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Bis[μ-bis(pyridin-2-yl)methanone oxime-κ^3N:,N',N'']bis[diacetato-κ^2O,O';κO-zinc(II)]

Guy Crundwell,* Nigel E. Crundwell and Barry L. Westcott

Central Connecticut State University, Department of Chemistry & Biochemistry, 1619 Stanley Street, New Britain, CT 06053, USA. *Correspondence e-mail: crundwellg@ccsu.edu

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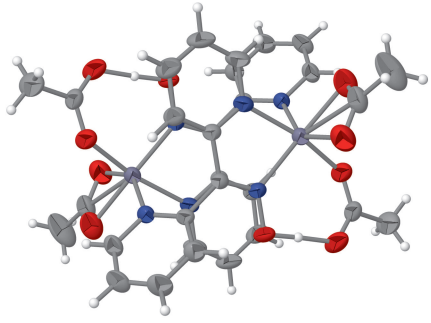
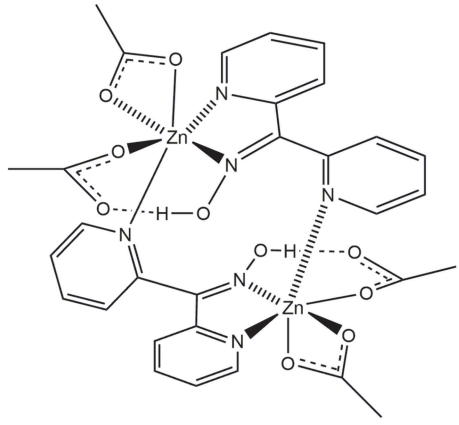
The structure of the title complex, $[Zn_2(C_2H_3O_2)_4(C_{11}H_9N_3O)_2]$, is triclinic containing half of the molecule in the asymmetric unit. Each zinc atom is coordinated to a pyridyl and oxime nitrogen from one di-2-pyridyl ketone oxime (dpko) ligand and a third nitrogen from the other dpko pyridyl ring. Additionally, each zinc is coordinated to two acetato anions, one of which is bidentate and the other monodentate. The uncoordinated oxygen of the monodentate acetato group is involved in a hydrogen bond with the oxime hydrogen. The packing in the crystal is assisted by weak C—H···O interactions between acetato groups and neighboring pyridyl rings.

3D view



Chemical scheme



Structure description

The three N atoms in dpko can act as ligands in a variety of ways. Previous reactions of Zn^{II} with dpko led to molecules of the form $Zn(dpko)Cl_2$ (Alexiou *et al.*, 2003; Gökce *et al.*, 2019) and $Zn(dpko)Br_2$ (Westcott *et al.*, 2016) where both pyridyl N atoms are bonding to the metal and the oxime group is directed away from the metal center. Dpko ligands with zinc have also been shown to retain their bidentate nature, yet they opt to bond *via* one pyridyl nitrogen and the oxime nitrogen (Tarushi *et al.*, 2013). Finally, in this complex a third motif is seen; one where a pyridyl nitrogen and oxime nitrogen bond to one zinc and the other pyridyl nitrogen binds to another. In this case a dimer is made and is analogous to Cu^{2+} complexes with dpko (Goher & Mautner, 1999) and to Mg^{2+} complexes with dpko (Milios *et al.*, 2005).

The asymmetric-unit of the the title complex, Fig. 1, comprises one-half molecule with the full molecule generated by inversion symmetry. Two acetate anions are also coordinated to the zinc. The first acetato group bonds with both O atoms at bond lengths of 2.1369 (17) and 2.289 (2) Å and the second acetato group coordinates through one oxygen at 2.0513 (14) Å. The second oxygen on the monodentate acetate is hydrogen bonded to the hydrogen on the oxime, Table 1. The packing in the crystal is assisted by

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O5	1.11 (4)	1.32 (4)	2.428 (2)	176 (3)
C2—H2···O1^{ii}	0.93	2.34	3.245 (2)	164
C3—H3···O3^{iii}	0.93	2.58	3.293 (3)	134
C9—H9···03^{iv}	0.93	2.59	3.361 (3)	141
C11—H11···O2^{i}	0.93	2.38	2.941 (3)	119

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

weak C—H···O interactions between acetato groups and neighboring pyridyl rings(Table 1).

