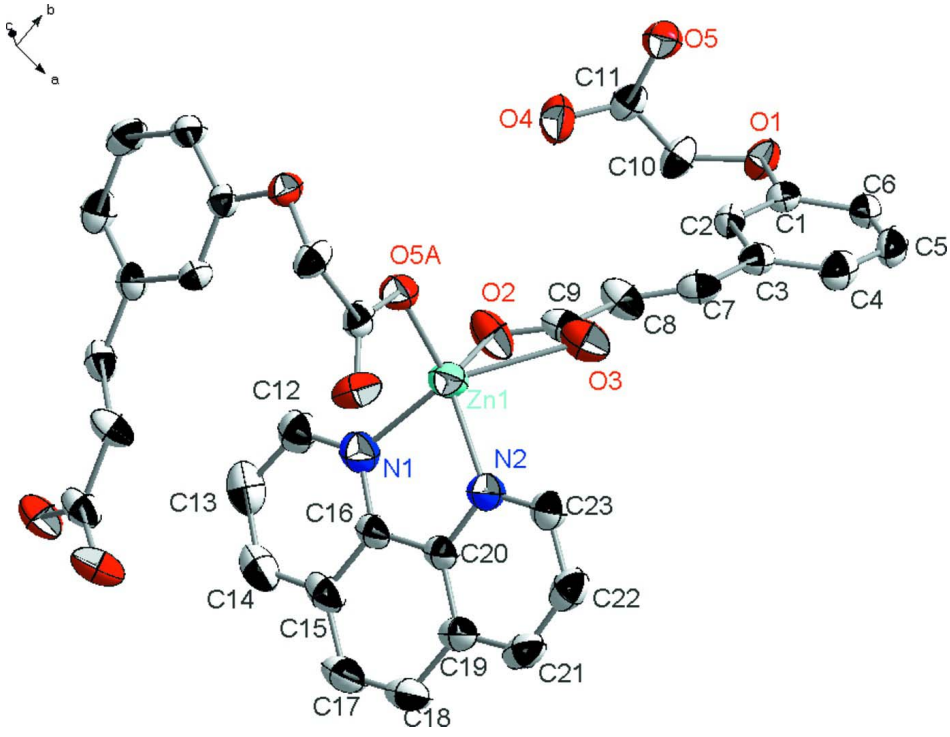

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code:(A) -*x* - 1,*y* - 1/2,-*z* + 1/2]

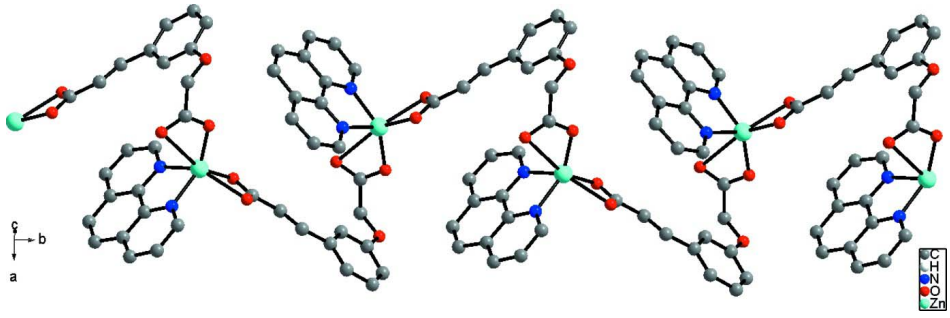

Figure 2

The one-dimensional chain structure in the title compound along the *b* axis.

