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Di-μ-adipato-$\kappa^4O^1,O^{1'}:O^6,O^{6'}$-bis[(2,2′-dipyridylamine-κ^2N,N')zinc(II)] trihydrate

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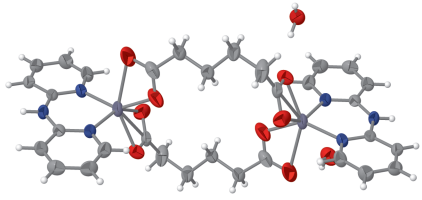
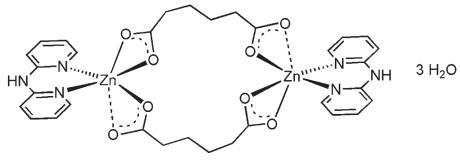
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Zn_2(C_6H_8O_4)_2(C_{10}H_9N_3)_2]\cdot 3H_2O$ or $\{Zn_2[(C_5H_4N)_2NH]_2[\mu\text{-}(CH_2)_4(COO)_2]_2\}\cdot 3H_2O$, was separated from the solvothermal reaction of zinc(II) sulfate heptahydrate, 2,2′-dipyridylamine and sodium adipate. The dinuclear metal complex has a centrosymmetric structure, with the Zn^{II} atom adopting a highly distorted octahedral coordination sphere composed of four oxygen atoms from bridging adipato ligands and two pyridine nitrogen atoms. In the crystal, the title compound aggregates into a tri-periodic supramolecular structure through intermolecular hydrogen-bonding networks of the form O—H···O and N—H···O.

3D view



Chemical scheme



Structure description

Polynitrile and bis-carboxylate compounds derived from transition-metal ions are of great interest with respect to their magnetic and luminescence properties, diverse molecular structures and for their topologies (Addala *et al.* 2019; Benmansour *et al.*, 2010; Klongdee *et al.*, 2023).

As a part of our continuing studies of the structural, magnetic and luminescence properties of coordination complexes containing polynitrile and/or bis-carboxylate and polypyridyl units (Setifi *et al.*, 2006, 2016; Lehchili *et al.*, 2017), we report here the molecular and crystal structure of the dinuclear compound, $[Zn_2(adp)_2(dpa)_2]\cdot 3H_2O$, based on the adipate dianion (adp) as ligand and the 2,2′-dipyridylamine (dpa) as co-ligand.

The asymmetric unit of the title compound consists of half of the metal complex molecule and two water molecules (one of which exhibits half-occupancy). The molecule

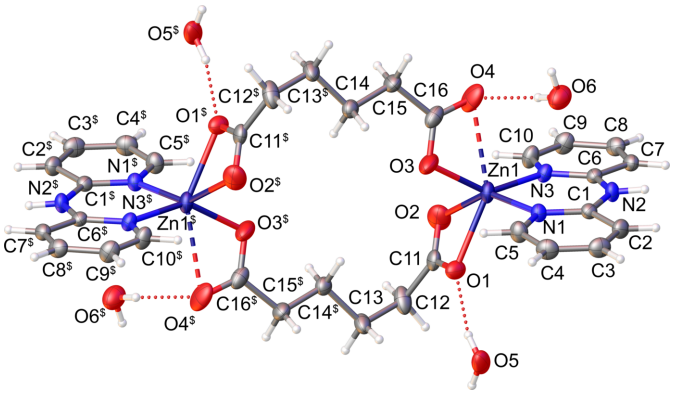


Figure 1
The molecular structure of the title compound showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: ($) $-x+1, -y+1, -z+1$.]

is completed by inversion symmetry. The Zn^{II} atom is octahedrally coordinated by two (O,O') donor sets of carboxylato groups from two different adp ligands and one (N,N)-chelating dpa co-ligand (Fig. 1). Except the Zn—O4 contact with a significantly long bond of 2.567 (2) Å, the lengths of other Zn—O bonds are in the range of 2.0073 (19)–2.2146 (17) Å, while Zn1—N1 and Zn1—N3 bond lengths are 2.0473 (16) and 2.0470 (16) Å, respectively. As a result of the long Zn—O4 bond, the highly distorted octahedral coordination environment of Zn^{II} ion is best described as [5 + 1]. This bonding situation of the present dinuclear Zn^{II} compound closely resembles Ni^{II} and Cu^{II} counterparts previously reported (Setifi *et al.*, 2014).