Synthesis and crystallization

Zinc acetate dihydrate and di-2-pyridyl ketone oxime (dpko) were used as received from Mallinckrodt and Sigma-Aldrich, respectively. A 15 ml solution of 0.3474 g (1.58 mmol) of zinc acetate dihydrate in acetonitrile was combined with a 15 ml acetonitrile solution of 0.3227 g (1.62 mmol) of dpko and stirred for 10 minutes, producing a colorless solution. Diffraction-quality, colorless crystals formed *via* slow evaporation of solvent within 24 h. Crystals were harvested from the evaporating solutions and decompose upon heating. IR (cm^{-1}) 1960(*wb*), 1710(*mb*), 1590(*s*), 1560(*s*), 1480(*m*), 1420(*s*), 1300(*w*), 1210(*w*), 1110(*w*), 1080(*sb*), 1010(*s*), 789(*s*), 754(*m*), 698(*m*), 675(*m*), 659(*s*).

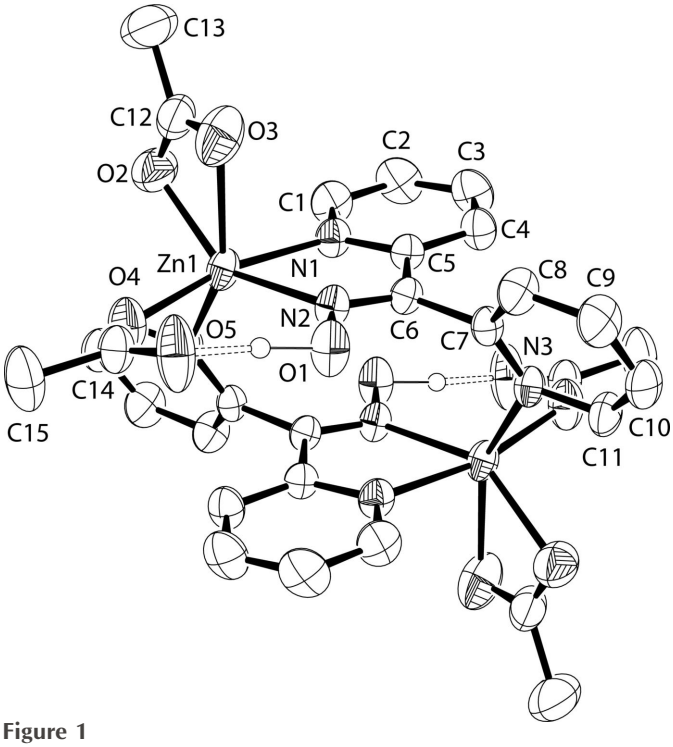


Figure 1
An *ORTEP* style (Farrugia, 2012) view of the title compound. Displacement ellipsoids are drawn at the 50% probability level. All hydrogen atoms not involved in hydrogen bonding have been omitted and non-H atoms generated by the inversion center have not been labeled.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn_2(C_2H_3O_2)_4(C_{11}H_9N_3O)_2]$
M_r	765.34
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	8.3549 (7), 9.3366 (8), 12.3971 (7)
α, β, γ (°)	69.409 (7), 75.524 (6), 65.217 (8)
V (Å^3)	815.88 (13)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.54
Crystal size (mm)	0.35 × 0.32 × 0.31
Data collection	
Diffractometer	Xcalibur, Sapphire3
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2019)
T_{min}, T_{max}	0.907, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10420, 5737, 4546
R_{int}	0.022
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.778
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.098, 1.03
No. of reflections	5737
No. of parameters	223
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.66, −0.22

Computer programs: *CrysAlis PRO* (Rigaku OD, 2019), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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References