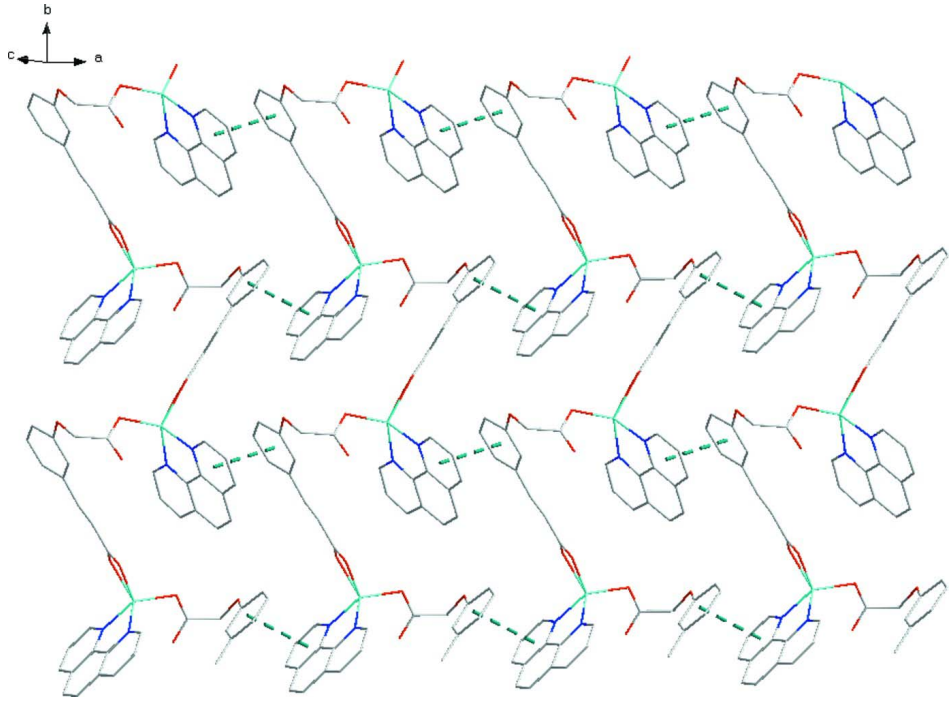

Figure 3

View of the two-dimensional supramolecular network connected by π-π stacking interactions.

catena-Poly[[(1,10-phenanthroline)zinc]-μ-3-[3-(carboxylatomethoxy)phenyl]acrylato]

Crystal data

$[Zn(C_{11}H_8O_5)(C_{12}H_8N_2)]$
$M_r = 465.75$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.2744$ (4) Å
$b = 14.9979$ (6) Å
$c = 15.9060$ (6) Å
$\beta = 127.347$ (2)°
$V = 1948.51$ (13) Å^3
$Z = 4$
$F(000) = 952$
$D_x = 1.588$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9958 reflections
$\theta = 2.1$–25.0°
$\mu = 1.30$ mm^{-1}
$T = 296$ K
Prism, colourless
0.46 × 0.42 × 0.26 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.56$, $T_{max} = 0.71$
26006 measured reflections
3430 independent reflections
2980 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -12 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.070$
$S = 1.02$
3430 reflections
280 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
$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.5701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ 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	−0.30637 (2)	−0.253939 (12)	0.368035 (16)	0.03728 (9)
O1	−0.33062 (15)	0.25494 (8)	0.04670 (10)	0.0419 (3)
O2	−0.36123 (19)	−0.15717 (9)	0.26359 (11)	0.0591 (4)
O3	−0.13946 (19)	−0.12441 (9)	0.42086 (11)	0.0567 (4)
O4	−0.66285 (17)	0.13485 (10)	0.00573 (12)	0.0591 (4)
O5	−0.56836 (17)	0.26740 (9)	0.07863 (12)	0.0482 (3)
N1	−0.41141 (18)	−0.35805 (9)	0.25550 (12)	0.0408 (3)
N2	−0.10093 (17)	−0.33092 (9)	0.42815 (12)	0.0373 (3)
C1	−0.20554 (19)	0.21845 (11)	0.14171 (12)	0.0320 (3)
C2	−0.22189 (19)	0.14486 (10)	0.18669 (13)	0.0335 (4)
H2A	−0.3230	0.1168	0.1518	0.040*
C3	−0.0880 (2)	0.11214 (11)	0.28402 (13)	0.0353 (4)
C4	0.0613 (2)	0.15579 (13)	0.33550 (14)	0.0442 (4)
H4A	0.1511	0.1361	0.4015	0.053*
C5	0.0764 (2)	0.22891 (13)	0.28838 (15)	0.0449 (4)
H5A	0.1773	0.2571	0.3227	0.054*
C6	−0.0547 (2)	0.26020 (11)	0.19240 (15)	0.0377 (4)
H6A	−0.0429	0.3089	0.1614	0.045*
C7	−0.1050 (2)	0.03192 (12)	0.32975 (14)	0.0412 (4)
H7A	−0.0254	0.0223	0.4017	0.049*
C8	−0.2224 (3)	−0.02701 (12)	0.27791 (15)	0.0473 (5)
H8A	−0.3011	−0.0182	0.2056	0.057*
C9	−0.2398 (3)	−0.10691 (12)	0.32551 (15)	0.0457 (4)
C10	−0.4780 (2)	0.20433 (14)	−0.01510 (13)	0.0433 (4)
H10A	−0.4506	0.1438	−0.0206	0.052*
H10B	−0.5465	0.2291	−0.0859	0.052*

