Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(1-methyl-4-oxoimidazolidin-2-iminium) diaquabis(pyridine-2,4-dicarboxylato-κ^2N,O^2)zincate(II) dihydrate

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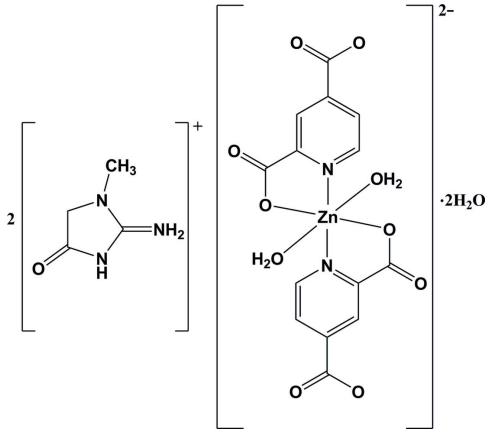
Received 24 February 2011; accepted 6 March 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.090; data-to-parameter ratio = 16.8.

In the title compound, $(C_4H_8N_3O)_2[Zn(C_7H_3NO_4)_2(H_2O)_2]\cdot 2H_2O$, the Zn^{II} ion is six-coordinated in a distorted octahedral geometry by two pyridine-2,4-dicarboxylate (pydc) ligands in the equatorial plane and two water molecules in the axial positions. The pydc ligands act as bidentate chelating ligands through one carboxylate O atom and the pyridine N atom. Intermolecular N—H···O, O—H···O and weak C—H···O hydrogen bonds stabilize the crystal structure.

Related literature

For a review article on proton-transfer compounds, see: Aghabozorg *et al.* (2008*b*). For related structures, see: Aghabozorg *et al.* (2008*a*,*c*); Attar Gharamaleki *et al.* (2009); Moghimi *et al.* (2004, 2005).



Experimental

Crystal data

$(C_4H_8N_3O)_2[Zn(C_7H_3NO_4)_2(H_2O)_2]\cdot 2H_2O$
M_r = 695.93
Triclinic, $P\overline{1}$
a = 5.3209 (11) Å
b = 8.3893 (17) Å
c = 16.621 (3) Å
α = 81.58 (3)°
β = 85.26 (3)°
γ = 74.09 (3)°
V = 705.1 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.96 mm^{-1}
T = 298 K
0.30 × 0.20 × 0.15 mm

Data collection

Stoe IPDS-2 diffractometer
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)
T_{min} = 0.793, T_{max} = 0.862
7743 measured reflections
3787 independent reflections
3206 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.05
3787 reflections
226 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O3^{i}	0.91 (3)	1.87 (3)	2.764 (2)	165 (3)
N4—H4A···O4^{i}	0.86	1.86	2.706 (2)	168
N4—H4B···O2^{ii}	0.86	1.92	2.771 (2)	169
O5—H5A···O4^{i}	0.79 (2)	1.95 (3)	2.729 (2)	171 (3)
O5—H5B···O1^{ii}	0.85 (3)	1.98 (3)	2.8088 (17)	165 (2)
O7—H7A···O3	0.73 (4)	2.32 (4)	2.968 (3)	148 (4)
O7—H7B···O6^{iii}	0.82 (4)	2.26 (4)	2.993 (3)	149 (4)
C5—H5···O5^{iv}	0.93	2.46	3.308 (2)	152
C11—H11A···O2^{ii}	0.96	2.48	3.425 (3)	167

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We are grateful to the Islamic Azad University, North Tehran Branch, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2411).

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supporting information

Acta Cryst. (2011). E**67**, m435–m436 [doi:10.1107/S1600536811008452]

Bis(1-methyl-4-oxoimidazolidin-2-iminium) diaquabis(pyridine-2,4-dicarboxylato-κ^2N,O^2)zincate(II) dihydrate

