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

# *catena*-Poly[[aquazinc(II)]-$\mu$-*N*,*N*′-bis(2-cyano-3-ethoxy-3-oxoprop-1-enyl)-benzene-1,2-diaminido]

**Monica Fuchs, Thomas Zevaco, Eckhard Dinjus and Olaf Walter*‡**

IKFT, KIT-Campus Nord, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
Correspondence e-mail: olaf.walter@ec.europa.eu

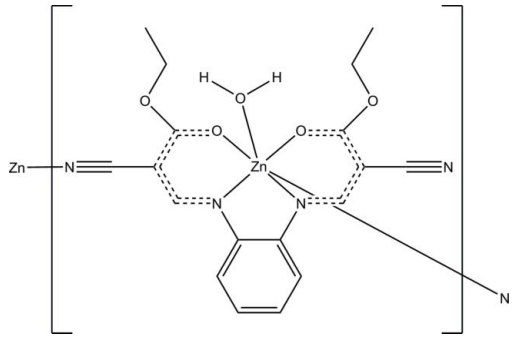
Received 21 February 2014; accepted 14 April 2014

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.023; $wR$ factor = 0.063; data-to-parameter ratio = 16.0.

The slightly yellow-coloured title complex, $[Zn(C_{18}H_{16}N_4O_4)(H_2O)]_n$, crystallizes with one molecule in the asymmetric unit. The structure clearly shows the *mer*-$\eta^4$*O*,*O*,*N*,*N*-binding mode of the *N*,*N*′-bis-(2-cyano-ethylpropenoyl)-1,2-diamidobenzene ligand stabilizing the Zn centre of a distorted octahedral environment. The fifth coordination site in one apical position is held by a coordinating solvent water molecule whereas the complete octahedral coordination sphere is completed by coordination of one N atom from a CN group of a neighbouring molecule, leading to the final polymeric structure consisting of zigzag staggered chains in parallel orientation along the *c*-axis direction. Between the coordinated water solvent molecule and the N atoms of uncoordinated cyano-groups of neighboured units, two H-bridge bonds are formed. One of these H-bridge bonds is of inter- whereas the other of intra-strand nature, leading to a two-dimensional network parallel to (110) stabilizing the supramolecular structure. Six Zn—O or Zn—N bonds are found with lengths ranging from 2.061 (1) to 2.185 (1) Å and bond angles about the Zn atom are clustered in the ranges 79.83 (4)–104.21 (4) and 167.05 (4)–170.28 (4)°.

## Related literature

The structures of $Zn^{II}$ complexes with ligands stabilizing comparable complex geometries can be found in Barnard *et al.* (2009), Ryu *et al.* (2003) or Tanase *et al.* (2001). In Tanase *et al.* (2001), the ligands show comparable *N*,*N*,*O*,*O*-coordination with respect to a different ligand backbone whereas in Ryu *et al.* (2003) and Barnard *et al.* (2009), the ligands with *N*,*N*,*N*,*N*-coordination are diaminobenzene derivatives. In Fuchs *et al.* (2014), a mononuclear Zn complex is presented with the same ligand but a dmso molecule in the coordination sphere of the metal stabilizing a different complex geometry. For the synthesis, see: Jäger *et al.* (1985).




## Experimental

### Crystal data

$[Zn(C_{18}H_{16}N_4O_4)(H_2O)]$
$M_r$ = 435.73
Orthorhombic, *Pbca*
$a$ = 13.9312 (11) Å
$b$ = 9.2315 (7) Å
$c$ = 27.423 (2) Å
$V$ = 3526.7 (5) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.43 mm$^{-1}$
$T$ = 100 K
0.10 × 0.09 × 0.07 mm

### Data collection

Bruker APEXII Quazar diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.928, $T_{max}$ = 0.953
60234 measured reflections
4294 independent reflections
3812 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.063
$S$ = 1.04
4294 reflections
268 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H51···N4$^{i}$ | 0.79 (2) | 2.21 (2) | 2.9823 (17) | 168 (2) |
| O5—H52···N4$^{ii}$ | 0.83 (2) | 2.12 (2) | 2.9405 (16) | 174 (2) |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors gratefully acknowledge financial support for their work from the Karlsruhe Institute for Technology.