In the crystal, complex molecules aggregate into a tri-periodic supramolecular hydrogen-bonding network. The NH groups of dpa form hydrogen bonds with the O5 water molecules, which in turn provide hydrogen bonds to carboxylate oxygen atoms (O1 and O4) of adp (Table 1, Fig. 2*a*). In addition, the half-occupied O6 water molecule is also involved in weaker hydrogen bonds with adp through O2 and O4 atoms (Table 1, Fig. 2*b*).

Synthesis and crystallization

The title compound was prepared solvothermally under autogenous pressure from a mixture of zinc(II) sulfate heptahydrate (29 mg, 0.1 mmol), 2,2′-dipyridylamine (24 mg, 0.2 mmol) and sodium adipate (0.2 mol l^{-1}) in a mixture of water and ethanol (4:1 *v*/*v*, 25 ml). This mixture was sealed in a Teflon-lined autoclave and held at 393 K for 2 d, and then cooled to ambient temperature at a rate of 10 K h^{-1} to give the product in form of colorless needles (yield 36%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The O6 atom and associated H atoms of the second water molecule were refined with an occupancy of 0.5. Hydrogen atoms of the water molecules were included in calculated positions and were refined in a riding model, with O—H distances of 0.85 Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*A*···O1	0.85	1.89	2.728 (3)	167
O5—H5*B*···O4^{i}	0.85	2.10	2.877 (3)	151
O6—H6*A*···O4	0.85	2.26	3.107 (5)	173
O6—H6*B*···O2^{ii}	0.85	2.58	3.275 (5)	140
N2—H2···O5^{iii}	0.86	1.97	2.824 (2)	177

