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catena-Poly[[[bis(methylamine)zinc(II)]- μ -4,4'-oxydibenzoato] *N,N*-dimethylacetamide solvate]

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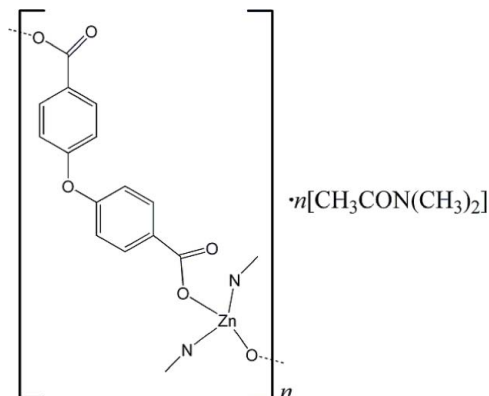
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.053; wR factor = 0.149; data-to-parameter ratio = 17.9.

In the title zinc(II) coordination polymer, $\{[\text{Zn}(\text{C}_{14}\text{H}_8\text{O}_5)(\text{CH}_5\text{N})_2] \cdot \text{C}_4\text{H}_9\text{NO}\}_n$, each Zn(II) cation is tetrahedrally coordinated by two carboxylato O atoms of two oba anions (H_2oba is 4,4'-oxydibenzoic acid), and two N atoms from two methylamine molecules. Each oba anion bridges two Zn(II) cations through the two carboxylate groups in a monodentate fashion, forming one-dimensional polymeric chains. These chains are linked *via* N-H...O hydrogen bonds, forming a two-dimensional supramolecular network.

Related literature

For related literature, see: Kondo *et al.* (2004); Luo *et al.* (2003); Sun *et al.* (2005); Yaghi *et al.* (1998).



Experimental

Crystal data

$[\text{Zn}(\text{C}_{14}\text{H}_8\text{O}_5)(\text{CH}_5\text{N})_2] \cdot \text{C}_4\text{H}_9\text{NO}$
 $M_r = 470.82$

Monoclinic, $C2/c$
 $a = 27.617$ (6) Å

$b = 8.9276$ (18) Å
 $c = 21.212$ (4) Å
 $\beta = 122.46$ (3)°
 $V = 4413$ (2) Å³
 $Z = 8$

Mo $K\alpha$ radiation
 $\mu = 1.15$ mm⁻¹
 $T = 293$ (2) K
 $0.35 \times 0.34 \times 0.15$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (Higashi, 1995)
 $T_{\text{min}} = 0.690$, $T_{\text{max}} = 0.850$

20180 measured reflections
4942 independent reflections
2843 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.149$
 $S = 1.04$
4942 reflections

276 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.43$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.47$ e Å⁻³

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1B...O4 ⁱ	0.90	2.21	2.991 (5)	145
N2—H2A...O2 ⁱⁱ	0.90	2.11	2.966 (4)	159
N2—H2B...O6 ⁱⁱⁱ	0.90	2.40	3.276 (6)	164

Symmetry codes: (i) $-x + \frac{3}{2}, -y + \frac{3}{2}, -z + 1$; (ii) $-x + 2, -y + 2, -z + 1$; (iii) $x + \frac{1}{2}, y + \frac{1}{2}, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 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: FJ2083).

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supplementary materials

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***catena*-Poly[[[bis(methylamine)zinc(II)]- μ -4,4'-oxydibenzoato] *N,N*-dimethylacetamide solvate]**

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Comment

Recently, great interest has been focused on the design and synthesis of coordination polymers because of their intriguing network topologies and promising applications (Yaghi *et al.*, 1998). It is well known that the selection of appropriate organic ligands is crucial to the design and synthesis of the supramolecular architectures. In preparing target metal complexes, carboxylate and organic amine ligands have been frequently employed (Luo *et al.*, 2003). More and more interest has focused on long flexible ligands recently, and how to avoid, or make use of, their interpenetration to construct novel coordination polymers is an interesting challenge. 4,4'-oxybis(benzoic acid) (H₂oba) ligand, in which two benzene moieties are linked together by a μ_2 -O bridge, is the typical example of flexible ligand and may offer more possibilities in geometry configuration and coordination modes towards the metal ions. As far as we know, several coordination polymers based on 4,4'-oxybis(benzoic acid) have been obtained (Kondo *et al.*, 2004; Sun *et al.*, 2005). We present here the solvothermal synthesis and crystal structure of title coordination polymer, [Zn(C₁₄H₈O₅)(CNH₅)₂(C₄NOH₉)]_n, (I).