‡ present address: European Commission, Joint Research Centre, Institute for Transuranium Elements, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany.

Supporting information for this paper is available from the IUCr electronic archives (Reference: NK2220).

## References


Barnard, P. J., Holland, J. P., Bayly, S. R., Wadas, T. J., Anderson, C. J. & Dilworth, J. R. (2009). *Inorg. Chem.* **48**, 7117–7126.

Bruker (2007). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Fuchs, M. A., Staudt, S., Altesleben, C., Walter, O., Zevaco, T. A. & Dinjus, E. (2014). *Dalton Trans.* **43**, 2344–2347.

Jäger, E.-G., Häussler, E., Rudolph, M. & Schneider, A. (1985). *Z. Anorg. Allg. Chem.* **525**, 67–85.

Ryu, J. Y., Lee, J. Y., Seo, J. S., Kim, C. & Kim, Y. (2003). *Appl. Organomet. Chem.* **17**, 803–804.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Tanase, T., Inukai, H., Onaka, T., Kato, M., Yano, S. & Lippard, S. J. (2001). *Inorg. Chem.* **40**, 3943–3953.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supporting information

*Acta Cryst.* (2014). E**70**, m187–m188 [doi:10.1107/S1600536814008381]

## *catena*-Poly[[aquazinc(II)]-$\mu$-*N*,*N*′-bis(2-cyano-3-ethoxy-3-oxoprop-1-enyl)benzene-1,2-diaminido]

**Monica Fuchs, Thomas Zevaco, Eckhard Dinjus and Olaf Walter**

### S1. Comment

The polymeric chain structure of title compound can be described by single units of to a Zn-centre *mer*-$\eta^4$-O,*O*-N,*N*-coordinated *N*,*N*′-bis-(2-cyano-ethylpropenoyl)-1,2-diamidobenzene ligand with a water solvent molecule in one apical position over the coordination plane. The polymeric structure and completeness of the coordination sphere is obtained by intermolecular coordination of a N-atom of a neighboured molecule finally forming the polymeric catena-structure with Zn-atoms in distorted octahedral geometry. The Zn-O bond distances involving the ligand are accordingly determined to 2.061 (1) and 2.111 (1) Å and agree with the corresponding Zn-N bond lengths of 2.063 (1) and 2.075 (1) Å. The Zn-O bond distance to the coordinated water solvent molecule is elongated to 2.185 (1) Å but still shorter than the one to the N-atom of the cyano-group of a neighbour molecule (2.232 (1) Å) which finally leads to the formation of the polymeric catena structure. The four donor atoms of the ligand in its mer-coordination form a coordination plane, they deviate from this by in the mean 0.09 Å so that the position of the central Zn-atom with a deviation from this plane of 0.04 Å can be regarded as placed well within this plane. These findings are in agreement with its embedding in the centre of a distorted octahedron. With respect to the flexibility of Zn(ii) in the formation of different complex geometries the complex fits within Fuchs *et al.* (2014), Barnard *et al.* (2009), Ryu *et al.* (2003), or Tanase *et al.* (2001), even if for the latter case larger structural deviations are observed due to larger structural differences in the ligand constitution.