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

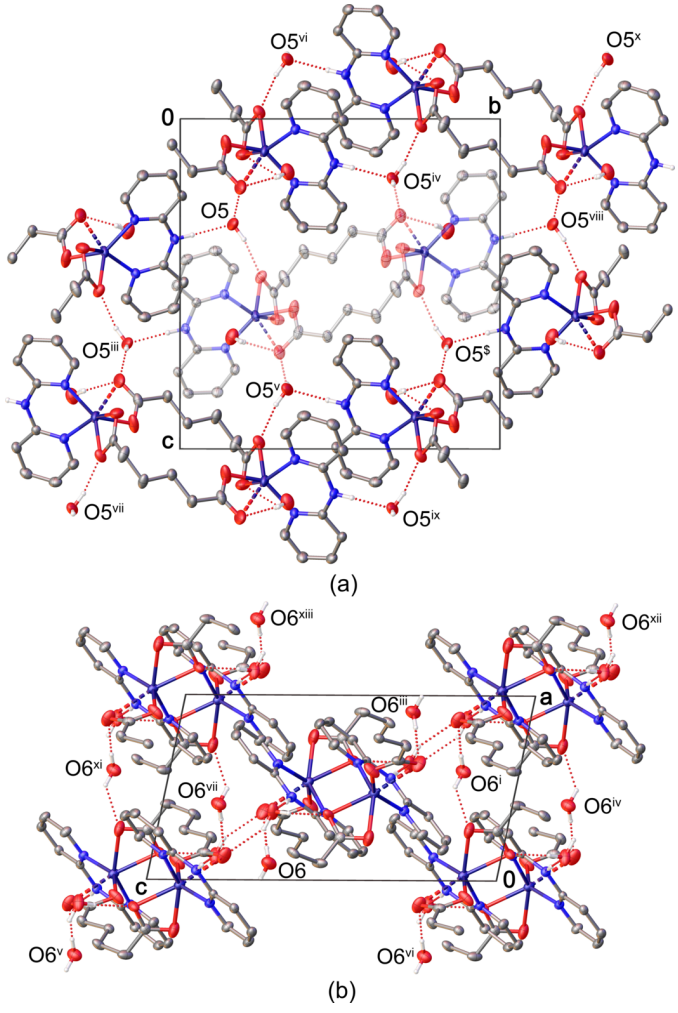


Figure 2
Partial packing diagram showing the hydrogen-bonding interactions involving (*a*) O5 water molecules (shown in projection down the *a* axis) and (*b*) O6 water molecules (shown in projection down the *b* axis). Hydrogen atoms bonded to carbon atoms were omitted for clarity. [Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y, -z+1$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (vi) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (vii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (viii) $x, y+1, z$; (ix) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (*x*) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (xi) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (xii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (xiii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$].

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Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn_2(C_6H_8O_4)_2(C_{10}H_9N_3)_2]\cdot 3H_2O$
M_r	815.44
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	302
a, b, c (Å)	8.2105 (3), 14.4478 (6), 15.2042 (8)
β (°)	101.694 (2)
V (Å^3)	1766.14 (14)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.43
Crystal size (mm)	0.18 × 0.11 × 0.06
Data collection	
Diffractometer	Oxford Diffraction Xcalibur with Sapphire CCD
Absorption correction	Multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min}, T_{max}	0.492, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20158, 6416, 4033
R_{int}	0.038
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.762
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.102, 1.02
No. of reflections	6416
No. of parameters	241
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.48, −0.86

Computer programs: *CrysAlis CCD* (Oxford Diffraction, 2009), *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *OLEX2* 1.5 (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2024). **9**, x240906 [https://doi.org/10.1107/S2414314624009064]

Di-μ-adipato-$\kappa^4O^1,O^{1'}:O^6,O^{6'}$-bis[(2,2′-dipyridylamine-κ^2N,N')zinc(II)] trihydrate

Fatima Setifi, Zouaoui Setifi, Thang Pham Chien, Mohammad Hadi Al-Douh and Abderezak Addala

Di-μ-adipato-$\kappa^4O^1,O^{1'}:O^6,O^{6'}$-bis{[*N*-(pyridin-2-yl-$\kappa N$)pyridin-2-amine-$\kappa N^1$]zinc(II)} trihydrate