The asymmetric unit of (I) consists of one crystallographically independent Zn(II) cation, one oba ligand, two methylamine and one dimethylacetamide molecule. Fig.1 shows the molecular structure of (I) with the atom-labelling scheme. The Zn(II) cation has a slightly distorted tetrahedral coordination geometry and formed by two carboxy oxygen atoms (O1 and O5A) from two oba ligands and two nitrogen atoms (N1 and N2) from two methylamine molecule, with Zn—O distances of 1.949 (3)–1.952 (3) Å and Zn—N distances in the range of 1.996 (4)–2.047 (4) Å. These values are in good agreement with those found in other extended structures (Kondo *et al.*, 2004). The O—Zn—O and N—Zn—N bond angles are 106.28 (11)° and 106.15 (19)°, respectively. The N—Zn—O angles are in the range from 98.65 (12) to 115.75 (14)°. In (I), two carboxylate groups of each oba exhibit bis-monodentate coordination modes, namely oba anion acts as μ_2 -bridging ligand to connect with two Zn(II) centers and each Zn(II) center connects with two oba anions to form the chain arrangement with ZnⁱⁱⁱZn distance of 14.512 (4) Å (Fig. 2). It is found that there are hydrogen bonding interactions between adjacent chains. The N—HⁱⁱⁱO hydrogen bonds involve the uncoordinated carboxylic oxygen atoms of oba and N—H groups of methylamine molecules from adjacent chains (Table 2). In addition, dimethylacetamide molecules located in the crystal lattice with N—HⁱⁱⁱO hydrogen bonding interactions involving the oxygen atoms of dimethylacetamide molecules and N—H groups of methylamine molecules (Table 2). Finally, the chains are linked together by hydrogen bonds to form two-dimensional supramolecular network (Fig. 2).

Experimental

(I) was solvothermally prepared from a mixture of Zn(NO₃)₂·6H₂O (0.044 g, 0.2 mmol), 4,4'-oxybis(benzoic acid) (0.051 g, 0.2 mmol), methylamine (0.05 ml) and dimethylacetamide (10 ml). The slurry was stirred for 30 min and heated at 120 °C for 72 h in a Teflon-lined stainless steel autoclave (25 ml) under autogenous pressure. After cooling to room temperature, the block-shaped crystals were washed with water and dried in air.

Refinement

The H atoms were placed in geometrical calculated positions, with C—H distances of 0.93–0.96 Å and N—H distances of 0.90 Å. A common displacement parameter was refined for all H atoms.

Figures

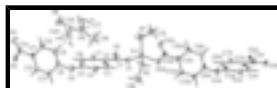


Fig. 1. A perspective view of molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii. [symmetry code: (A) $x + 1/2, y - 1/2, z$.].



Fig. 2. A packing diagram of (I). The dashed lines indicate the hydrogen bonds.

catena-Poly[[[bis(methylamine)zinc(II)]- μ -4,4'-oxydibenzoato] *N,N*-dimethylacetamide]

Crystal data

$[\text{Zn}(\text{C}_{14}\text{H}_8\text{O}_5)(\text{CH}_5\text{N})_2] \cdot \text{C}_4\text{H}_9\text{NO}$

$M_r = 470.82$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 27.617(6) \text{ \AA}$

$b = 8.9276(18) \text{ \AA}$

$c = 21.212(4) \text{ \AA}$

$\beta = 122.46(3)^\circ$

$V = 4413(2) \text{ \AA}^3$

$Z = 8$

$F_{000} = 1968$

$D_x = 1.417 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 11100 reflections

$\theta = 3.0\text{--}27.5^\circ$

$\mu = 1.15 \text{ mm}^{-1}$

$T = 293(2) \text{ K}$

Block, colorless

$0.35 \times 0.34 \times 0.15 \text{ mm}$

Data collection

Rigaku RAXIS-RAPID
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: $10.0 \text{ pixels mm}^{-1}$