Alexiou, M., Dendrinou-Samara, D., Raptopolou, C. P., Terzis, A. & Kessissoglou, D. P. (2003). *Inorg. Chem.* **41**, 4732–4738.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Goher, M. A. S. & Mautner, F. A. (1999). *Polyhedron*, **18**, 3425–3431.
Gökce, H., Alpaslan, G. & Alaşalvar, C. (2019). *J. Coord. Chem.* **72**, 1075–1096.
Milios, C. J., Kyritsis, P., Raptopoulou, C. P., Terzis, A., Vicente, R., Escuer, A. & Perlepes, S. P. (2005). *Dalton Trans.* pp. 501–511.
Rigaku OD (2019). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3–8.
Tarushi, A., Karaflou, Z., Kljun, J., Turel, I., Psomas, G., Papadopoulos, A. N. & Kessissoglou, D. P. (2013). *J. Inorg. Biochem.* **128**, 86–96.
Westcott, B. L., Crundwell, G., Remesic, M., Knopf, K., Chandler, K., McMaster, J. & Davies, E. S. (2016). *Inorg. Chem. Commun.* **74**, 79–81.

full crystallographic data

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Crystal data

$[Zn_2(C_2H_3O_2)_4(C_{11}H_9N_3O)_2]$
M_r = 765.34
Triclinic, $P\overline{1}$
a = 8.3549 (7) Å
b = 9.3366 (8) Å
c = 12.3971 (7) Å
α = 69.409 (7)°
β = 75.524 (6)°
γ = 65.217 (8)°
V = 815.88 (13) Å^3
Z = 1
$F(000)$ = 392
D_x = 1.558 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4170 reflections
θ = 4.5–33.0°
μ = 1.54 mm^{-1}
T = 293 K
Block, colorless
0.35 × 0.32 × 0.31 mm