### S2. Experimental

*N*,*N*′-Bis(2-cyano-2-ethoxycarbonylethenyl)benzene-1,2-diamine was synthesized from 1,2-diaminobenzene and 2-cyano-3-methoxypropanoic acid ethyl ester according to Jäger *et al.* (1985). Under an argon atmosphere 5.00 g (14.1 mmol) *N*,*N*′-bis(2-cyanoethylpropenoyl)-1,2-diaminobenzene is suspended in 75 ml thf. 14.1 ml diethyl zinc solution (1*M* in hexane, 14.1 mmol) is added under stirring. The reaction mixture is stirred overnight, the solvent is removed under reduced pressure leaving 2 as a deep yellow solid (5.88 g, 14.1 mmol, 99.8%). Single crystals are obtained by re-crystallization from dimethylsulfoxide in an open laboratory beaker glass.

### S3. Refinement

The positions of the H atoms are calculated on geometrical positions according to the hybridization of the atoms they are bound to. The isotropic U values of these hydrogen atoms are refined in groups with respect to the hybridization of the atoms where they are bound to. A riding model was applied for the refinement of the H-atoms of the methyl-groups. The positions of H51 and H52 are located in the fourier map and refined together with their isotropic displacement parameter leading to O—H distances of 0.785 (24) and 0.826 (24) Å and a bond angle H—O—H of 111 (2)°.

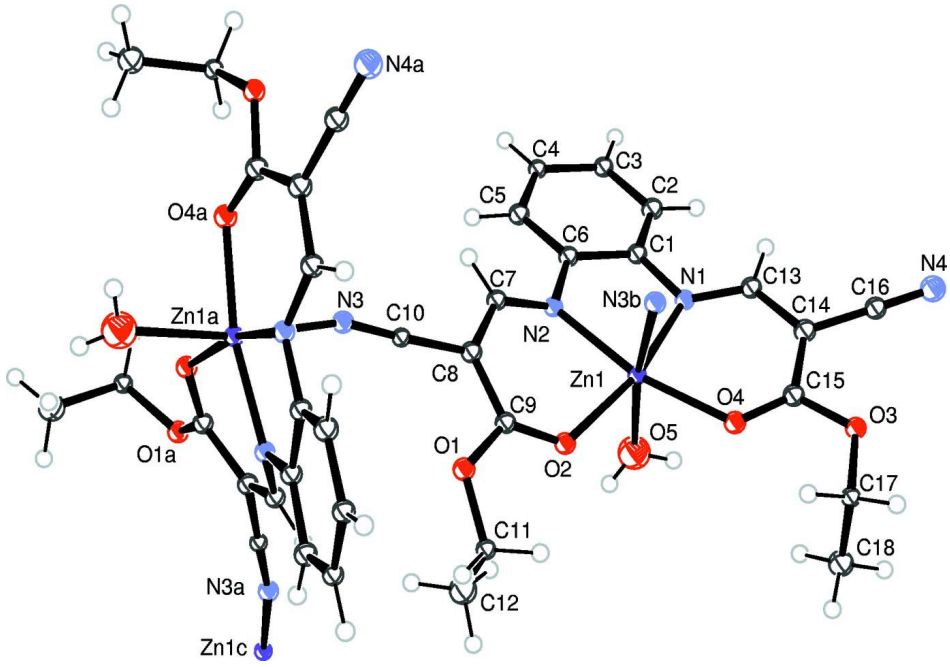



**Figure 1**

View to the a part of the polymeric chain in the molecular structure of *catena*-Poly-{*aqua*-$\eta^4$-*N*,*N*,*O*,*O*- $\mu$-*N*′-cyano-[*N*,*N*′-bis-(2-cyano-ethylpropenoyl)- 1,2-diamidobenzene]zinc(II)}; ellipsoids at 50% probability level (Symmetry codes for atoms with suffix a: -*x*, -0.5 + *y*, 0.5 - *z*, -*z* + 1; with suffix b: -*x*, 0.5 + *y*, 0.5 - *z*; and with suffix c: *x*, *y* - 1, *z*. For the residues with suffix b, c there is only one atom of the unit represented in the drawing).