Hossein Aghabozorg, Fatemeh Jafarbak, Masoud Mirzaei and Behrouz Notash

S1. Comment

Many organic aromatic ligands and metal ions may aggregate into supramolecular networks using coordination and hydrogen bonds and π–π stacking interactions (Aghabozorg *et al.*, 2008*b*). Metal complexes of pyridine-(di)carboxylates possess versatile structural motifs, which finally aggregate to various supramolecular architectures with interesting properties. We have previously reported several compounds containing creatinine (creat), pyridine-2,6-dicarboxylic acid ($pydcH_2$) and various metals, such as (creatH)(pydcH).H_2O (Moghimi *et al.*, 2004), (creatH)$_2$[Bi(pydc)$_2$]$_2$.4H_2O (Moghimi *et al.*, 2005), (creatH)[Zn(pydc)(pydcH)].4H_2O (Aghabozorg *et al.*, 2008*c*), (creatH)[Cr(pydc)$_2$](pydcH_2).6H_2O (Aghabozorg *et al.*, 2008*a*) and (H_3O)(creatH)[Ni(pydc)$_2$].3H_2O (Attar Gharamaleki *et al.*, 2009). For more details and related literature see our recent review article on proton-transfer compounds (Aghabozorg *et al.*, 2008*b*).

We describe here the crystal structure of the title compound. The compound contains a $[Zn(pydc)_2(H_2O)_2]^{2-}$ anion, two $(creatH)^+$ cations and two uncoordinated water molecules (Fig. 1). In the anion, the Zn^{II} atom is six-coordinated by two N atoms and two O atoms from two pydc ligands and two water molecules, with the bond length range of 2.0819 (14)–2.1957 (15) Å. The coordination environment around Zn^{II} is distorted octahedral. Intermolecular N—H···O, O—H···O, and weak C—H···O hydrogen bonds play an important role in the stabilization of the crystal structure (Fig. 2 and Table 1).

S2. Experimental

The reaction of pyridine-2,4-dicarboxylic acid (83 mg, 0.5 mmol) in 10 ml distilled water, creatinine (56 mg, 0.5 mmol) in 5 ml distilled water and $Zn(NO_3)_2$.4H_2O (65 mg, 0.25 mmol) in 10 ml distilled water in a 2:2:1 molar ratio gave colorless block crystals of the title compound after slow evaporation of the solvent at the room temperature. The crystals obtained were stable in air.

S3. Refinement

H atoms of water molecules and NH group were found in a difference Fourier map and refined isotropically. H5A was refined with a distance restraint of O—H = 0.79 (2) Å. H atoms on C atoms and NH_2 group were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH), 0.97 (CH_2) and 0.96 (CH_3) Å and N—H = 0.86 Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C, N).

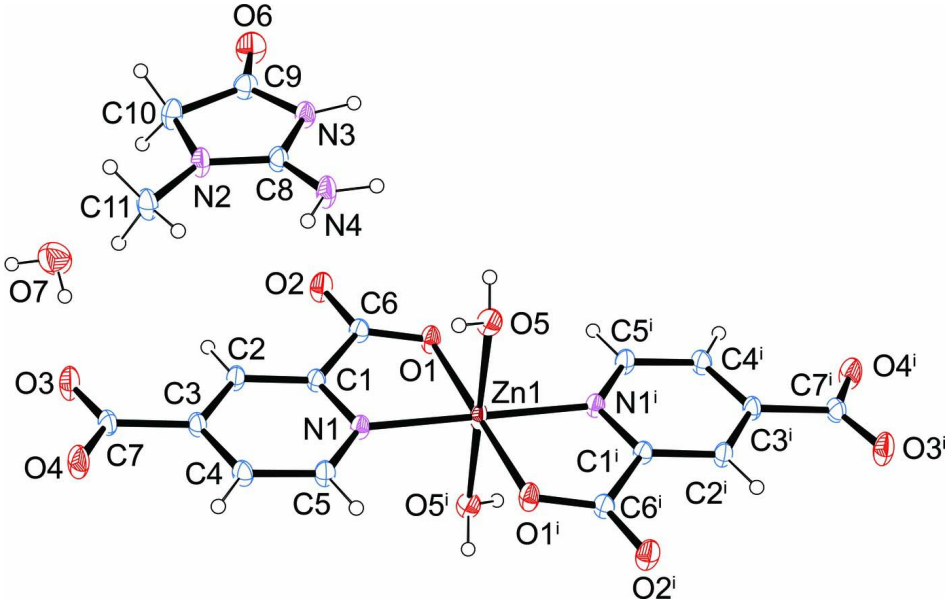

Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i) -*x*+1, -*y*, -*z*+1.]

