Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *catena*-Poly[[[bis(methylamine)zinc(II)]-$\mu$-4,4′-oxydibenzoato] *N*,*N*-dimethylacetamide solvate]

**Xianzhu Xu,* Peng Wang and Shujie Shi**

School of Municipal and Environmental Engineering, Harbin Institute of Technology, Harbin 150090, People's Republic of China.
Correspondence e-mail: xianzhuxu@yahoo.com.cn

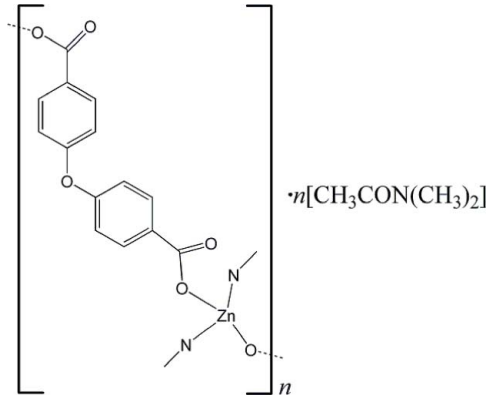
Received 18 November 2007; accepted 25 November 2007

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–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, $\{[Zn(C_{14}H_8O_5)(CH_5N)_2]\cdot C_4H_9NO\}_n$, each Zn(II) cation is tetrahedrally coordinated by two carboxylato O atoms of two oba anions ($H_2$oba 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

$[Zn(C_{14}H_8O_5)(CH_5N)_2]\cdot C_4H_9NO$
$M_r$ = 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) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.15 mm$^{-1}$
$T$ = 293 (2) K
0.35 × 0.34 × 0.15 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (Higashi, 1995)
$T_{min}$ = 0.690, $T_{max}$ = 0.850
20180 measured reflections
4942 independent reflections
2843 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$B$···O4$^{i}$ | 0.90 | 2.21 | 2.991 (5) | 145 |
| N2—H2$A$···O2$^{ii}$ | 0.90 | 2.11 | 2.966 (4) | 159 |
| N2—H2$B$···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*.

This work was supported by the National Science Foundation of China (50678045), the Science Foundation of Heilongjiang Province (E200519), the China Postdoctoral Science Foundation and Heilongjiang Postdoctoral Financial Assistance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2083).

## References

Bruker (2000). *SHELXTL*. Version 6.14. Bruker AXS Inc., Madison, Wisconsin, USA.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Kondo, M., Irie, Y., Shimizu, Y., Miyazawa, M., Kawaguchi, H., Nakamura, A., Naito, T., Maeda, K. & Uchida, F. (2004). *Inorg. Chem.* **43**, 6139–6141.
Luo, J., Hong, M., Wang, R., Cao, R., Han, L. & Lin, Z. (2003). *Eur. J. Inorg. Chem.* pp. 2705–2710.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sun, C.-Y., Zheng, X.-J., Song, G., Li, L.-C. & Jin, L.-P. (2005). *Eur. J. Inorg. Chem.* pp. 4150–4159.
Yaghi, O. M., Li, H., Davis, C., Richardson, D. & Groy, T. L. (1998). *Acc. Chem. Res.* **31**, 474–484.

# supporting information

*Acta Cryst.* (2008). E**64**, m90 [https://doi.org/10.1107/S1600536807063155]

## *catena*-Poly[[[bis(methylamine)zinc(II)]-$\mu$-4,4′-oxydibenzoato] *N*,*N*-dimethylacetamide solvate]

**Xianzhu Xu, Peng Wang and Shujie Shi**

### S1. 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) ($H_2$oba) ligand, in which two benzene moieties are linked together by a $\mu_2$-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, $[Zn(C_{14}H_8O_5)(CNH_5)_2\cdot(C_4NOH_9)]_n$, (I).

The asymmetric unit of (I) consists of one crystallogaphically 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 $\mu_2$-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 Zn···Zn distance of 14.512 (4) Å (Fig. 2). It is found that there are hydrogen bonding interactions between adjacent chains. The N—H···O 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—H···O 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).