C11	−0.5770 (2)	0.20077 (12)	0.02659 (13)	0.0386 (4)
C12	−0.5648 (2)	−0.37041 (13)	0.17056 (16)	0.0511 (5)
H12A	−0.6440	−0.3295	0.1562	0.061*
C13	−0.6122 (3)	−0.44236 (15)	0.10171 (17)	0.0602 (6)
H13A	−0.7209	−0.4489	0.0429	0.072*
C14	−0.4975 (3)	−0.50280 (14)	0.12172 (17)	0.0583 (5)
H14A	−0.5279	−0.5515	0.0771	0.070*
C15	−0.3334 (3)	−0.49139 (12)	0.20977 (16)	0.0486 (5)
C16	−0.2961 (2)	−0.41737 (11)	0.27537 (14)	0.0382 (4)
C17	−0.2041 (3)	−0.55048 (13)	0.23654 (19)	0.0583 (6)
H17A	−0.2280	−0.5997	0.1938	0.070*
C18	−0.0487 (3)	−0.53644 (13)	0.32207 (19)	0.0564 (6)
H18A	0.0330	−0.5756	0.3367	0.068*
C19	−0.0068 (2)	−0.46234 (12)	0.39092 (16)	0.0447 (4)
C20	−0.1308 (2)	−0.40297 (11)	0.36709 (14)	0.0369 (4)
C21	0.1518 (2)	−0.44575 (13)	0.48294 (17)	0.0506 (5)
H21A	0.2373	−0.4837	0.5020	0.061*
C22	0.1806 (2)	−0.37366 (14)	0.54458 (16)	0.0503 (5)
H22A	0.2852	−0.3625	0.6061	0.060*
C23	0.0510 (2)	−0.31708 (12)	0.51406 (15)	0.0443 (4)
H23A	0.0720	−0.2675	0.5557	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.04366 (15)	0.02930 (13)	0.04777 (15)	0.00345 (7)	0.03236 (12)	0.00291 (8)
O1	0.0319 (6)	0.0483 (8)	0.0439 (7)	0.0026 (5)	0.0221 (6)	0.0141 (5)
O2	0.0862 (11)	0.0392 (7)	0.0518 (8)	−0.0111 (7)	0.0418 (8)	0.0017 (6)
O3	0.0772 (9)	0.0435 (8)	0.0504 (8)	0.0091 (7)	0.0393 (8)	0.0136 (6)
O4	0.0534 (8)	0.0638 (9)	0.0682 (9)	−0.0194 (7)	0.0411 (7)	−0.0084 (7)
O5	0.0560 (8)	0.0423 (7)	0.0640 (9)	0.0012 (6)	0.0456 (8)	0.0041 (6)
N1	0.0480 (9)	0.0336 (7)	0.0481 (9)	−0.0012 (6)	0.0330 (8)	0.0024 (6)
N2	0.0435 (8)	0.0309 (7)	0.0492 (9)	0.0005 (6)	0.0342 (8)	0.0025 (6)
C1	0.0317 (9)	0.0319 (8)	0.0352 (9)	0.0016 (6)	0.0217 (8)	−0.0012 (7)
C2	0.0284 (8)	0.0327 (8)	0.0368 (9)	−0.0036 (6)	0.0184 (7)	−0.0016 (7)
C3	0.0363 (9)	0.0358 (9)	0.0343 (9)	0.0028 (7)	0.0217 (8)	−0.0015 (7)
C4	0.0329 (9)	0.0543 (11)	0.0327 (9)	0.0013 (8)	0.0132 (8)	−0.0043 (8)
C5	0.0327 (9)	0.0508 (10)	0.0453 (11)	−0.0119 (8)	0.0205 (9)	−0.0131 (8)
C6	0.0390 (10)	0.0334 (9)	0.0477 (11)	−0.0064 (7)	0.0300 (9)	−0.0061 (7)
C7	0.0447 (10)	0.0411 (10)	0.0382 (9)	0.0121 (8)	0.0254 (8)	0.0091 (8)
C8	0.0663 (12)	0.0362 (9)	0.0389 (10)	0.0006 (9)	0.0316 (10)	0.0053 (8)
C9	0.0702 (13)	0.0329 (9)	0.0505 (12)	0.0086 (9)	0.0452 (11)	0.0040 (8)
C10	0.0311 (9)	0.0620 (12)	0.0338 (9)	0.0001 (8)	0.0182 (8)	0.0049 (8)
C11	0.0306 (8)	0.0460 (10)	0.0341 (9)	0.0058 (8)	0.0170 (8)	0.0110 (8)
C12	0.0493 (11)	0.0481 (11)	0.0543 (12)	−0.0018 (9)	0.0305 (10)	0.0058 (9)
C13	0.0628 (13)	0.0589 (13)	0.0528 (12)	−0.0191 (11)	0.0319 (11)	−0.0051 (10)
C14	0.0806 (15)	0.0440 (11)	0.0616 (13)	−0.0192 (11)	0.0491 (13)	−0.0127 (10)
C15	0.0738 (14)	0.0333 (9)	0.0597 (12)	−0.0089 (9)	0.0514 (12)	−0.0034 (8)
C16	0.0541 (11)	0.0273 (8)	0.0509 (10)	−0.0009 (7)	0.0410 (9)	0.0031 (7)
C17	0.0897 (17)	0.0348 (10)	0.0808 (16)	−0.0005 (10)	0.0675 (15)	−0.0061 (10)

