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catena-Poly[[bis(pyridine-κ*N*)zinc]-μ-5-carboxybenzene-1,3-dicarboxylato-κ^2*O*^{1}:*O*^{3}]

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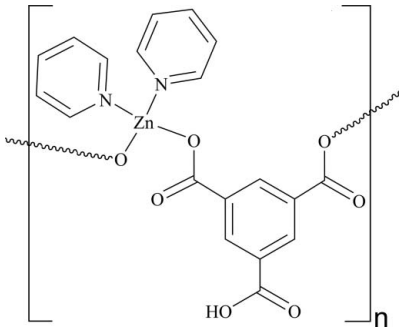
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.075; data-to-parameter ratio = 17.1.

The title one-dimensional coordination polymer, $[Zn(C_9H_4O_6)(C_5H_5N)_2]_n$ or $[Zn(HBTC)(py)_2]_n$, (I), where BTC is benzene-1,3,5-tricarboxylate and py is pyridine, is a solvent-free polymorph of $[Zn(HBTC)(py)_2]\cdot 2C_2H_5OH$ [Yaghi *et al.* (1997). *Chem. Mater.* **9**, 1074–1076]. Differences in the spatial arrangements and supramolecular packing of the $[Zn(HBTC)(py)_2]_n$ chains in the two structures are described. The chain in (I) extends parallel to [100] and is severely puckered, with a Zn···Zn distance of 8.3599 (3) Å and a Zn···Zn···Zn angle of 107.516 (3)°, as a result of hydrogen-bonding interactions of the types O—H···O and C—H···O. There is no evidence for π–π interactions in (I). The differences between the solvent-free and solvent-containing structures can be accounted for by the absence of the ethanol solvent molecule and the use of the converging pair of O atoms in the bis-monodentate bridging $HBTC^{2-}$ ligand in (I).

Related literature

For the ethanol monosolvate of (I), see: Yaghi *et al.* (1997). For a review on supramolecular isomerism in coordination compounds, see: Zhang *et al.* (2009).



Experimental

Crystal data

$[Zn(C_9H_4O_6)(C_5H_5N)_2]$
M_r = 431.69
Orthorhombic, *Pbca*
a = 13.4850 (4) Å
b = 15.7677 (4) Å
c = 16.7252 (4) Å
V = 3556.24 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 293 K
0.40 × 0.32 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.638, T_{max} = 0.746
18851 measured reflections
4402 independent reflections
3448 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.075
S = 1.03
4402 reflections
257 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*W*···O3^{i}	0.86 (3)	1.74 (3)	2.5813 (19)	164 (3)
C1—H1···O1	0.93	2.45	3.053 (2)	122
C5—H5···O6^{ii}	0.93	2.39	3.129 (3)	136
C17—H17···O5	0.93	2.37	2.693 (2)	100
C17—H17···O5^{i}	0.93	2.42	3.309 (2)	159

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) and *WinGX* (Farrugia, 2012); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008) and *WinGX*; molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CQ2004).

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supporting information

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catena-Poly[[bis(pyridine-κN)zinc]-μ-5-carboxybenzene-1,3-dicarboxylato-κ^2O^1:O^3]

Bunlawee Yotnoi and Apinpus Rujiwatra

S1. Comment

The reported complex $[Zn(HBTC)(py)_2]_n$ (**I**), where BTC = 1,3,5-benzenetricarboxylate and pyr = pyridine (C_5H_5N), is a supramolecular isomer of the previously reported $[Zn(HBTC)(py)_2].2C_2H_5OH$ (Yaghi *et al.*, 1997). It is clear that the two isomers result from differences in the synthesis method. In order to synthesize **I**, a simple solution route was adopted, whereas the crystals of $[Zn(HBTC)(py)_2].2C_2H_5OH$ have only been synthesized when poly(ethyleneoxide) (PEO) gel is used as the reaction medium in the presence of C_2H_5OH as solvent (Yaghi *et al.*, 1997). The absence or presence of the C_2H_5OH solvent molecules results in different spatial arrangements and supramolecular packing in the two isomers.