**_catena_-Poly[[aquazinc(II)]-$\mu$-*N*,*N*′-bis(2-cyano-3-ethoxy-3-oxoprop-1-enyl)benzene-1,2-diaminido]**

*Crystal data*

$[Zn(C_{18}H_{16}N_4O_4)(H_2O)]$
$M_r$ = 435.73
Orthorhombic, *Pbca*
*a* = 13.9312 (11) Å
*b* = 9.2315 (7) Å
*c* = 27.423 (2) Å
*V* = 3526.7 (5) Å$^3$
*Z* = 8
*F*(000) = 1792
$D_x$ = 1.641 Mg m$^{-3}$
Mo *K*$\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9786 reflections
$\theta$ = 5.5–56.7°
$\mu$ = 1.43 mm$^{-1}$
*T* = 100 K
Quader, light yellow
0.10 × 0.09 × 0.07 mm

*Data collection*

Bruker APEXII Quazar diffractometer
Radiation source: microfocus sealed I$\mu$s tube
Detector resolution: 66 pixels mm$^{-1}$
combined $\varphi$– and $\omega$–scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.928, $T_{max}$ = 0.953
60234 measured reflections
4294 independent reflections
3812 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025
$\theta_{max}$ = 28.6°, $\theta_{min}$ = 1.5°
*h* = −18→18
*k* = −11→12
*l* = −36→36

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.063$
$S = 1.04$
4294 reflections
268 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 2.5256P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ e Å$^{-3}$

*Special details*

**Experimental**. Spectroscopic data: $^1$H NMR (400 MHz, dmso-$d_6$): $\delta$ = 7.56, dd, $^3J_{HH}$= 6.1 Hz, $^4J_{HH}$= 3.1 Hz, 2H, H(arom); 7.05, dd, $^3J_{HH}$= 6.1 Hz, $^4J_{HH}$= 3.1 Hz, 2H, H(arom); 4.25, q, $^3J_{HH}$= 7.1 Hz, 4H, $OCH_2$; 1.29, t, $^3J_{HH}$= 7.1 Hz, 3H, $CH_3$. $^{13}$C NMR (100 MHz, dmso-$d_6$): $\delta$ = 177.77; 156.27; 138.01; 124.39; 121.19; 114.89; 68.05; 60.24; 14.13. ESI-MS (m/*z*, %): 417 (100) $[M]^+$, 418 (23) $[M+H]^+$, 835 (15) $[2M+H]^+$. IR (KBr, cm$^{-1}$): 2203; 1625; 1023; 748. UV/VIS ($CH_2Cl_2$): $\lambda$max ($\varepsilon$) (nm, mol$^{-1}$dm$^3$cm$^{-1}$): 241 (16522),

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.50231 (2) | 0.19828 (2) | 0.37062 (2) | 0.00984 (6) |
| O1 | 0.36966 (7) | −0.12202 (11) | 0.28089 (3) | 0.0161 (2) |
| O2 | 0.41756 (7) | 0.03163 (10) | 0.34019 (3) | 0.01339 (19) |
| O3 | 0.34564 (7) | 0.50414 (11) | 0.45261 (4) | 0.0178 (2) |
| O4 | 0.40466 (7) | 0.31264 (10) | 0.41189 (3) | 0.01378 (19) |
| O5 | 0.51731 (9) | 0.06806 (12) | 0.43673 (4) | 0.0195 (2) |
| H51 | 0.5088 (13) | −0.014 (3) | 0.4428 (7) | 0.026 (5)* |
| H52 | 0.5083 (14) | 0.119 (3) | 0.4611 (9) | 0.035 (6)* |
| N1 | 0.61097 (8) | 0.33622 (12) | 0.39350 (4) | 0.0107 (2) |
| N2 | 0.61290 (8) | 0.12889 (12) | 0.32640 (4) | 0.0105 (2) |
| N3 | 0.53603 (9) | −0.15532 (13) | 0.19114 (4) | 0.0150 (2) |
| N4 | 0.50550 (9) | 0.76393 (14) | 0.47291 (4) | 0.0168 (2) |
| C1 | 0.70235 (10) | 0.29789 (13) | 0.37492 (4) | 0.0104 (2) |
| C2 | 0.79016 (10) | 0.35644 (14) | 0.38978 (5) | 0.0127 (2) |
| H2 | 0.7915 | 0.4271 | 0.4150 | 0.017 (2)* |
| C3 | 0.87537 (10) | 0.31270 (14) | 0.36822 (5) | 0.0131 (3) |
| H3 | 0.9342 | 0.3561 | 0.3779 | 0.017 (2)* |
| C4 | 0.87557 (10) | 0.20536 (14) | 0.33235 (5) | 0.0133 (3) |
| H4 | 0.9342 | 0.1760 | 0.3177 | 0.017 (2)* |
| C5 | 0.78987 (10) | 0.14213 (14) | 0.31837 (5) | 0.0129 (3) |
| H5 | 0.7900 | 0.0664 | 0.2949 | 0.017 (2)* |
| C6 | 0.70280 (10) | 0.18889 (14) | 0.33858 (4) | 0.0106 (2) |
| C7 | 0.60147 (10) | 0.06126 (13) | 0.28535 (4) | 0.0109 (2) |