Data collection

Xcalibur, Sapphire3 diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1790 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2019)
T_{min} = 0.907, T_{max} = 1.000
10420 measured reflections
5737 independent reflections
4546 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 33.6°, θ_{min} = 4.2°
h = −11→12
k = −13→13
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.098
S = 1.03
5737 reflections
223 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.1935P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Hydrogen atoms on sp2 and sp3 carbons were placed at calculated positions with a C—H distance of 0.93?Å and 0.96?Å and were included in the refinement in riding motion approximation with Uiso = 1.2Ueq or 1.5Ueq of the carrier atom, respectively. The position and thermal parameters for the oxime hydrogen were allowed to refine freely.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.34622 (3)	0.46689 (2)	0.21836 (2)	0.03562 (8)
O1	0.3171 (2)	0.81600 (16)	0.04557 (12)	0.0489 (4)
O2	0.2284 (2)	0.3158 (2)	0.35870 (14)	0.0625 (4)
O3	0.0490 (3)	0.5591 (2)	0.28225 (15)	0.0738 (5)
O4	0.4272 (2)	0.56182 (17)	0.31195 (12)	0.0517 (4)
O5	0.3442 (3)	0.83015 (19)	0.23171 (15)	0.0721 (6)
N1	0.3011 (2)	0.38026 (17)	0.08947 (13)	0.0362 (3)
N2	0.3064 (2)	0.66897 (16)	0.06028 (12)	0.0338 (3)
N3	0.3964 (2)	0.73732 (16)	−0.23140 (12)	0.0327 (3)
C1	0.2935 (3)	0.2329 (2)	0.10808 (19)	0.0475 (5)
H1A	0.318212	0.155161	0.179385	0.057*
C2	0.2505 (3)	0.1924 (2)	0.0253 (2)	0.0549 (6)
H2	0.247728	0.088449	0.040771	0.066*
C3	0.2119 (3)	0.3053 (3)	−0.0797 (2)	0.0523 (5)
H3	0.180763	0.280147	−0.135924	0.063*
C4	0.2202 (3)	0.4589 (2)	−0.10074 (17)	0.0410 (4)
H4	0.194267	0.538517	−0.171163	0.049*
C5	0.2675 (2)	0.49042 (19)	−0.01513 (14)	0.0314 (3)
C6	0.2823 (2)	0.64842 (18)	−0.03036 (13)	0.0300 (3)
C7	0.2681 (2)	0.77575 (19)	−0.14482 (14)	0.0310 (3)
C8	0.1286 (3)	0.9258 (2)	−0.15985 (17)	0.0434 (4)
H8	0.042857	0.949951	−0.097911	0.052*
C9	0.1179 (3)	1.0396 (2)	−0.26807 (19)	0.0523 (5)
H9	0.025274	1.141321	−0.279936	0.063*
C10	0.2468 (3)	0.9997 (2)	−0.35777 (18)	0.0489 (5)
H10	0.241831	1.073160	−0.431699	0.059*
C11	0.3830 (3)	0.8493 (2)	−0.33611 (15)	0.0419 (4)
H11	0.470518	0.823590	−0.396915	0.050*
C12	0.0764 (3)	0.4213 (3)	0.35166 (18)	0.0533 (5)
C13	−0.0764 (4)	0.3756 (5)	0.4298 (3)	0.0938 (12)
H13A	−0.181804	0.435492	0.391611	0.141*
H13B	−0.096138	0.402581	0.501117	0.141*
H13C	−0.047996	0.259790	0.446085	0.141*
C14	0.4072 (3)	0.7035 (2)	0.30937 (16)	0.0426 (4)
C15	0.4641 (4)	0.7266 (3)	0.4055 (2)	0.0684 (7)
H15A	0.461453	0.638302	0.474543	0.103*
H15B	0.384817	0.829313	0.420185	0.103*
H15C	0.582636	0.726925	0.383512	0.103*
H1	0.325 (5)	0.821 (4)	0.132 (3)	0.116 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.04561 (13)	0.02653 (10)	0.02801 (10)	−0.00898 (8)	−0.00571 (8)	−0.00425 (7)
O1	0.0854 (11)	0.0274 (6)	0.0412 (7)	−0.0243 (7)	−0.0195 (7)	−0.0054 (5)
O2	0.0476 (9)	0.0701 (11)	0.0524 (9)	−0.0126 (8)	−0.0018 (7)	−0.0110 (8)
O3	0.0920 (14)	0.0576 (11)	0.0510 (10)	−0.0185 (10)	−0.0065 (9)	−0.0037 (8)
O4	0.0768 (11)	0.0382 (7)	0.0431 (7)	−0.0183 (7)	−0.0202 (7)	−0.0095 (6)
O5	0.1310 (17)	0.0374 (8)	0.0516 (9)	−0.0177 (9)	−0.0432 (10)	−0.0107 (7)
N1	0.0459 (8)	0.0255 (6)	0.0353 (7)	−0.0141 (6)	−0.0083 (6)	−0.0028 (5)
N2	0.0482 (8)	0.0231 (6)	0.0302 (6)	−0.0126 (6)	−0.0065 (6)	−0.0068 (5)
N3	0.0411 (8)	0.0261 (6)	0.0263 (6)	−0.0082 (6)	−0.0082 (5)	−0.0043 (5)
C1	0.0612 (12)	0.0276 (8)	0.0519 (11)	−0.0198 (8)	−0.0135 (10)	0.0001 (7)
C2	0.0700 (15)	0.0314 (9)	0.0726 (15)	−0.0253 (10)	−0.0184 (12)	−0.0104 (9)
C3	0.0655 (14)	0.0443 (11)	0.0614 (13)	−0.0246 (10)	−0.0176 (11)	−0.0188 (9)
C4	0.0533 (11)	0.0351 (9)	0.0398 (9)	−0.0190 (8)	−0.0126 (8)	−0.0083 (7)
C5	0.0364 (8)	0.0251 (7)	0.0319 (7)	−0.0107 (6)	−0.0055 (6)	−0.0070 (6)
C6	0.0360 (8)	0.0231 (7)	0.0281 (7)	−0.0092 (6)	−0.0046 (6)	−0.0052 (5)
C7	0.0396 (8)	0.0241 (7)	0.0292 (7)	−0.0109 (6)	−0.0097 (6)	−0.0046 (5)
C8	0.0458 (10)	0.0310 (8)	0.0399 (9)	−0.0036 (7)	−0.0058 (8)	−0.0069 (7)
C9	0.0523 (12)	0.0321 (9)	0.0515 (12)	−0.0005 (8)	−0.0151 (9)	0.0004 (8)
C10	0.0546 (12)	0.0396 (10)	0.0379 (9)	−0.0120 (9)	−0.0167 (9)	0.0073 (7)
C11	0.0472 (10)	0.0395 (9)	0.0291 (8)	−0.0110 (8)	−0.0084 (7)	−0.0014 (7)
C12	0.0519 (12)	0.0612 (13)	0.0353 (9)	−0.0152 (10)	−0.0035 (8)	−0.0081 (9)
C13	0.0545 (16)	0.121 (3)	0.0676 (18)	−0.0295 (18)	0.0021 (13)	0.0081 (17)
C14	0.0539 (11)	0.0412 (9)	0.0349 (9)	−0.0148 (8)	−0.0078 (8)	−0.0149 (7)
C15	0.107 (2)	0.0603 (14)	0.0537 (13)	−0.0356 (15)	−0.0343 (14)	−0.0118 (11)