While the two supramolecular isomers are built up of the same structural building motifs, *i.e.* a tetrahedral Zn(II) ion, two monodentate pyr molecules and a bridging $HBTC^{2-}$ anion, the architecture of the one-dimensional chains of the two isomers notably differs. In the case of **I**, an asymmetric unit comprises a tetrahedral Zn(II) ion (Fig. 1), coordinated by two N atoms (N1 and N2) from two crystallographically independent pyr molecules and two O atoms (O1 and O2) from two distinct carboxylato groups of the $HBTC^{2-}$ anion. The $HBTC^{2-}$ ligand in structure **I** adopts a *bis*-monodentate bridging mode (μ_2-η^1:η^1:η^0:η^0:η^0:η^0) (Fig. 2), linking two adjacent Zn(II) ions to form a one-dimensional chain of chemical composition $[Zn(HBTC)(py)_2]_n$, extending in the [1 0 0] direction. Because of the converging positions of the coordinating O1 and O2 atoms, the derived chain is severely puckered with a Zn···Zn distance of 8.3599 (3) Å and a Zn···Zn···Zn angle of 107.516 (3)°. In comparison, the one-dimensional chain of the previously reported $[Zn(HBTC)(py)_2].2C_2H_5OH$ isomer is almost linear with corresponding distance and angle values of 10.162 (2) Å and 180°, respectively. The presence of the C_2H_5OH solvent molecule in the vicinity of the two coordinating carboxylato groups in the $[Zn(HBTC)(py)_2].2C_2H_5OH$ isomer ostensibly forces the coordinating atoms to be the diverging pair of O atoms (equivalent to O3 and O6 in **I**), rather than the converging pair as in **I**.

A larger degree of puckering in **I** compared to that of the previously reported isomer imparts an immense influence on the corresponding supramolecular interactions and packing. While there are no π–π interactions in **I**, which is in contrast to the $[Zn(HBTC)(py)_2].2C_2H_5OH$ case, an acidic proton of the bridging $HBTC^{2-}$ anion is involved in the hydrogen bonding interactions with the O atom of the $HBTC^{2-}$ anion from the adjacent chain (Fig. 3). Weak C—H···O hydrogen bonding interactions further link these one-dimensional chains into a dense, three-dimensional supramolecular structure.

S2. Experimental

A small fraction of pyridine (0.50 ml, 6.18 mmol; 99.8% Sigma-Aldrich) was gradually added to a 2.50 ml of a 0.204 $molL^{-1}$ aqueous solution of 1,3,5-benzenetricarboxylic acid (H_3BTC; 0.509 mmol; 95% Sigma-Aldrich) with stirring until the acid was completely dissolved. Then 2.50 ml of 0.296 $molL^{-1}$ $ZnSO_4.7H_2O$ (aq) solution (0.741 mmol; 99% Sigma-Aldrich) was added, giving a clear solution. The solution was left at ambient temperature for 2 days before the colourless crystals of **I** started to crystallize.

S3. Refinement

Atom H5W atom was located in a difference Fourier map. The aromatic H-atoms were treated as riding groups on the bonded C-atoms using a C—H bond length of 0.93 Å.