Crystal data

$[Zn_2(C_6H_8O_4)_2(C_{10}H_9N_3)_2]\cdot 3H_2O$
M_r = 815.44
Monoclinic, $P2_1/n$
a = 8.2105 (3) Å
b = 14.4478 (6) Å
c = 15.2042 (8) Å
β = 101.694 (2)°
V = 1766.14 (14) Å^3
Z = 2
$F(000)$ = 844
D_x = 1.533 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1439 reflections
θ = 2.3–26.3°
μ = 1.43 mm^{-1}
T = 302 K
Needle, colourless
0.18 × 0.11 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur with Sapphire CCD diffractometer
Radiation source: Enhance (Mo) X-ray source
ω scans
Absorption correction: multi-scan (Crysalis Red; Oxford Diffraction, 2009)
T_{min} = 0.492, T_{max} = 1.000
20158 measured reflections
6416 independent reflections
4033 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 32.8°, θ_{min} = 3.6°
h = −10→12
k = −22→21
l = −23→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.102
S = 1.02
6416 reflections
241 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 0.9459P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 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}	Occ. (<1)
Zn1	0.52923 (3)	0.23563 (2)	0.59713 (2)	0.03924 (9)	
O4	0.3690 (3)	0.31102 (13)	0.70690 (14)	0.0791 (7)	
O2	0.7724 (3)	0.30383 (15)	0.60833 (13)	0.0752 (6)	
O1	0.6465 (2)	0.25296 (11)	0.47921 (12)	0.0498 (4)	
O5	0.6289 (3)	0.16459 (13)	0.31903 (14)	0.0725 (6)	
H5A	0.639294	0.199470	0.364850	0.109*	
H5B	0.722914	0.167391	0.303780	0.109*	
O6	0.0902 (5)	0.1631 (3)	0.6599 (3)	0.0730 (11)	0.5
H6A	0.171671	0.199984	0.675684	0.109*	0.5
H6B	0.008471	0.190701	0.674841	0.109*	0.5
N1	0.3655 (2)	0.13927 (11)	0.53175 (11)	0.0347 (4)	
N2	0.4477 (2)	0.01757 (11)	0.63553 (12)	0.0375 (4)	
H2	0.420818	−0.037731	0.647937	0.045*	
N3	0.6264 (2)	0.14173 (11)	0.69451 (11)	0.0352 (4)	
O3	0.4049 (3)	0.35591 (12)	0.57654 (16)	0.0757 (6)	
C1	0.3528 (2)	0.05144 (13)	0.55665 (13)	0.0320 (4)	
C2	0.2422 (3)	−0.01017 (15)	0.50387 (15)	0.0423 (5)	
H2A	0.235752	−0.071351	0.521863	0.051*	
C3	0.1439 (3)	0.02034 (18)	0.42585 (16)	0.0488 (6)	
H3	0.069354	−0.019799	0.390602	0.059*	
C4	0.1559 (3)	0.11133 (18)	0.39960 (16)	0.0503 (6)	
H4	0.090285	0.133564	0.346685	0.060*	
C5	0.2670 (3)	0.16751 (16)	0.45378 (16)	0.0462 (5)	
H5	0.275555	0.228659	0.436171	0.055*	
C6	0.5767 (2)	0.05380 (13)	0.69865 (13)	0.0315 (4)	
C7	0.6539 (3)	−0.00637 (14)	0.76730 (14)	0.0369 (4)	
H7	0.618034	−0.067305	0.768749	0.044*	
C8	0.7820 (3)	0.02557 (16)	0.83172 (15)	0.0434 (5)	
H8	0.834264	−0.013415	0.877486	0.052*	
C9	0.8335 (3)	0.11660 (16)	0.82839 (16)	0.0485 (5)	
H9	0.919951	0.139854	0.871929	0.058*	
C10	0.7542 (3)	0.17143 (15)	0.75964 (16)	0.0456 (5)	
H10	0.789670	0.232347	0.757327	0.055*	
C16	0.3524 (3)	0.36974 (15)	0.64708 (19)	0.0480 (6)	
C15	0.2705 (3)	0.46125 (15)	0.65891 (17)	0.0473 (5)	
H15A	0.341863	0.494613	0.707215	0.057*	
H15B	0.167041	0.448608	0.678170	0.057*	
C14	0.2323 (3)	0.52446 (14)	0.57801 (15)	0.0403 (5)	
H14A	0.161271	0.492051	0.528875	0.048*	
H14B	0.335121	0.539790	0.559240	0.048*	
C13	0.8531 (3)	0.38678 (15)	0.40257 (19)	0.0519 (6)	
H13A	0.949705	0.402554	0.377984	0.062*	
H13B	0.777494	0.351921	0.357227	0.062*	
C12	0.9082 (3)	0.32560 (18)	0.4846 (2)	0.0611 (7)	
H12A	0.965667	0.272054	0.467267	0.073*	