### S2. Experimental

(I) was solvothermally prepared from a mixture of $Zn(NO_3)_2\cdot 6H_2O$ (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.

### S3. 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.

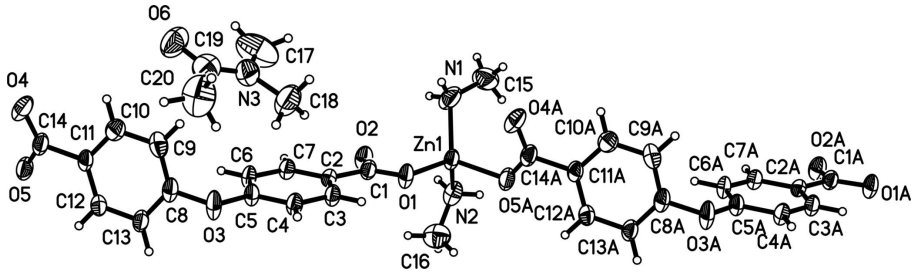



**Figure 1**

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*.].

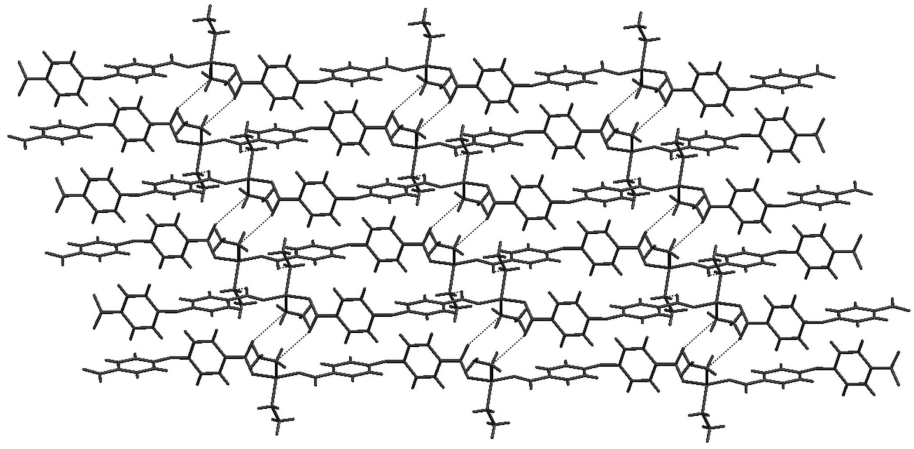


**Figure 2**

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*

$[Zn(C_{14}H_8O_5)(CH_5N)_2]\cdot C_4H_9NO$
$M_r$ = 470.82
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
*a* = 27.617 (6) Å
*b* = 8.9276 (18) Å
*c* = 21.212 (4) Å
*β* = 122.46 (3)°
*V* = 4413 (2) Å$^3$
*Z* = 8
*F*(000) = 1968
$D_x$ = 1.417 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 11100 reflections
*θ* = 3.0–27.5°
*μ* = 1.15 mm$^{-1}$
*T* = 293 K
Block, colorless
0.35 × 0.34 × 0.15 mm

*Data collection*

Rigaku RAXIS-RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (Higashi, 1995)
$T_{min}$ = 0.690, $T_{max}$ = 0.850
20180 measured reflections
4942 independent reflections
2843 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 3.0°
$h$ = −34→35
$k$ = −11→11
$l$ = −27→27

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.149
$S$ = 1.04
4942 reflections
276 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
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 3.5742P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.016
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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* |
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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 |
| 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 (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*B*···O4$^{iii}$ | 0.90 | 2.21 | 2.991 (5) | 145 |
| N2—H2*A*···O2$^{iv}$ | 0.90 | 2.11 | 2.966 (4) | 159 |
| N2—H2*B*···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) $x+1/2, y+1/2, z$.