$T = 293(2) \text{ K}$

ω scan

Absorption correction: multi-scan
(Higashi, 1995)

$T_{\min} = 0.690, T_{\max} = 0.850$

20180 measured reflections

4942 independent reflections

2843 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 27.5^\circ$

$\theta_{\min} = 3.0^\circ$

$h = -34 \rightarrow 35$

$k = -11 \rightarrow 11$

$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 3.5742P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
4942 reflections	$(\Delta/\sigma)_{\max} = 0.016$
276 parameters	$\Delta\rho_{\max} = 0.43 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.47 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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	1.006041 (17)	0.74836 (5)	0.42522 (2)	0.05793 (17)
O1	0.92334 (11)	0.7166 (3)	0.37118 (16)	0.0679 (7)
O2	0.92687 (11)	0.9063 (3)	0.44038 (16)	0.0727 (8)
O3	0.66245 (11)	0.7259 (3)	0.26587 (18)	0.0794 (9)
O4	0.53662 (14)	0.9180 (4)	0.43119 (19)	0.0892 (10)
O5	0.53394 (11)	1.1281 (3)	0.37427 (16)	0.0699 (7)
O6	0.6660 (2)	0.4181 (4)	0.4624 (3)	0.1244 (15)
N1	1.04661 (18)	0.7142 (7)	0.5352 (2)	0.1189 (18)
H1A	1.0413	0.7967	0.5552	0.143*
H1B	1.0284	0.6387	0.5422	0.143*
N2	1.03183 (15)	0.9546 (4)	0.4121 (2)	0.0781 (11)
H2A	1.0374	1.0144	0.4497	0.094*
H2B	1.0657	0.9447	0.4159	0.094*
N3	0.7274 (2)	0.3980 (5)	0.4262 (3)	0.1002 (14)
C1	0.90007 (16)	0.8060 (4)	0.3942 (2)	0.0561 (9)
C2	0.83754 (14)	0.7855 (4)	0.3618 (2)	0.0489 (8)
C3	0.80568 (15)	0.6814 (4)	0.3053 (2)	0.0563 (9)
H3	0.8241	0.6228	0.2881	0.068*

supplementary materials

C4	0.74798 (15)	0.6634 (4)	0.2745 (2)	0.0588 (9)
H4	0.7275	0.5935	0.2367	0.071*
C5	0.72034 (15)	0.7500 (4)	0.3001 (2)	0.0550 (9)
C6	0.75117 (15)	0.8530 (4)	0.3565 (2)	0.0581 (9)
H6	0.7328	0.9103	0.3741	0.070*
C7	0.80910 (15)	0.8709 (4)	0.3866 (2)	0.0538 (9)
H7	0.8294	0.9414	0.4241	0.065*
C8	0.63392 (16)	0.7940 (5)	0.2969 (2)	0.0612 (10)
C9	0.63948 (19)	0.7328 (4)	0.3591 (3)	0.0736 (12)
H9	0.6631	0.6501	0.3817	0.088*
C10	0.60983 (17)	0.7938 (4)	0.3885 (2)	0.0660 (11)
H10	0.6126	0.7505	0.4302	0.079*
C11	0.57618 (14)	0.9188 (4)	0.3560 (2)	0.0532 (9)
C12	0.57183 (15)	0.9781 (4)	0.2931 (2)	0.0578 (9)
H12	0.5493	1.0627	0.2710	0.069*
C13	0.60007 (15)	0.9151 (4)	0.2624 (2)	0.0615 (10)
H13	0.5961	0.9543	0.2192	0.074*
C14	0.54638 (16)	0.9909 (5)	0.3901 (2)	0.0618 (10)
C15	1.1043 (2)	0.6820 (8)	0.5769 (3)	0.1136 (18)
H15A	1.1097	0.5759	0.5765	0.170*
H15B	1.1203	0.7151	0.6274	0.170*
H15C	1.1231	0.7325	0.5559	0.170*
C16	0.9915 (2)	1.0269 (6)	0.3416 (3)	0.1081 (17)
H16A	0.9865	0.9662	0.3012	0.162*
H16B	1.0061	1.1234	0.3399	0.162*
H16C	0.9553	1.0388	0.3372	0.162*
C17	0.7729 (4)	0.4772 (9)	0.4917 (4)	0.176 (3)
H17A	0.7756	0.5780	0.4781	0.264*
H17B	0.8088	0.4268	0.5102	0.264*
H17C	0.7642	0.4790	0.5298	0.264*
C18	0.7438 (3)	0.3428 (8)	0.3747 (4)	0.135 (2)
H18A	0.7627	0.2477	0.3920	0.202*
H18B	0.7694	0.4132	0.3731	0.202*
H18C	0.7101	0.3315	0.3256	0.202*
C19	0.6771 (3)	0.3747 (5)	0.4157 (4)	0.0996 (17)
C20	0.6342 (3)	0.3043 (9)	0.3452 (5)	0.155 (3)
H20A	0.6380	0.1973	0.3502	0.233*
H20B	0.6398	0.3363	0.3064	0.233*
H20C	0.5965	0.3329	0.3326	0.233*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0438 (3)	0.0778 (3)	0.0601 (3)	0.00039 (19)	0.0331 (2)	-0.0105 (2)
O1	0.0482 (14)	0.0878 (19)	0.0793 (19)	-0.0015 (12)	0.0420 (14)	-0.0218 (14)
O2	0.0553 (16)	0.092 (2)	0.077 (2)	-0.0088 (14)	0.0396 (15)	-0.0233 (16)
O3	0.0444 (15)	0.107 (2)	0.092 (2)	-0.0008 (13)	0.0398 (15)	-0.0396 (17)
O4	0.094 (2)	0.116 (2)	0.095 (2)	-0.0078 (19)	0.076 (2)	-0.0023 (19)