H12B	0.986835	0.359756	0.529059	0.073*
C11	0.7690 (3)	0.29305 (14)	0.52654 (16)	0.0420 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.04188 (14)	0.02539 (11)	0.04678 (16)	−0.00240 (9)	0.00029 (10)	0.00485 (10)
O4	0.1090 (17)	0.0462 (11)	0.0712 (14)	0.0344 (11)	−0.0072 (12)	0.0039 (9)
O2	0.1084 (17)	0.0698 (13)	0.0417 (11)	−0.0076 (12)	0.0020 (10)	0.0048 (9)
O1	0.0475 (8)	0.0476 (9)	0.0585 (11)	−0.0147 (7)	0.0204 (8)	−0.0152 (7)
O5	0.1197 (18)	0.0454 (10)	0.0540 (12)	−0.0324 (11)	0.0216 (11)	−0.0117 (8)
O6	0.068 (3)	0.060 (2)	0.095 (3)	−0.0104 (19)	0.027 (2)	−0.015 (2)
N1	0.0350 (8)	0.0316 (8)	0.0364 (9)	−0.0025 (6)	0.0044 (7)	0.0024 (7)
N2	0.0445 (9)	0.0270 (8)	0.0396 (10)	−0.0074 (7)	0.0050 (7)	0.0037 (7)
N3	0.0383 (8)	0.0266 (7)	0.0388 (9)	0.0020 (6)	0.0028 (7)	−0.0011 (6)
O3	0.0923 (14)	0.0387 (9)	0.1157 (18)	−0.0024 (9)	0.0674 (14)	−0.0157 (10)
C1	0.0309 (9)	0.0323 (9)	0.0342 (10)	−0.0020 (7)	0.0100 (7)	−0.0012 (7)
C2	0.0439 (11)	0.0360 (10)	0.0468 (13)	−0.0097 (8)	0.0090 (9)	−0.0051 (9)
C3	0.0393 (11)	0.0579 (14)	0.0463 (14)	−0.0089 (10)	0.0022 (9)	−0.0121 (11)
C4	0.0464 (12)	0.0623 (15)	0.0379 (13)	0.0038 (11)	−0.0015 (10)	0.0010 (11)
C5	0.0489 (12)	0.0428 (12)	0.0432 (13)	−0.0014 (9)	0.0011 (10)	0.0067 (9)
C6	0.0338 (9)	0.0289 (9)	0.0336 (10)	0.0031 (7)	0.0112 (7)	−0.0011 (7)
C7	0.0436 (11)	0.0317 (9)	0.0374 (11)	0.0049 (8)	0.0128 (8)	0.0034 (8)
C8	0.0459 (12)	0.0439 (12)	0.0389 (12)	0.0116 (9)	0.0052 (9)	0.0050 (9)
C9	0.0479 (12)	0.0467 (13)	0.0443 (13)	0.0032 (10)	−0.0063 (10)	−0.0024 (10)
C10	0.0490 (12)	0.0327 (10)	0.0486 (13)	−0.0028 (9)	−0.0059 (10)	−0.0032 (9)
C16	0.0352 (10)	0.0348 (11)	0.0721 (17)	−0.0011 (8)	0.0067 (10)	−0.0129 (11)
C15	0.0572 (13)	0.0351 (11)	0.0547 (14)	0.0089 (9)	0.0237 (11)	0.0008 (10)
C14	0.0405 (10)	0.0337 (10)	0.0482 (13)	−0.0049 (8)	0.0126 (9)	−0.0022 (9)
C13	0.0521 (13)	0.0379 (11)	0.0749 (18)	0.0038 (10)	0.0342 (12)	0.0127 (11)
C12	0.0382 (12)	0.0476 (13)	0.097 (2)	−0.0029 (10)	0.0115 (12)	0.0249 (13)
C11	0.0505 (12)	0.0241 (8)	0.0501 (14)	0.0025 (8)	0.0071 (10)	0.0064 (8)

Geometric parameters (Å, º)

Zn1—O4	2.567 (2)	C3—C4	1.383 (4)
Zn1—O2	2.202 (2)	C4—H4	0.9300
Zn1—O1	2.2146 (17)	C4—C5	1.366 (3)
Zn1—N1	2.0473 (16)	C5—H5	0.9300
Zn1—N3	2.0470 (16)	C6—C7	1.407 (3)
Zn1—O3	2.0073 (19)	C7—H7	0.9300
Zn1—C11	2.563 (2)	C7—C8	1.364 (3)
O4—C16	1.231 (3)	C8—H8	0.9300
O2—C11	1.248 (3)	C8—C9	1.385 (3)
O1—C11	1.253 (3)	C9—H9	0.9300
O5—H5A	0.8500	C9—C10	1.367 (3)
O5—H5B	0.8504	C10—H10	0.9300
O6—H6A	0.8508	C16—C15	1.511 (3)