C18	0.0836 (16)	0.0334 (10)	0.0880 (16)	0.0105 (10)	0.0708 (15)	0.0066 (10)
C19	0.0605 (12)	0.0332 (9)	0.0658 (12)	0.0073 (8)	0.0516 (11)	0.0114 (8)
C20	0.0501 (10)	0.0272 (8)	0.0509 (10)	0.0006 (7)	0.0398 (9)	0.0049 (7)
C21	0.0528 (11)	0.0457 (11)	0.0734 (14)	0.0138 (9)	0.0488 (11)	0.0213 (10)
C22	0.0436 (10)	0.0563 (12)	0.0571 (12)	0.0029 (9)	0.0336 (10)	0.0148 (10)
C23	0.0491 (11)	0.0414 (10)	0.0514 (11)	−0.0023 (8)	0.0352 (10)	0.0019 (8)

Geometric parameters (Å, º)

Zn1—O5^{i}	1.9502 (13)	C7—C8	1.307 (3)
Zn1—O2	2.0119 (13)	C7—H7A	0.9300
Zn1—N2	2.0626 (14)	C8—C9	1.485 (2)
Zn1—N1	2.1126 (15)	C8—H8A	0.9300
Zn1—O3	2.3818 (15)	C10—C11	1.515 (2)
Zn1—C9	2.5197 (19)	C10—H10A	0.9700
O1—C1	1.371 (2)	C10—H10B	0.9700
O1—C10	1.425 (2)	C12—C13	1.398 (3)
O2—C9	1.266 (2)	C12—H12A	0.9300
O3—C9	1.239 (2)	C13—C14	1.363 (3)
O4—C11	1.229 (2)	C13—H13A	0.9300
O5—C11	1.266 (2)	C14—C15	1.403 (3)
O5—Zn1^{ii}	1.9502 (13)	C14—H14A	0.9300
N1—C12	1.327 (2)	C15—C16	1.408 (2)
N1—C16	1.357 (2)	C15—C17	1.430 (3)
N2—C23	1.326 (2)	C16—C20	1.433 (3)
N2—C20	1.358 (2)	C17—C18	1.345 (3)
C1—C2	1.380 (2)	C17—H17A	0.9300
C1—C6	1.389 (2)	C18—C19	1.431 (3)
C2—C3	1.395 (2)	C18—H18A	0.9300
C2—H2A	0.9300	C19—C21	1.402 (3)
C3—C4	1.388 (2)	C19—C20	1.405 (2)
C3—C7	1.470 (2)	C21—C22	1.366 (3)
C4—C5	1.389 (3)	C21—H21A	0.9300
C4—H4A	0.9300	C22—C23	1.394 (3)
C5—C6	1.367 (3)	C22—H22A	0.9300
C5—H5A	0.9300	C23—H23A	0.9300
C6—H6A	0.9300		