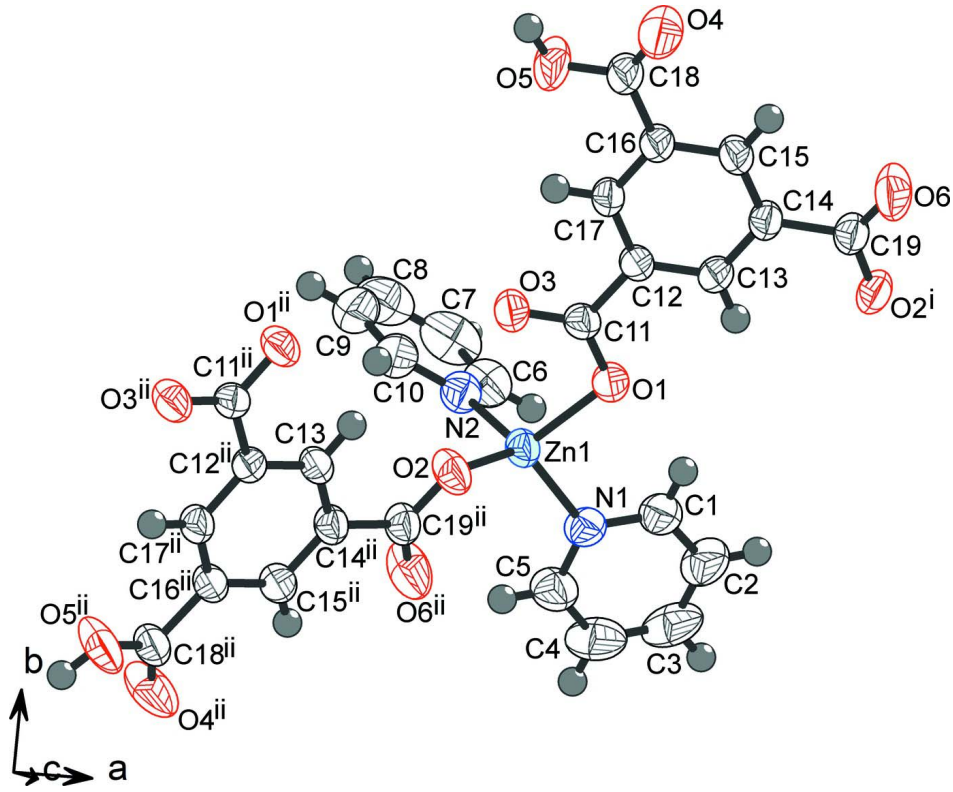

Figure 1

View of an extended unit of **I** with atom numbering scheme. Displacement ellipsoids are drawn at the 70% probability level. [Symmetry codes: (i) 1/2 + *x*, 0.5 - *y*, 1 - *z*; (ii) -1/2 + *x*, 0.5 - *y*, 1 - *z*]

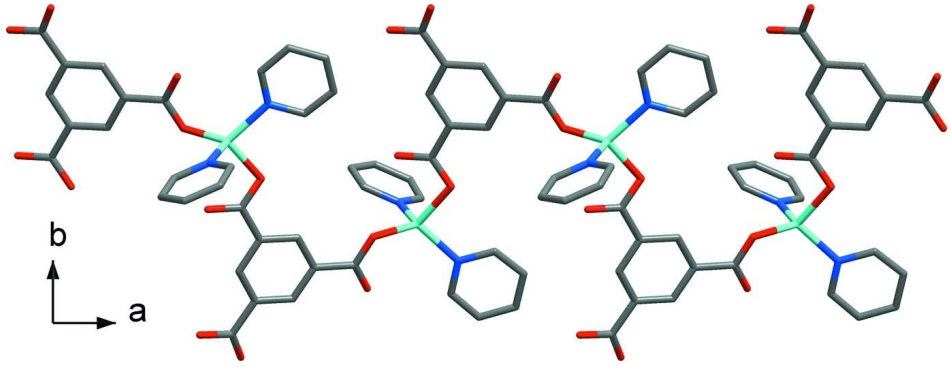

Figure 2

View of the one-dimensional chain of **I**. Hydrogen atoms are omitted for clarity.