O5	0.0635 (17)	0.086 (2)	0.078 (2)	0.0096 (14)	0.0498 (15)	-0.0068 (15)
O6	0.172 (4)	0.111 (3)	0.147 (4)	0.017 (3)	0.123 (4)	0.000 (3)
N1	0.062 (3)	0.237 (6)	0.069 (3)	0.002 (3)	0.043 (2)	0.012 (3)
N2	0.069 (2)	0.094 (3)	0.084 (3)	-0.0183 (19)	0.049 (2)	-0.030 (2)
N3	0.104 (4)	0.096 (3)	0.117 (4)	0.025 (3)	0.070 (3)	0.018 (3)
C1	0.048 (2)	0.069 (2)	0.060 (2)	0.0024 (18)	0.0350 (19)	-0.0031 (19)
C2	0.0444 (19)	0.061 (2)	0.049 (2)	0.0049 (14)	0.0307 (17)	0.0014 (15)
C3	0.047 (2)	0.069 (2)	0.060 (2)	0.0050 (17)	0.0333 (19)	-0.0123 (19)
C4	0.047 (2)	0.076 (2)	0.058 (2)	0.0005 (17)	0.0308 (18)	-0.0182 (19)
C5	0.0406 (18)	0.066 (2)	0.064 (2)	0.0024 (16)	0.0320 (17)	-0.0103 (19)
C6	0.052 (2)	0.063 (2)	0.074 (3)	0.0047 (17)	0.044 (2)	-0.0121 (19)
C7	0.049 (2)	0.060 (2)	0.059 (2)	0.0008 (15)	0.0335 (18)	-0.0095 (17)
C8	0.042 (2)	0.078 (2)	0.071 (3)	-0.0061 (17)	0.0349 (19)	-0.020 (2)
C9	0.063 (3)	0.064 (2)	0.099 (4)	0.0134 (19)	0.046 (3)	0.000 (2)
C10	0.060 (2)	0.071 (2)	0.076 (3)	-0.0045 (19)	0.042 (2)	0.005 (2)
C11	0.0364 (18)	0.067 (2)	0.063 (2)	-0.0029 (15)	0.0306 (17)	-0.0053 (18)
C12	0.0427 (19)	0.070 (2)	0.064 (2)	0.0070 (16)	0.0313 (18)	0.0011 (19)
C13	0.045 (2)	0.085 (3)	0.064 (2)	0.0033 (18)	0.0356 (19)	-0.005 (2)
C14	0.044 (2)	0.088 (3)	0.064 (3)	-0.0047 (19)	0.0354 (19)	-0.009 (2)
C15	0.080 (4)	0.155 (5)	0.082 (4)	0.006 (4)	0.028 (3)	0.022 (4)
C16	0.105 (4)	0.109 (4)	0.104 (4)	-0.023 (3)	0.052 (4)	0.005 (3)
C17	0.157 (7)	0.146 (6)	0.115 (6)	-0.024 (6)	0.000 (5)	-0.023 (5)
C18	0.159 (6)	0.149 (6)	0.153 (6)	0.025 (5)	0.121 (6)	0.012 (5)
C19	0.126 (5)	0.068 (3)	0.117 (5)	0.005 (3)	0.073 (4)	0.005 (3)
C20	0.125 (6)	0.154 (6)	0.180 (8)	-0.054 (5)	0.077 (6)	-0.062 (6)