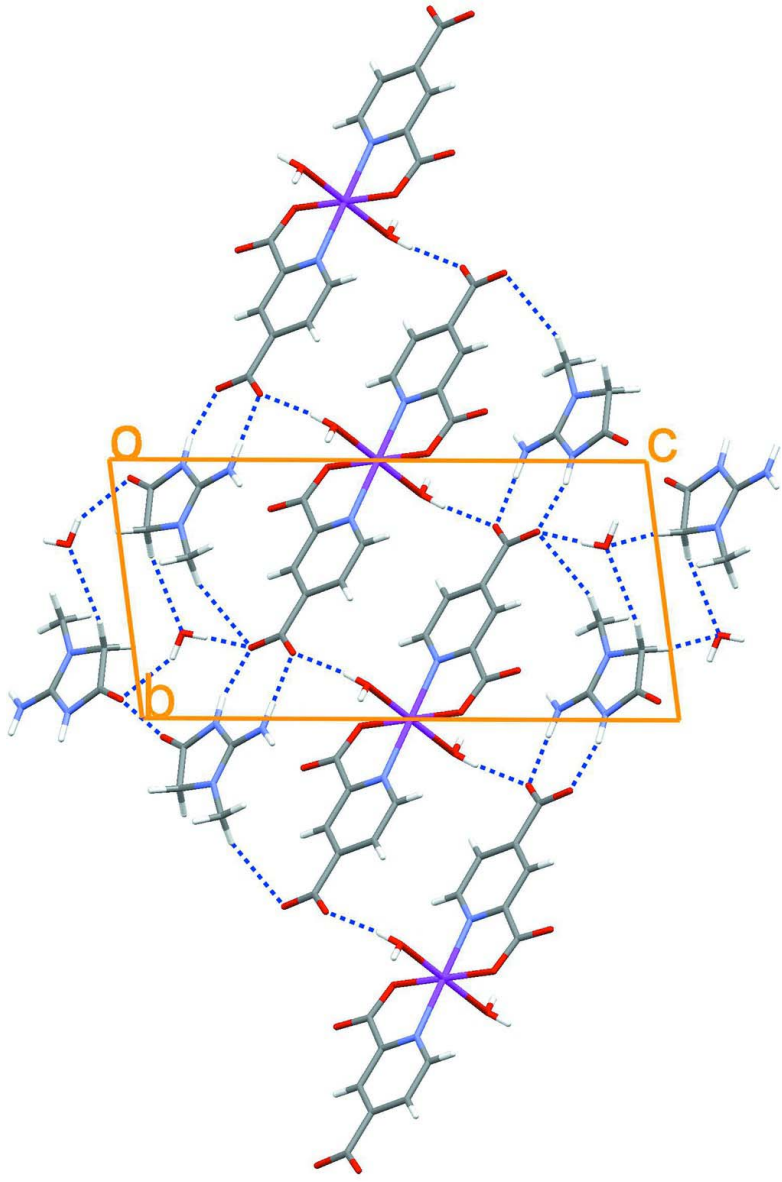

Figure 2

The packing diagram of the title compound. Intermolecular hydrogen bonds are shown as blue dashed lines.

Bis(1-methyl-4-oxoimidazolidin-2-iminium) diaquabis(pyridine-2,4-dicarboxylato-κ^2N,O^2)zincate(II) dihydrate

Crystal data

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$M_r = 695.93$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.3209$ (11) Å
$b = 8.3893$ (17) Å
$c = 16.621$ (3) Å
$\alpha = 81.58$ (3)°
$\beta = 85.26$ (3)°
$\gamma = 74.09$ (3)°
$V = 705.1$ (3) Å^3
$Z = 1$
$F(000) = 360.0$
$D_x = 1.639$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3787 reflections
$\theta = 2.5$–29.2°
$\mu = 0.96$ mm^{-1}

T = 298 K
Block, colorless

0.30 × 0.20 × 0.15 mm

Data collection

Stoe IPDS-2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)
T_{min} = 0.793, T_{max} = 0.862