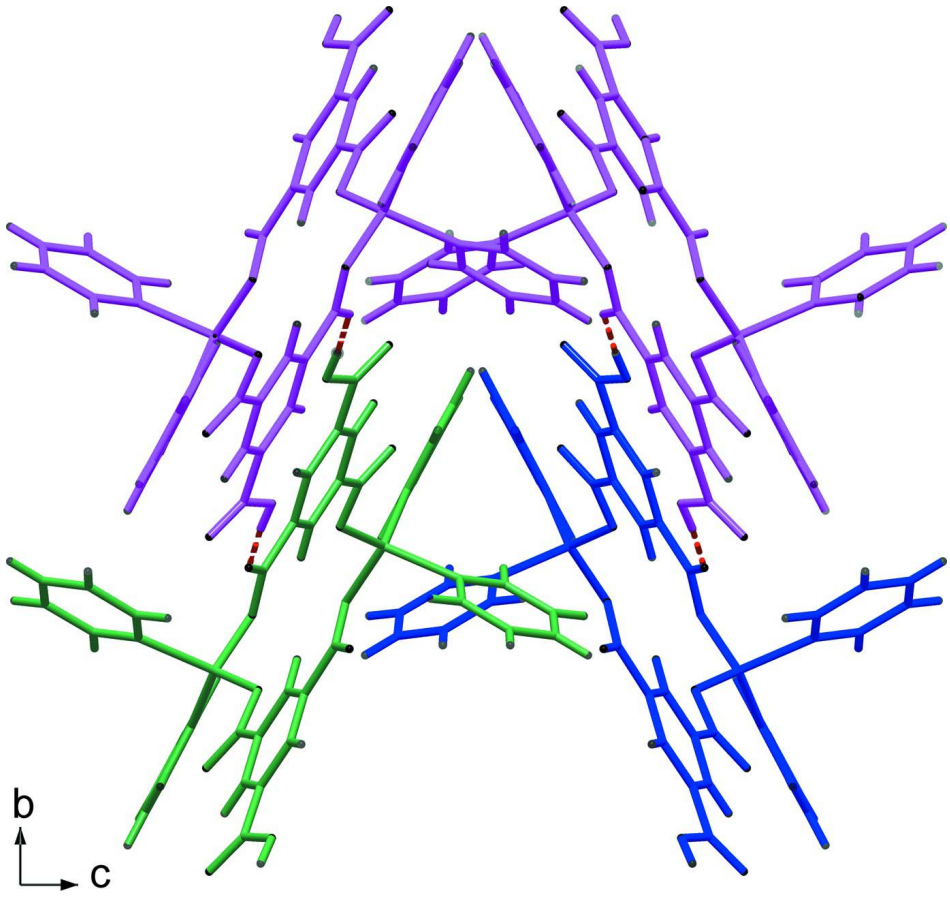

Figure 3

View of supramolecular packing in **I**, directed primarily by the O—H···O hydrogen bonding interactions (dotted lines).

catena-Poly[[bis(pyridine-κN)zinc]-μ-5-carboxybenzene-1,3-dicarboxylato-κ²O¹:O³]