Geometric parameters (Å, °)

Zn1—O1	1.949 (3)	C6—H6	0.9300
Zn1—O5 ⁱ	1.952 (3)	C7—H7	0.9300
Zn1—N1	1.996 (4)	C8—C9	1.358 (6)
Zn1—N2	2.047 (4)	C8—C13	1.358 (5)
O1—C1	1.275 (4)	C9—C10	1.380 (6)
O2—C1	1.238 (4)	C9—H9	0.9300
O3—C5	1.372 (4)	C10—C11	1.377 (5)
O3—C8	1.407 (4)	C10—H10	0.9300
O4—C14	1.228 (5)	C11—C12	1.379 (5)
O5—C14	1.267 (5)	C11—C14	1.501 (5)
O5—Zn1 ⁱⁱ	1.952 (3)	C12—C13	1.378 (5)
O6—C19	1.246 (6)	C12—H12	0.9300
N1—C15	1.374 (7)	C13—H13	0.9300
N1—H1A	0.9000	C15—H15A	0.9600
N1—H1B	0.9000	C15—H15B	0.9600
N2—C16	1.450 (6)	C15—H15C	0.9600
N2—H2A	0.9000	C16—H16A	0.9600
N2—H2B	0.9000	C16—H16B	0.9600
N3—C19	1.302 (7)	C16—H16C	0.9600
N3—C17	1.462 (8)	C17—H17A	0.9600
N3—C18	1.472 (7)	C17—H17B	0.9600