| | | | | |
|---|---|---|---|---|
| H7 | 0.6540 | 0.0611 | 0.2633 | 0.011 (3)* |
| C8 | 0.51716 (10) | −0.01222 (15) | 0.27076 (5) | 0.0117 (2) |
| C9 | 0.43345 (10) | −0.02889 (14) | 0.30044 (4) | 0.0116 (2) |
| C10 | 0.52453 (9) | −0.09216 (15) | 0.22679 (5) | 0.0117 (2) |
| C11 | 0.29041 (10) | −0.17030 (16) | 0.31142 (5) | 0.0173 (3) |
| H11A | 0.2381 | −0.2080 | 0.2906 | 0.027 (2)* |
| H11B | 0.2650 | −0.0872 | 0.3303 | 0.027 (2)* |
| C12 | 0.32314 (12) | −0.28751 (16) | 0.34613 (6) | 0.0219 (3) |
| H12A | 0.3535 | −0.3660 | 0.3276 | 0.027 (2)* |
| H12B | 0.2677 | −0.3256 | 0.3640 | 0.027 (2)* |
| H12C | 0.3695 | −0.2470 | 0.3693 | 0.027 (2)* |
| C13 | 0.59711 (10) | 0.46053 (14) | 0.41516 (4) | 0.0111 (2) |
| H13 | 0.6510 | 0.5226 | 0.4188 | 0.011 (3)* |
| C14 | 0.50756 (10) | 0.51032 (15) | 0.43377 (5) | 0.0121 (3) |
| C16 | 0.50610 (9) | 0.64963 (16) | 0.45565 (5) | 0.0132 (3) |
| C15 | 0.41851 (10) | 0.43285 (14) | 0.43127 (4) | 0.0126 (3) |
| C17 | 0.25169 (11) | 0.43452 (17) | 0.45179 (5) | 0.0218 (3) |
| H17A | 0.2435 | 0.3821 | 0.4206 | 0.037 (2)* |
| H17B | 0.2010 | 0.5093 | 0.4539 | 0.037 (2)* |
| C18 | 0.24101 (12) | 0.32972 (19) | 0.49360 (5) | 0.0272 (4) |
| H18A | 0.2945 | 0.2609 | 0.4932 | 0.037 (2)* |
| H18B | 0.1803 | 0.2770 | 0.4903 | 0.037 (2)* |
| H18C | 0.2412 | 0.3832 | 0.5245 | 0.037 (2)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.01164 (9) | 0.00914 (9) | 0.00874 (8) | −0.00053 (5) | 0.00045 (5) | −0.00140 (5) |
| O1 | 0.0152 (5) | 0.0196 (5) | 0.0134 (4) | −0.0059 (4) | 0.0007 (3) | −0.0042 (4) |
| O2 | 0.0143 (5) | 0.0136 (5) | 0.0122 (4) | −0.0016 (4) | 0.0011 (3) | −0.0024 (3) |