O6—H6B	0.8500	C15—H15A	0.9700
N1—C1	1.334 (2)	C15—H15B	0.9700
N1—C5	1.355 (3)	C15—C14	1.513 (3)
N2—H2	0.8600	C14—H14A	0.9700
N2—C1	1.381 (2)	C14—H14B	0.9700
N2—C6	1.380 (2)	C14—C13^{i}	1.519 (3)
N3—C6	1.340 (2)	C13—H13A	0.9700
N3—C10	1.358 (3)	C13—H13B	0.9700
O3—C16	1.250 (3)	C13—C12	1.520 (3)
C1—C2	1.402 (3)	C12—H12A	0.9700
C2—H2A	0.9300	C12—H12B	0.9700
C2—C3	1.365 (3)	C12—C11	1.493 (3)
C3—H3	0.9300		

O2—Zn1—O4	109.63 (8)	C4—C5—H5	118.1
O2—Zn1—O1	58.38 (7)	N2—C6—C7	116.65 (17)
O2—Zn1—C11	29.12 (7)	N3—C6—N2	121.67 (17)
O1—Zn1—O4	147.40 (6)	N3—C6—C7	121.68 (18)
O1—Zn1—C11	29.26 (6)	C6—C7—H7	120.3
N1—Zn1—O4	103.40 (7)	C8—C7—C6	119.32 (19)
N1—Zn1—O2	146.89 (8)	C8—C7—H7	120.3
N1—Zn1—O1	91.96 (6)	C7—C8—H8	120.3
N1—Zn1—C11	120.07 (7)	C7—C8—C9	119.4 (2)
N3—Zn1—O4	89.24 (6)	C9—C8—H8	120.3
N3—Zn1—O2	91.51 (7)	C8—C9—H9	120.8
N3—Zn1—O1	119.40 (7)	C10—C9—C8	118.5 (2)
N3—Zn1—N1	91.24 (6)	C10—C9—H9	120.8
N3—Zn1—C11	107.32 (7)	N3—C10—C9	123.5 (2)
O3—Zn1—O4	54.76 (7)	N3—C10—H10	118.2
O3—Zn1—O2	92.81 (8)	C9—C10—H10	118.2
O3—Zn1—O1	93.82 (7)	O4—C16—O3	121.2 (2)
O3—Zn1—N1	104.48 (8)	O4—C16—C15	120.0 (2)
O3—Zn1—N3	142.92 (8)	O3—C16—C15	118.8 (2)
O3—Zn1—C11	93.66 (7)	C16—C15—H15A	108.0
C11—Zn1—O4	132.29 (7)	C16—C15—H15B	108.0
C16—O4—Zn1	78.85 (16)	C16—C15—C14	117.1 (2)
C11—O2—Zn1	91.72 (15)	H15A—C15—H15B	107.3
C11—O1—Zn1	90.99 (15)	C14—C15—H15A	108.0
H5A—O5—H5B	104.5	C14—C15—H15B	108.0
H6A—O6—H6B	104.4	C15—C14—H14A	109.1
C1—N1—Zn1	126.18 (13)	C15—C14—H14B	109.1
C1—N1—C5	117.85 (18)	C15—C14—C13^{i}	112.29 (19)
C5—N1—Zn1	115.89 (14)	H14A—C14—H14B	107.9
C1—N2—H2	113.3	C13^{i}—C14—H14A	109.1
C6—N2—H2	113.3	C13^{i}—C14—H14B	109.1
C6—N2—C1	133.48 (16)	C14^{i}—C13—H13A	108.8
C6—N3—Zn1	125.79 (13)	C14^{i}—C13—H13B	108.8
C6—N3—C10	117.58 (17)	C14^{i}—C13—C12	113.8 (2)