supplementary materials

C1—C2	1.488 (5)	C17—H17C	0.9600
C2—C7	1.386 (4)	C18—H18A	0.9600
C2—C3	1.393 (5)	C18—H18B	0.9600
C3—C4	1.369 (5)	C18—H18C	0.9600
C3—H3	0.9300	C19—C20	1.460 (9)
C4—C5	1.386 (5)	C20—H20A	0.9600
C4—H4	0.9300	C20—H20B	0.9600
C5—C6	1.380 (5)	C20—H20C	0.9600
C6—C7	1.377 (5)		
O1—Zn1—O5 ⁱ	106.28 (11)	C10—C9—H9	120.2
O1—Zn1—N1	114.24 (15)	C11—C10—C9	119.9 (4)
O5 ⁱ —Zn1—N1	114.99 (17)	C11—C10—H10	120.1
O1—Zn1—N2	115.75 (14)	C9—C10—H10	120.1
O5 ⁱ —Zn1—N2	98.65 (12)	C10—C11—C12	118.7 (3)
N1—Zn1—N2	106.15 (19)	C10—C11—C14	120.2 (4)
C1—O1—Zn1	110.9 (2)	C12—C11—C14	121.0 (3)
C5—O3—C8	118.1 (3)	C13—C12—C11	121.6 (4)
C14—O5—Zn1 ⁱⁱ	121.1 (3)	C13—C12—H12	119.2
C15—N1—Zn1	120.9 (3)	C11—C12—H12	119.2
C15—N1—H1A	107.1	C8—C13—C12	118.0 (4)
Zn1—N1—H1A	107.1	C8—C13—H13	121.0
C15—N1—H1B	107.1	C12—C13—H13	121.0
Zn1—N1—H1B	107.1	O4—C14—O5	124.7 (4)
H1A—N1—H1B	106.8	O4—C14—C11	120.0 (4)
C16—N2—Zn1	114.2 (3)	O5—C14—C11	115.3 (4)
C16—N2—H2A	108.7	N1—C15—H15A	109.5
Zn1—N2—H2A	108.7	N1—C15—H15B	109.5
C16—N2—H2B	108.7	H15A—C15—H15B	109.5
Zn1—N2—H2B	108.7	N1—C15—H15C	109.5
H2A—N2—H2B	107.6	H15A—C15—H15C	109.5
C19—N3—C17	122.3 (6)	H15B—C15—H15C	109.5
C19—N3—C18	123.1 (6)	N2—C16—H16A	109.5
C17—N3—C18	114.7 (6)	N2—C16—H16B	109.5
O2—C1—O1	123.1 (3)	H16A—C16—H16B	109.5
O2—C1—C2	120.5 (3)	N2—C16—H16C	109.5
O1—C1—C2	116.4 (3)	H16A—C16—H16C	109.5
C7—C2—C3	117.9 (3)	H16B—C16—H16C	109.5
C7—C2—C1	120.7 (3)	N3—C17—H17A	109.5
C3—C2—C1	121.3 (3)	N3—C17—H17B	109.5
C4—C3—C2	121.7 (3)	H17A—C17—H17B	109.5
C4—C3—H3	119.2	N3—C17—H17C	109.5
C2—C3—H3	119.2	H17A—C17—H17C	109.5
C3—C4—C5	119.5 (3)	H17B—C17—H17C	109.5
C3—C4—H4	120.3	N3—C18—H18A	109.5
C5—C4—H4	120.3	N3—C18—H18B	109.5
O3—C5—C6	124.4 (3)	H18A—C18—H18B	109.5
O3—C5—C4	115.8 (3)	N3—C18—H18C	109.5
C6—C5—C4	119.8 (3)	H18A—C18—H18C	109.5

C7—C6—C5	120.2 (3)	H18B—C18—H18C	109.5
C7—C6—H6	119.9	O6—C19—N3	120.7 (6)
C5—C6—H6	119.9	O6—C19—C20	122.5 (7)
C6—C7—C2	120.9 (3)	N3—C19—C20	116.7 (6)
C6—C7—H7	119.5	C19—C20—H20A	109.5
C2—C7—H7	119.5	C19—C20—H20B	109.5
C9—C8—C13	122.1 (4)	H20A—C20—H20B	109.5
C9—C8—O3	118.7 (4)	C19—C20—H20C	109.5
C13—C8—O3	119.2 (4)	H20A—C20—H20C	109.5
C8—C9—C10	119.7 (4)	H20B—C20—H20C	109.5
C8—C9—H9	120.2		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1B \cdots O4 ⁱⁱⁱ	0.90	2.21	2.991 (5)	145
N2—H2A \cdots O2 ^{iv}	0.90	2.11	2.966 (4)	159
N2—H2B \cdots O6 ^v	0.90	2.40	3.276 (6)	164

Symmetry codes: (iii) $-x+3/2, -y+3/2, -z+1$; (iv) $-x+2, -y+2, -z+1$; (v) $x+1/2, y+1/2, z$.

Fig. 1

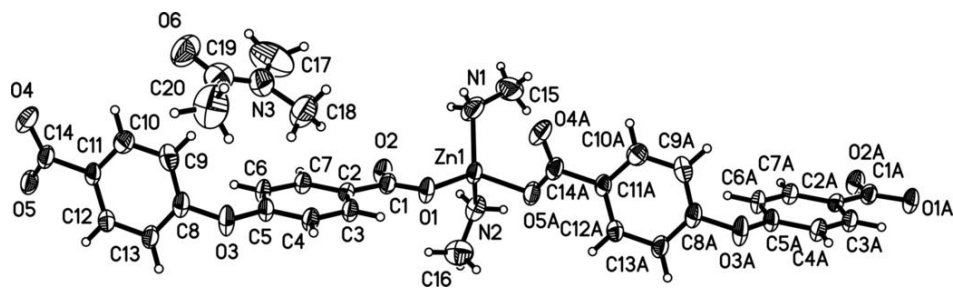


Fig. 2