| O3 | 0.0141 (5) | 0.0166 (5) | 0.0226 (5) | 0.0008 (4) | 0.0038 (4) | −0.0058 (4) |
| O4 | 0.0156 (5) | 0.0132 (5) | 0.0126 (4) | −0.0006 (4) | 0.0013 (4) | −0.0028 (3) |
| O5 | 0.0387 (7) | 0.0089 (5) | 0.0110 (5) | 0.0003 (4) | 0.0024 (4) | −0.0005 (4) |
| N1 | 0.0131 (5) | 0.0096 (5) | 0.0095 (5) | 0.0002 (4) | 0.0000 (4) | −0.0002 (4) |
| N2 | 0.0121 (5) | 0.0092 (5) | 0.0102 (5) | −0.0003 (4) | −0.0010 (4) | −0.0007 (4) |
| N3 | 0.0143 (6) | 0.0172 (6) | 0.0136 (5) | −0.0040 (5) | −0.0001 (4) | −0.0026 (4) |
| N4 | 0.0218 (7) | 0.0124 (6) | 0.0161 (6) | 0.0003 (5) | 0.0043 (4) | −0.0015 (5) |
| C1 | 0.0134 (6) | 0.0088 (6) | 0.0092 (5) | 0.0013 (5) | −0.0007 (4) | 0.0015 (4) |
| C2 | 0.0163 (7) | 0.0097 (6) | 0.0120 (6) | −0.0008 (5) | −0.0023 (5) | −0.0005 (4) |
| C3 | 0.0138 (6) | 0.0111 (6) | 0.0142 (6) | −0.0024 (5) | −0.0030 (5) | 0.0020 (5) |
| C4 | 0.0122 (6) | 0.0136 (6) | 0.0140 (6) | 0.0007 (5) | 0.0015 (5) | 0.0016 (5) |
| C5 | 0.0153 (6) | 0.0116 (6) | 0.0120 (6) | 0.0004 (5) | −0.0004 (5) | −0.0018 (5) |
| C6 | 0.0137 (6) | 0.0086 (6) | 0.0097 (5) | −0.0005 (5) | −0.0010 (4) | 0.0013 (4) |
| C7 | 0.0130 (6) | 0.0095 (6) | 0.0101 (5) | 0.0006 (5) | 0.0006 (4) | 0.0004 (4) |
| C8 | 0.0140 (6) | 0.0113 (6) | 0.0098 (6) | −0.0011 (5) | −0.0008 (5) | −0.0012 (5) |
| C9 | 0.0137 (6) | 0.0095 (6) | 0.0116 (5) | −0.0001 (5) | −0.0022 (5) | 0.0006 (4) |
| C10 | 0.0106 (6) | 0.0118 (6) | 0.0126 (6) | −0.0026 (5) | −0.0014 (5) | 0.0021 (5) |
| C11 | 0.0121 (6) | 0.0193 (7) | 0.0205 (6) | −0.0047 (5) | 0.0026 (5) | −0.0045 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12 | 0.0253 (8) | 0.0162 (7) | 0.0243 (7) | −0.0028 (6) | 0.0065 (6) | −0.0015 (5) |