7743 measured reflections
3787 independent reflections
3206 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 29.2°, θ_{min} = 2.5°
h = −7→7
k = −11→11
l = −18→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.05
3787 reflections
226 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.5000	0.0000	0.5000	0.02707 (9)
O1	0.2451 (2)	0.02688 (14)	0.40534 (7)	0.0301 (2)
O2	0.1143 (3)	0.18980 (16)	0.28950 (8)	0.0395 (3)
O3	0.4093 (3)	0.72611 (16)	0.22032 (9)	0.0432 (3)
O4	0.7237 (3)	0.74523 (17)	0.29581 (9)	0.0462 (4)
O5	0.8365 (2)	−0.13001 (16)	0.42711 (8)	0.0325 (3)
O6	0.1878 (3)	0.07267 (19)	0.03511 (9)	0.0476 (3)
O7	0.0855 (4)	0.6692 (3)	0.09580 (15)	0.0641 (5)
N1	0.5314 (2)	0.22674 (15)	0.43582 (8)	0.0239 (2)
N2	0.6139 (3)	0.25207 (17)	0.11654 (9)	0.0313 (3)
N3	0.4814 (3)	0.02055 (17)	0.13579 (9)	0.0305 (3)
N4	0.7948 (3)	0.03970 (18)	0.22119 (10)	0.0379 (4)
H4B	0.8947	0.0943	0.2359	0.045*
H4A	0.7965	−0.0579	0.2462	0.045*
C1	0.3894 (3)	0.27280 (17)	0.36902 (9)	0.0228 (3)
C2	0.3856 (3)	0.41957 (18)	0.31741 (9)	0.0266 (3)
H2	0.2819	0.4505	0.2724	0.032*
C3	0.5398 (3)	0.51957 (17)	0.33430 (9)	0.0252 (3)
C4	0.6886 (3)	0.46909 (18)	0.40272 (10)	0.0282 (3)
H4	0.7951	0.5326	0.4151	0.034*
C5	0.6774 (3)	0.32360 (19)	0.45239 (10)	0.0277 (3)
H5	0.7746	0.2921	0.4988	0.033*

C6	0.2358 (3)	0.15364 (18)	0.35239 (9)	0.0251 (3)
C7	0.5555 (3)	0.67753 (19)	0.27867 (10)	0.0302 (3)
C8	0.6413 (3)	0.10458 (19)	0.16135 (10)	0.0275 (3)
C9	0.3457 (3)	0.1124 (2)	0.07056 (11)	0.0322 (3)
C10	0.4348 (3)	0.2712 (2)	0.05257 (11)	0.0348 (4)
H10A	0.5227	0.2790	−0.0008	0.042*
H10B	0.2887	0.3694	0.0555	0.042*
C11	0.7495 (4)	0.3769 (2)	0.12415 (12)	0.0360 (4)
H11A	0.8693	0.3364	0.1673	0.054*
H11B	0.6247	0.4781	0.1362	0.054*
H11C	0.8445	0.3988	0.0739	0.054*
H3	0.453 (6)	−0.081 (4)	0.155 (2)	0.076 (9)*
H7A	0.113 (8)	0.685 (5)	0.136 (2)	0.085 (13)*
H5B	0.952 (5)	−0.078 (3)	0.4112 (15)	0.048 (7)*
H7B	0.025 (7)	0.763 (5)	0.072 (2)	0.083 (11)*
H5A	0.818 (6)	−0.174 (3)	0.3900 (14)	0.060 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03224 (15)	0.02409 (13)	0.02854 (15)	−0.01705 (9)	−0.01220 (10)	0.00935 (9)
O1	0.0344 (6)	0.0286 (5)	0.0326 (6)	−0.0204 (4)	−0.0115 (5)	0.0074 (4)
O2	0.0513 (7)	0.0399 (6)	0.0359 (7)	−0.0273 (6)	−0.0237 (6)	0.0088 (5)
O3	0.0569 (8)	0.0353 (6)	0.0435 (7)	−0.0273 (6)	−0.0233 (6)	0.0156 (5)
O4	0.0700 (9)	0.0397 (7)	0.0419 (7)	−0.0400 (7)	−0.0218 (7)	0.0124 (5)
O5	0.0335 (6)	0.0362 (6)	0.0326 (6)	−0.0182 (5)	−0.0065 (5)	−0.0004 (5)
O6	0.0467 (8)	0.0542 (8)	0.0483 (8)	−0.0211 (6)	−0.0229 (6)	−0.0009 (7)
O7	0.0781 (13)	0.0550 (10)	0.0624 (12)	−0.0174 (9)	−0.0188 (10)	−0.0093 (9)
N1	0.0256 (6)	0.0233 (5)	0.0251 (6)	−0.0117 (4)	−0.0077 (5)	0.0029 (4)
N2	0.0348 (7)	0.0267 (6)	0.0343 (7)	−0.0152 (5)	−0.0096 (6)	0.0081 (5)
N3	0.0394 (7)	0.0280 (6)	0.0295 (7)	−0.0187 (5)	−0.0106 (6)	0.0031 (5)
N4	0.0529 (9)	0.0315 (7)	0.0369 (8)	−0.0264 (6)	−0.0225 (7)	0.0119 (6)
C1	0.0247 (6)	0.0227 (6)	0.0242 (7)	−0.0125 (5)	−0.0057 (5)	0.0013 (5)
C2	0.0323 (7)	0.0246 (6)	0.0254 (7)	−0.0140 (6)	−0.0099 (6)	0.0053 (5)
C3	0.0301 (7)	0.0208 (6)	0.0268 (7)	−0.0121 (5)	−0.0059 (6)	0.0028 (5)
C4	0.0328 (8)	0.0247 (7)	0.0321 (8)	−0.0164 (6)	−0.0092 (6)	0.0013 (6)
C5	0.0313 (7)	0.0266 (7)	0.0286 (7)	−0.0141 (6)	−0.0130 (6)	0.0041 (6)
C6	0.0269 (7)	0.0254 (6)	0.0273 (7)	−0.0149 (5)	−0.0071 (6)	0.0010 (5)
C7	0.0424 (9)	0.0228 (6)	0.0296 (8)	−0.0173 (6)	−0.0054 (6)	0.0024 (6)
C8	0.0335 (8)	0.0254 (7)	0.0269 (7)	−0.0152 (6)	−0.0047 (6)	0.0024 (6)
C9	0.0321 (8)	0.0349 (8)	0.0308 (8)	−0.0108 (6)	−0.0080 (6)	−0.0005 (6)
C10	0.0338 (8)	0.0338 (8)	0.0354 (9)	−0.0111 (6)	−0.0113 (7)	0.0094 (7)
C11	0.0402 (9)	0.0273 (7)	0.0435 (10)	−0.0180 (6)	−0.0069 (7)	0.0055 (7)