Crystal data

$[Zn(C_9H_4O_6)(C_5H_5N)_2]$
$M_r = 431.69$
Orthorhombic, *Pbca*
$a = 13.4850\ (4)$ Å
$b = 15.7677\ (4)$ Å
$c = 16.7252\ (4)$ Å
$V = 3556.24\ (16)$ Å^3
$Z = 8$
$F(000) = 1760$
$D_x = 1.613$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 12396 reflections
$\theta = 2.3$–$28.3°$
$\mu = 1.42$ mm^{-1}
$T = 293$ K
Block, colorless
0.40 × 0.32 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.638$, $T_{max} = 0.746$
18851 measured reflections
4402 independent reflections
3448 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.3°$
$h = -17 \rightarrow 16$
$k = -18 \rightarrow 21$
$l = -22 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.075$
$S = 1.03$
4402 reflections
257 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 1.2882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.13687 (2)	0.15689 (2)	0.38115 (2)	0.02934 (7)
O1	0.22574 (9)	0.24099 (8)	0.43444 (8)	0.0387 (3)
O2	0.02076 (9)	0.12804 (8)	0.44224 (8)	0.0380 (3)
O3	0.08532 (9)	0.31056 (8)	0.42911 (9)	0.0403 (3)
O4	0.17223 (13)	0.64303 (10)	0.62643 (11)	0.0636 (5)
O5	0.06430 (11)	0.59328 (10)	0.53854 (11)	0.0610 (5)
O6	0.50499 (11)	0.48839 (11)	0.63064 (10)	0.0572 (4)
N1	0.24456 (11)	0.07341 (9)	0.34795 (9)	0.0344 (3)
N2	0.08742 (12)	0.20600 (9)	0.27386 (9)	0.0351 (3)
C1	0.34018 (14)	0.09488 (13)	0.35799 (13)	0.0403 (4)
H1	0.3551	0.1456	0.3837	0.048*
C2	0.41665 (16)	0.04472 (14)	0.33178 (15)	0.0526 (6)
H2	0.4821	0.0612	0.3398	0.063*
C3	0.39544 (18)	−0.02992 (14)	0.29374 (14)	0.0554 (6)
H3	0.4463	−0.0645	0.2749	0.066*
C4	0.29877 (19)	−0.05299 (13)	0.28377 (14)	0.0554 (6)
H4	0.2829	−0.1038	0.2586	0.066*
C5	0.22515 (16)	−0.00031 (13)	0.31132 (12)	0.0451 (5)
H5	0.1594	−0.0164	0.3043	0.054*
C6	0.14604 (16)	0.21440 (13)	0.21013 (12)	0.0455 (5)
H6	0.2091	0.1906	0.2119	0.055*
C7	0.1175 (2)	0.25651 (16)	0.14217 (13)	0.0581 (6)
H7	0.1607	0.2614	0.0991	0.070*
C8	0.0245 (2)	0.29120 (16)	0.13863 (15)	0.0639 (7)
H8	0.0034	0.3200	0.0932	0.077*
C9	−0.03721 (19)	0.28258 (14)	0.20360 (15)	0.0570 (6)
H9	−0.1010	0.3050	0.2025	0.068*
C10	−0.00334 (15)	0.24024 (12)	0.27043 (12)	0.0424 (5)
H10	−0.0449	0.2353	0.3145	0.051*
C11	0.17367 (13)	0.30629 (11)	0.44909 (10)	0.0290 (3)