Geometric parameters (Å, º)

Zn1—O2	2.1369 (17)	C3—H3	0.9300
Zn1—O3	2.289 (2)	C3—C4	1.393 (3)
Zn1—O4	2.0513 (14)	C4—H4	0.9300
Zn1—N1	2.1944 (16)	C4—C5	1.377 (3)
Zn1—N2	2.1702 (14)	C5—C6	1.474 (2)
Zn1—N3^{i}	2.1921 (14)	C6—C7	1.490 (2)
Zn1—C12	2.538 (2)	C7—C8	1.383 (2)
O1—N2	1.3581 (18)	C8—H8	0.9300
O1—H1	1.11 (4)	C8—C9	1.384 (3)
O2—C12	1.240 (3)	C9—H9	0.9300
O3—C12	1.233 (3)	C9—C10	1.375 (3)
O4—C14	1.251 (2)	C10—H10	0.9300
O5—C14	1.238 (2)	C10—C11	1.374 (3)
O5—H1	1.32 (4)	C11—H11	0.9300
N1—C1	1.339 (2)	C12—C13	1.516 (4)
N1—C5	1.349 (2)	C13—H13A	0.9600
N2—C6	1.279 (2)	C13—H13B	0.9600
N3—C7	1.343 (2)	C13—H13C	0.9600

N3—C11	1.346 (2)	C14—C15	1.498 (3)
C1—H1A	0.9300	C15—H15A	0.9600
C1—C2	1.377 (3)	C15—H15B	0.9600
C2—H2	0.9300	C15—H15C	0.9600
C2—C3	1.368 (3)		

O2—Zn1—O3	58.16 (6)	C5—C4—C3	118.68 (18)
O2—Zn1—N1	92.26 (6)	C5—C4—H4	120.7
O2—Zn1—N2	146.35 (6)	N1—C5—C4	122.62 (15)
O2—Zn1—N3^{i}	89.78 (6)	N1—C5—C6	114.95 (14)
O2—Zn1—C12	29.18 (7)	C4—C5—C6	122.42 (15)
O3—Zn1—C12	29.01 (7)	N2—C6—C5	115.96 (14)
O4—Zn1—O2	99.02 (7)	N2—C6—C7	122.71 (14)
O4—Zn1—O3	98.14 (7)	C5—C6—C7	121.32 (14)
O4—Zn1—N1	168.00 (6)	N3—C7—C6	116.84 (14)
O4—Zn1—N2	98.84 (6)	N3—C7—C8	122.22 (15)
O4—Zn1—N3^{i}	88.29 (6)	C8—C7—C6	120.94 (16)
O4—Zn1—C12	100.79 (7)	C7—C8—H8	120.4
N1—Zn1—O3	91.27 (7)	C7—C8—C9	119.26 (18)
N1—Zn1—C12	91.05 (7)	C9—C8—H8	120.4
N2—Zn1—O3	91.18 (6)	C8—C9—H9	120.6
N2—Zn1—N1	73.40 (5)	C10—C9—C8	118.83 (18)
N2—Zn1—N3^{i}	119.03 (6)	C10—C9—H9	120.6
N2—Zn1—C12	118.85 (7)	C9—C10—H10	120.6
N3^{i}—Zn1—O3	147.87 (6)	C11—C10—C9	118.74 (17)
N3^{i}—Zn1—N1	87.66 (6)	C11—C10—H10	120.6
N3^{i}—Zn1—C12	118.87 (6)	N3—C11—C10	123.36 (18)
N2—O1—H1	107.4 (19)	N3—C11—H11	118.3
C12—O2—Zn1	93.65 (15)	C10—C11—H11	118.3
C12—O3—Zn1	86.75 (16)	O2—C12—Zn1	57.18 (12)
C14—O4—Zn1	134.88 (14)	O2—C12—C13	118.1 (2)
C14—O5—H1	120.5 (16)	O3—C12—Zn1	64.23 (14)
C1—N1—Zn1	125.79 (13)	O3—C12—O2	121.3 (2)
C1—N1—C5	117.95 (16)	O3—C12—C13	120.6 (2)
C5—N1—Zn1	116.13 (11)	C13—C12—Zn1	173.8 (2)
O1—N2—Zn1	125.25 (11)	C12—C13—H13A	109.5
C6—N2—Zn1	119.18 (11)	C12—C13—H13B	109.5
C6—N2—O1	115.40 (13)	C12—C13—H13C	109.5
C7—N3—Zn1^{i}	127.73 (11)	H13A—C13—H13B	109.5
C7—N3—C11	117.57 (15)	H13A—C13—H13C	109.5
C11—N3—Zn1^{i}	113.67 (12)	H13B—C13—H13C	109.5
N1—C1—H1A	118.9	O4—C14—C15	119.21 (19)
N1—C1—C2	122.28 (18)	O5—C14—O4	125.11 (18)
C2—C1—H1A	118.9	O5—C14—C15	115.68 (19)
C1—C2—H2	120.1	C14—C15—H15A	109.5
C3—C2—C1	119.88 (18)	C14—C15—H15B	109.5
C3—C2—H2	120.1	C14—C15—H15C	109.5
C2—C3—H3	120.7	H15A—C15—H15B	109.5