| C13 | 0.0147 (6) | 0.0103 (6) | 0.0085 (5) | −0.0008 (5) | −0.0014 (5) | 0.0003 (4) |
| C14 | 0.0165 (7) | 0.0095 (6) | 0.0105 (6) | 0.0014 (5) | 0.0005 (4) | −0.0012 (5) |
| C16 | 0.0156 (7) | 0.0137 (7) | 0.0103 (6) | 0.0005 (5) | 0.0021 (4) | 0.0016 (5) |
| C15 | 0.0151 (7) | 0.0131 (6) | 0.0096 (5) | 0.0024 (5) | 0.0008 (5) | 0.0009 (5) |
| C17 | 0.0116 (7) | 0.0269 (8) | 0.0268 (7) | 0.0002 (6) | 0.0006 (5) | −0.0103 (6) |
| C18 | 0.0210 (8) | 0.0365 (9) | 0.0242 (7) | −0.0136 (7) | 0.0030 (6) | −0.0085 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—O4 | 2.0606 (9) | C3—H3 | 0.9500 |
| Zn1—N2 | 2.0626 (11) | C4—C5 | 1.3831 (19) |
| Zn1—N1 | 2.0754 (11) | C4—H4 | 0.9500 |
| Zn1—O2 | 2.1112 (9) | C5—C6 | 1.4016 (18) |
| Zn1—O5 | 2.1852 (11) | C5—H5 | 0.9500 |
| Zn1—N3$^{i}$ | 2.2317 (11) | C7—C8 | 1.4141 (18) |
| O1—C9 | 1.3476 (16) | C7—H7 | 0.9500 |
| O1—C11 | 1.4555 (16) | C8—C10 | 1.4175 (18) |
| O2—C9 | 1.2447 (15) | C8—C9 | 1.4304 (18) |
| O3—C15 | 1.3440 (16) | C11—C12 | 1.511 (2) |
| O3—C17 | 1.4582 (18) | C11—H11A | 0.9900 |
| O4—C15 | 1.2455 (16) | C11—H11B | 0.9900 |
| O5—H51 | 0.79 (2) | C12—H12A | 0.9800 |
| O5—H52 | 0.83 (2) | C12—H12B | 0.9800 |
| N1—C13 | 1.3064 (16) | C12—H12C | 0.9800 |
| N1—C1 | 1.4161 (17) | C13—C14 | 1.4242 (18) |
| N2—C7 | 1.2970 (16) | C13—H13 | 0.9500 |
| N2—C6 | 1.4097 (17) | C14—C16 | 1.4192 (19) |
| N3—C10 | 1.1493 (17) | C14—C15 | 1.4336 (19) |
| N3—Zn1$^{ii}$ | 2.2317 (11) | C17—C18 | 1.508 (2) |
| N4—C16 | 1.157 (2) | C17—H17A | 0.9900 |
| C1—C2 | 1.3982 (18) | C17—H17B | 0.9900 |
| C1—C6 | 1.4163 (17) | C18—H18A | 0.9800 |
| C2—C3 | 1.3862 (19) | C18—H18B | 0.9800 |
| C2—H2 | 0.9500 | C18—H18C | 0.9800 |
| C3—C4 | 1.3962 (18) | | |