C12	0.22248 (12)	0.37837 (10)	0.49276 (10)	0.0274 (3)
C13	0.32159 (13)	0.37427 (11)	0.51554 (10)	0.0290 (4)
H13	0.3589	0.3265	0.5029	0.035*
C14	0.36539 (12)	0.44093 (11)	0.55706 (10)	0.0296 (4)
C15	0.30929 (13)	0.51149 (11)	0.57672 (11)	0.0325 (4)
H15	0.3381	0.5560	0.6048	0.039*
C16	0.20993 (12)	0.51606 (11)	0.55457 (11)	0.0311 (4)
C17	0.16744 (13)	0.44966 (11)	0.51237 (11)	0.0306 (4)
H17	0.1013	0.4530	0.4970	0.037*
C18	0.14864 (13)	0.59105 (12)	0.57802 (13)	0.0377 (4)
C19	0.47177 (13)	0.43569 (11)	0.58439 (11)	0.0322 (4)
H5W	0.022 (2)	0.6310 (19)	0.5540 (18)	0.096 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02247 (11)	0.02948 (11)	0.03608 (12)	−0.00104 (8)	0.00170 (8)	−0.00546 (8)
O1	0.0273 (7)	0.0301 (6)	0.0587 (8)	0.0041 (5)	−0.0047 (6)	−0.0160 (6)
O2	0.0269 (7)	0.0399 (7)	0.0472 (7)	−0.0100 (5)	0.0077 (6)	−0.0080 (6)
O3	0.0262 (7)	0.0345 (7)	0.0604 (9)	0.0031 (5)	−0.0077 (6)	−0.0175 (6)
O4	0.0489 (9)	0.0533 (10)	0.0887 (13)	0.0178 (8)	−0.0231 (9)	−0.0421 (9)
O5	0.0303 (8)	0.0560 (10)	0.0967 (13)	0.0175 (7)	−0.0177 (8)	−0.0409 (9)
O6	0.0325 (8)	0.0634 (10)	0.0759 (11)	0.0070 (7)	−0.0159 (7)	−0.0354 (8)
N1	0.0317 (8)	0.0309 (8)	0.0407 (8)	0.0036 (6)	0.0055 (7)	−0.0024 (7)
N2	0.0352 (9)	0.0350 (8)	0.0352 (8)	0.0005 (7)	−0.0019 (7)	−0.0053 (7)
C1	0.0338 (10)	0.0344 (10)	0.0526 (11)	0.0012 (8)	0.0058 (9)	−0.0005 (9)
C2	0.0342 (11)	0.0496 (12)	0.0740 (16)	0.0100 (9)	0.0150 (10)	0.0077 (11)
C3	0.0593 (15)	0.0445 (12)	0.0625 (14)	0.0220 (11)	0.0265 (12)	0.0054 (11)
C4	0.0711 (16)	0.0364 (11)	0.0587 (14)	0.0090 (11)	0.0144 (12)	−0.0115 (10)
C5	0.0442 (12)	0.0368 (10)	0.0544 (12)	0.0002 (9)	0.0051 (10)	−0.0112 (9)
C6	0.0488 (13)	0.0469 (11)	0.0408 (11)	−0.0019 (10)	0.0059 (9)	−0.0068 (9)
C7	0.0817 (18)	0.0554 (14)	0.0373 (11)	−0.0166 (13)	0.0046 (11)	−0.0009 (11)
C8	0.094 (2)	0.0476 (13)	0.0500 (14)	−0.0149 (14)	−0.0259 (14)	0.0094 (11)
C9	0.0558 (15)	0.0443 (12)	0.0710 (16)	0.0029 (11)	−0.0223 (12)	0.0006 (11)
C10	0.0403 (11)	0.0397 (10)	0.0472 (11)	0.0016 (9)	−0.0036 (9)	−0.0043 (9)
C11	0.0273 (8)	0.0256 (8)	0.0342 (9)	−0.0003 (7)	0.0012 (7)	−0.0049 (7)
C12	0.0239 (8)	0.0256 (8)	0.0328 (8)	−0.0012 (6)	0.0005 (7)	−0.0037 (7)
C13	0.0239 (8)	0.0272 (8)	0.0358 (9)	0.0041 (7)	0.0006 (7)	−0.0042 (7)
C14	0.0224 (8)	0.0321 (9)	0.0342 (9)	0.0018 (7)	−0.0015 (7)	−0.0028 (7)
C15	0.0258 (9)	0.0304 (9)	0.0414 (10)	−0.0007 (7)	−0.0038 (7)	−0.0100 (8)
C16	0.0242 (8)	0.0287 (8)	0.0404 (9)	0.0023 (7)	−0.0015 (7)	−0.0080 (7)
C17	0.0215 (8)	0.0300 (9)	0.0404 (10)	0.0008 (7)	−0.0027 (7)	−0.0057 (7)
C18	0.0256 (9)	0.0338 (9)	0.0536 (12)	0.0040 (7)	−0.0019 (8)	−0.0114 (9)
C19	0.0246 (8)	0.0359 (9)	0.0361 (9)	0.0021 (7)	−0.0013 (7)	−0.0018 (8)

Geometric parameters (Å, º)