C2—C3—C4	118.55 (19)	H15A—C15—H15C	109.5
C4—C3—H3	120.7	H15B—C15—H15C	109.5
C3—C4—H4	120.7		

Zn1—O2—C12—O3	−3.7 (3)	N2—C6—C7—C8	−64.7 (3)
Zn1—O2—C12—C13	175.4 (2)	N3—C7—C8—C9	1.3 (3)
Zn1—O3—C12—O2	3.4 (3)	C1—N1—C5—C4	2.3 (3)
Zn1—O3—C12—C13	−175.6 (3)	C1—N1—C5—C6	−178.61 (17)
Zn1—O4—C14—O5	−10.1 (4)	C1—C2—C3—C4	1.0 (4)
Zn1—O4—C14—C15	170.56 (18)	C2—C3—C4—C5	0.2 (3)
Zn1—N1—C1—C2	174.66 (17)	C3—C4—C5—N1	−2.0 (3)
Zn1—N1—C5—C4	−173.72 (14)	C3—C4—C5—C6	179.04 (19)
Zn1—N1—C5—C6	5.3 (2)	C4—C5—C6—N2	171.92 (17)
Zn1—N2—C6—C5	5.5 (2)	C4—C5—C6—C7	−7.5 (3)
Zn1—N2—C6—C7	−175.07 (12)	C5—N1—C1—C2	−1.0 (3)
Zn1^{i}—N3—C7—C6	−14.1 (2)	C5—C6—C7—N3	−65.3 (2)
Zn1^{i}—N3—C7—C8	165.91 (14)	C5—C6—C7—C8	114.7 (2)
Zn1^{i}—N3—C11—C10	−168.65 (17)	C6—C7—C8—C9	−178.66 (19)
O1—N2—C6—C5	−179.02 (15)	C7—N3—C11—C10	0.6 (3)
O1—N2—C6—C7	0.4 (3)	C7—C8—C9—C10	0.1 (3)
N1—C1—C2—C3	−0.7 (4)	C8—C9—C10—C11	−1.1 (4)
N1—C5—C6—N2	−7.1 (2)	C9—C10—C11—N3	0.7 (3)
N1—C5—C6—C7	173.44 (16)	C11—N3—C7—C6	178.31 (16)
N2—C6—C7—N3	115.34 (19)	C11—N3—C7—C8	−1.6 (3)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O5	1.11 (4)	1.32 (4)	2.428 (2)	176 (3)
C2—H2···O1^{ii}	0.93	2.34	3.245 (2)	164
C3—H3···O3^{iii}	0.93	2.58	3.293 (3)	134
C9—H9···03^{iv}	0.93	2.59	3.361 (3)	141
C11—H11···O2^{i}	0.93	2.38	2.941 (3)	119

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