O5^{i}—Zn1—O2	108.22 (6)	O3—C9—C8	121.79 (19)
O5^{i}—Zn1—N2	130.55 (6)	O2—C9—C8	116.76 (17)
O2—Zn1—N2	118.81 (6)	O3—C9—Zn1	69.26 (10)
O5^{i}—Zn1—N1	110.93 (6)	O2—C9—Zn1	52.27 (9)
O2—Zn1—N1	95.18 (6)	C8—C9—Zn1	168.31 (14)
N2—Zn1—N1	80.34 (6)	O1—C10—C11	115.57 (15)
O5^{i}—Zn1—O3	103.69 (5)	O1—C10—H10A	108.4
O2—Zn1—O3	58.93 (5)	C11—C10—H10A	108.4
N2—Zn1—O3	88.72 (5)	O1—C10—H10B	108.4
N1—Zn1—O3	142.20 (5)	C11—C10—H10B	108.4
O5^{i}—Zn1—C9	109.35 (6)	H10A—C10—H10B	107.4
O2—Zn1—C9	29.86 (6)	O4—C11—O5	124.43 (17)

N2—Zn1—C9	104.25 (6)	O4—C11—C10	118.21 (17)
N1—Zn1—C9	120.11 (6)	O5—C11—C10	117.33 (16)
O3—Zn1—C9	29.10 (6)	N1—C12—C13	122.7 (2)
C1—O1—C10	116.18 (13)	N1—C12—H12A	118.7
C9—O2—Zn1	97.87 (11)	C13—C12—H12A	118.7
C9—O3—Zn1	81.63 (12)	C14—C13—C12	119.3 (2)
C11—O5—Zn1^{ii}	110.61 (11)	C14—C13—H13A	120.3
C12—N1—C16	118.40 (16)	C12—C13—H13A	120.3
C12—N1—Zn1	130.30 (13)	C13—C14—C15	119.82 (19)
C16—N1—Zn1	111.24 (12)	C13—C14—H14A	120.1
C23—N2—C20	118.40 (15)	C15—C14—H14A	120.1
C23—N2—Zn1	128.60 (12)	C14—C15—C16	117.25 (19)
C20—N2—Zn1	112.97 (11)	C14—C15—C17	123.94 (19)
O1—C1—C2	124.29 (14)	C16—C15—C17	118.80 (19)
O1—C1—C6	115.46 (15)	N1—C16—C15	122.52 (17)
C2—C1—C6	120.24 (15)	N1—C16—C20	117.81 (15)
C1—C2—C3	120.56 (15)	C15—C16—C20	119.67 (16)
C1—C2—H2A	119.7	C18—C17—C15	121.51 (19)
C3—C2—H2A	119.7	C18—C17—H17A	119.2
C4—C3—C2	118.79 (16)	C15—C17—H17A	119.2
C4—C3—C7	120.96 (16)	C17—C18—C19	121.12 (19)
C2—C3—C7	120.24 (15)	C17—C18—H18A	119.4
C3—C4—C5	119.93 (16)	C19—C18—H18A	119.4
C3—C4—H4A	120.0	C21—C19—C20	117.30 (17)
C5—C4—H4A	120.0	C21—C19—C18	123.79 (18)
C6—C5—C4	121.12 (17)	C20—C19—C18	118.90 (19)
C6—C5—H5A	119.4	N2—C20—C19	122.48 (17)
C4—C5—H5A	119.4	N2—C20—C16	117.53 (15)
C5—C6—C1	119.32 (17)	C19—C20—C16	119.99 (16)
C5—C6—H6A	120.3	C22—C21—C19	119.86 (17)
C1—C6—H6A	120.3	C22—C21—H21A	120.1
C8—C7—C3	125.61 (17)	C19—C21—H21A	120.1
C8—C7—H7A	117.2	C21—C22—C23	119.14 (19)
C3—C7—H7A	117.2	C21—C22—H22A	120.4
C7—C8—C9	125.05 (18)	C23—C22—H22A	120.4
C7—C8—H8A	117.5	N2—C23—C22	122.81 (18)
C9—C8—H8A	117.5	N2—C23—H23A	118.6
O3—C9—O2	121.44 (17)	C22—C23—H23A	118.6

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