C10—N3—Zn1	116.62 (13)	H13A—C13—H13B	107.7
C16—O3—Zn1	104.91 (17)	C12—C13—H13A	108.8
N1—C1—N2	121.38 (17)	C12—C13—H13B	108.8
N1—C1—C2	121.34 (18)	C13—C12—H12A	108.7
N2—C1—C2	117.28 (18)	C13—C12—H12B	108.7
C1—C2—H2A	120.2	H12A—C12—H12B	107.6
C3—C2—C1	119.5 (2)	C11—C12—C13	114.03 (19)
C3—C2—H2A	120.2	C11—C12—H12A	108.7
C2—C3—H3	120.2	C11—C12—H12B	108.7
C2—C3—C4	119.6 (2)	O2—C11—Zn1	59.17 (14)
C4—C3—H3	120.2	O2—C11—O1	118.9 (2)
C3—C4—H4	121.0	O2—C11—C12	121.4 (2)
C5—C4—C3	118.0 (2)	O1—C11—Zn1	59.75 (12)
C5—C4—H4	121.0	O1—C11—C12	119.6 (2)
N1—C5—C4	123.8 (2)	C12—C11—Zn1	179.3 (2)
N1—C5—H5	118.1		

Zn1—O4—C16—O3	4.8 (2)	C1—N1—C5—C4	0.0 (3)
Zn1—O4—C16—C15	−174.0 (2)	C1—N2—C6—N3	5.6 (3)
Zn1—O2—C11—O1	−0.5 (2)	C1—N2—C6—C7	−174.1 (2)
Zn1—O2—C11—C12	−179.62 (18)	C1—C2—C3—C4	0.6 (3)
Zn1—O1—C11—O2	0.5 (2)	C2—C3—C4—C5	−0.1 (4)
Zn1—O1—C11—C12	179.63 (18)	C3—C4—C5—N1	−0.2 (4)
Zn1—N1—C1—N2	3.8 (3)	C5—N1—C1—N2	−179.40 (19)
Zn1—N1—C1—C2	−176.34 (15)	C5—N1—C1—C2	0.4 (3)
Zn1—N1—C5—C4	177.1 (2)	C6—N2—C1—N1	−7.0 (3)
Zn1—N3—C6—N2	−1.2 (3)	C6—N2—C1—C2	173.1 (2)
Zn1—N3—C6—C7	178.48 (14)	C6—N3—C10—C9	−0.1 (3)
Zn1—N3—C10—C9	−179.1 (2)	C6—C7—C8—C9	0.0 (3)
Zn1—O3—C16—O4	−6.3 (3)	C7—C8—C9—C10	−0.5 (4)
Zn1—O3—C16—C15	172.52 (17)	C8—C9—C10—N3	0.5 (4)
O4—C16—C15—C14	−171.6 (2)	C10—N3—C6—N2	179.91 (19)
N1—C1—C2—C3	−0.7 (3)	C10—N3—C6—C7	−0.4 (3)
N2—C1—C2—C3	179.1 (2)	C16—C15—C14—C13^{i}	178.8 (2)
N2—C6—C7—C8	−179.88 (19)	C14^{i}—C13—C12—C11	61.0 (3)
N3—C6—C7—C8	0.4 (3)	C13—C12—C11—O2	−127.6 (3)
O3—C16—C15—C14	9.6 (3)	C13—C12—C11—O1	53.3 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O1	0.85	1.89	2.728 (3)	167
O5—H5*B*···O4^{ii}	0.85	2.10	2.877 (3)	151
O6—H6*A*···O4	0.85	2.26	3.107 (5)	173

O6—H6*B*···O2^{iii}	0.85	2.58	3.275 (5)	140
N2—H2···O5^{iv}	0.86	1.97	2.824 (2)	177

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