Zn1—O2	1.9241 (12)	C5—H5	0.9300
Zn1—O1	1.9973 (12)	C6—C7	1.371 (3)
Zn1—N1	2.0371 (14)	C6—H6	0.9300
Zn1—N2	2.0650 (15)	C7—C8	1.370 (4)
O1—C11	1.270 (2)	C7—H7	0.9300
O2—C19^{i}	1.283 (2)	C8—C9	1.375 (4)
O3—C11	1.239 (2)	C8—H8	0.9300
O4—C18	1.195 (2)	C9—C10	1.380 (3)
O5—C18	1.315 (2)	C9—H9	0.9300
O5—H5W	0.86 (3)	C10—H10	0.9300
O6—C19	1.220 (2)	C11—C12	1.503 (2)
N1—C5	1.340 (2)	C12—C17	1.386 (2)
N1—C1	1.344 (2)	C12—C13	1.391 (2)
N2—C6	1.334 (3)	C13—C14	1.391 (2)
N2—C10	1.339 (2)	C13—H13	0.9300
C1—C2	1.372 (3)	C14—C15	1.385 (2)
C1—H1	0.9300	C14—C19	1.508 (2)
C2—C3	1.368 (3)	C15—C16	1.392 (2)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.364 (3)	C16—C17	1.387 (2)
C3—H3	0.9300	C16—C18	1.495 (2)
C4—C5	1.374 (3)	C17—H17	0.9300
C4—H4	0.9300	C19—O2^{ii}	1.283 (2)
O2—Zn1—O1	114.10 (5)	C7—C8—C9	118.7 (2)
O2—Zn1—N1	124.90 (6)	C7—C8—H8	120.6
O1—Zn1—N1	97.06 (6)	C9—C8—H8	120.6
O2—Zn1—N2	106.70 (6)	C8—C9—C10	119.2 (2)
O1—Zn1—N2	109.43 (6)	C8—C9—H9	120.4
N1—Zn1—N2	103.63 (6)	C10—C9—H9	120.4
C11—O1—Zn1	107.01 (11)	N2—C10—C9	122.2 (2)
C19^{i}—O2—Zn1	114.84 (11)	N2—C10—H10	118.9
C18—O5—H5W	116 (2)	C9—C10—H10	118.9
C5—N1—C1	117.60 (17)	O3—C11—O1	121.57 (15)
C5—N1—Zn1	123.09 (13)	O3—C11—C12	120.73 (15)
C1—N1—Zn1	119.16 (13)	O1—C11—C12	117.69 (15)
C6—N2—C10	117.87 (18)	C17—C12—C13	119.16 (15)
C6—N2—Zn1	122.71 (14)	C17—C12—C11	119.58 (15)
C10—N2—Zn1	118.92 (13)	C13—C12—C11	121.25 (15)
N1—C1—C2	122.4 (2)	C12—C13—C14	120.63 (15)
N1—C1—H1	118.8	C12—C13—H13	119.7
C2—C1—H1	118.8	C14—C13—H13	119.7
C3—C2—C1	119.2 (2)	C15—C14—C13	119.57 (15)
C3—C2—H2	120.4	C15—C14—C19	119.45 (15)
C1—C2—H2	120.4	C13—C14—C19	120.92 (15)
C4—C3—C2	119.09 (19)	C14—C15—C16	120.28 (16)

C4—C3—H3	120.5	C14—C15—H15	119.9
C2—C3—H3	120.5	C16—C15—H15	119.9
C3—C4—C5	119.2 (2)	C17—C16—C15	119.61 (15)
C3—C4—H4	120.4	C17—C16—C18	120.15 (15)
C5—C4—H4	120.4	C15—C16—C18	120.22 (15)
N1—C5—C4	122.5 (2)	C12—C17—C16	120.75 (16)
N1—C5—H5	118.8	C12—C17—H17	119.6
C4—C5—H5	118.8	C16—C17—H17	119.6
N2—C6—C7	123.0 (2)	O4—C18—O5	123.49 (18)
N2—C6—H6	118.5	O4—C18—C16	124.95 (17)
C7—C6—H6	118.5	O5—C18—C16	111.55 (16)
C8—C7—C6	119.1 (2)	O6—C19—O2^{ii}	124.36 (17)
C8—C7—H7	120.5	O6—C19—C14	120.27 (16)
C6—C7—H7	120.5	O2^{ii}—C19—C14	115.32 (15)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*W*···O3^{iii}	0.86 (3)	1.74 (3)	2.5813 (19)	164 (3)
C1—H1···O1	0.93	2.45	3.053 (2)	122
C5—H5···O6^{i}	0.93	2.39	3.129 (3)	136
C17—H17···O5	0.93	2.37	2.693 (2)	100
C17—H17···O5^{iii}	0.93	2.42	3.309 (2)	159

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