| | | | |
|---|---|---|---|
| O4—Zn1—N2 | 167.20 (4) | N2—C6—C1 | 116.22 (12) |
| O4—Zn1—N1 | 90.06 (4) | N2—C7—C8 | 125.34 (12) |
| N2—Zn1—N1 | 79.83 (4) | N2—C7—H7 | 117.3 |
| O4—Zn1—O2 | 102.78 (4) | C8—C7—H7 | 117.3 |
| N2—Zn1—O2 | 87.65 (4) | C7—C8—C10 | 115.48 (12) |
| N1—Zn1—O2 | 167.05 (4) | C7—C8—C9 | 124.60 (12) |
| O4—Zn1—O5 | 83.64 (4) | C10—C8—C9 | 119.15 (12) |
| N2—Zn1—O5 | 104.21 (4) | O2—C9—O1 | 121.16 (12) |
| N1—Zn1—O5 | 90.97 (4) | O2—C9—C8 | 126.50 (12) |
| O2—Zn1—O5 | 88.89 (4) | O1—C9—C8 | 112.33 (11) |
| O4—Zn1—N3$^{i}$ | 87.06 (4) | N3—C10—C8 | 176.10 (14) |

| | | | |
|---|---|---|---|
| N2—Zn1—N3$^{i}$ | 85.45 (4) | O1—C11—C12 | 110.65 (12) |
| N1—Zn1—N3$^{i}$ | 91.86 (4) | O1—C11—H11A | 109.5 |
| O2—Zn1—N3$^{i}$ | 90.43 (4) | C12—C11—H11A | 109.5 |
| O5—Zn1—N3$^{i}$ | 170.28 (4) | O1—C11—H11B | 109.5 |
| C9—O1—C11 | 117.81 (10) | C12—C11—H11B | 109.5 |
| C9—O2—Zn1 | 125.02 (9) | H11A—C11—H11B | 108.1 |
| C15—O3—C17 | 117.09 (11) | C11—C12—H12A | 109.5 |
| C15—O4—Zn1 | 126.05 (9) | C11—C12—H12B | 109.5 |
| Zn1—O5—H51 | 133.8 (15) | H12A—C12—H12B | 109.5 |
| Zn1—O5—H52 | 110.0 (16) | C11—C12—H12C | 109.5 |
| H51—O5—H52 | 111 (2) | H12A—C12—H12C | 109.5 |
| C13—N1—C1 | 121.06 (11) | H12B—C12—H12C | 109.5 |
| C13—N1—Zn1 | 124.65 (9) | N1—C13—C14 | 125.16 (12) |
| C1—N1—Zn1 | 113.18 (8) | N1—C13—H13 | 117.4 |
| C7—N2—C6 | 120.25 (11) | C14—C13—H13 | 117.4 |
| C7—N2—Zn1 | 124.61 (9) | C16—C14—C13 | 117.16 (12) |
| C6—N2—Zn1 | 113.73 (8) | C16—C14—C15 | 117.38 (12) |
| C10—N3—Zn1$^{ii}$ | 156.83 (11) | C13—C14—C15 | 125.44 (12) |
| C2—C1—N1 | 125.81 (11) | N4—C16—C14 | 179.05 (15) |
| C2—C1—C6 | 118.41 (12) | O4—C15—O3 | 120.33 (12) |
| N1—C1—C6 | 115.77 (12) | O4—C15—C14 | 126.80 (12) |
| C3—C2—C1 | 120.83 (12) | O3—C15—C14 | 112.87 (11) |
| C3—C2—H2 | 119.6 | O3—C17—C18 | 111.08 (12) |
| C1—C2—H2 | 119.6 | O3—C17—H17A | 109.4 |
| C2—C3—C4 | 120.58 (13) | C18—C17—H17A | 109.4 |
| C2—C3—H3 | 119.7 | O3—C17—H17B | 109.4 |
| C4—C3—H3 | 119.7 | C18—C17—H17B | 109.4 |
| C5—C4—C3 | 119.55 (13) | H17A—C17—H17B | 108.0 |
| C5—C4—H4 | 120.2 | C17—C18—H18A | 109.5 |
| C3—C4—H4 | 120.2 | C17—C18—H18B | 109.5 |
| C4—C5—C6 | 120.49 (12) | H18A—C18—H18B | 109.5 |
| C4—C5—H5 | 119.8 | C17—C18—H18C | 109.5 |
| C6—C5—H5 | 119.8 | H18A—C18—H18C | 109.5 |
| C5—C6—N2 | 123.66 (11) | H18B—C18—H18C | 109.5 |
| C5—C6—C1 | 120.06 (12) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H51···N4$^{iii}$ | 0.79 (2) | 2.21 (2) | 2.9823 (17) | 168 (2) |
| O5—H52···N4$^{iv}$ | 0.83 (2) | 2.12 (2) | 2.9405 (16) | 174 (2) |

Symmetry codes: (iii) *x*, *y*−1, *z*; (iv) −*x*+1, −*y*+1, −*z*+1.