Geometric parameters (Å, º)

Zn1—N1	2.0819 (14)	N3—H3	0.91 (4)
Zn1—O1	2.1087 (13)	N4—C8	1.298 (2)

Zn1—O5	2.1957 (15)	N4—H4B	0.8600
O1—C6	1.2696 (18)	N4—H4A	0.8600
O2—C6	1.2303 (19)	C1—C2	1.390 (2)
O3—C7	1.244 (2)	C1—C6	1.520 (2)
O4—C7	1.254 (2)	C2—C3	1.393 (2)
O5—H5B	0.85 (3)	C2—H2	0.9300
O5—H5A	0.79 (2)	C3—C4	1.387 (2)
O6—C9	1.207 (2)	C3—C7	1.519 (2)
O7—H7A	0.74 (4)	C4—C5	1.383 (2)
O7—H7B	0.82 (4)	C4—H4	0.9300
N1—C5	1.3367 (19)	C5—H5	0.9300
N1—C1	1.3437 (19)	C9—C10	1.514 (3)
N2—C8	1.325 (2)	C10—H10A	0.9700
N2—C10	1.449 (2)	C10—H10B	0.9700
N2—C11	1.449 (2)	C11—H11A	0.9600
N3—C9	1.368 (2)	C11—H11B	0.9600
N3—C8	1.370 (2)	C11—H11C	0.9600
N1—Zn1—N1^{i}	180.000 (1)	C1—C2—H2	120.6
N1—Zn1—O1	79.39 (5)	C3—C2—H2	120.6
N1^{i}—Zn1—O1	100.61 (5)	C4—C3—C2	118.38 (13)
N1—Zn1—O1^{i}	100.61 (5)	C4—C3—C7	119.66 (14)
N1^{i}—Zn1—O1^{i}	79.39 (5)	C2—C3—C7	121.92 (14)
O1—Zn1—O1^{i}	180.00 (4)	C5—C4—C3	119.50 (14)
N1—Zn1—O5	89.26 (6)	C5—C4—H4	120.2
N1^{i}—Zn1—O5	90.74 (6)	C3—C4—H4	120.2
O1—Zn1—O5	91.70 (5)	N1—C5—C4	122.15 (14)
O1^{i}—Zn1—O5	88.30 (5)	N1—C5—H5	118.9
N1—Zn1—O5^{i}	90.74 (6)	C4—C5—H5	118.9
N1^{i}—Zn1—O5^{i}	89.26 (6)	O2—C6—O1	126.60 (14)
O1—Zn1—O5^{i}	88.30 (5)	O2—C6—C1	117.01 (13)
O1^{i}—Zn1—O5^{i}	91.70 (5)	O1—C6—C1	116.38 (13)
O5—Zn1—O5^{i}	180.000 (1)	O3—C7—O4	125.95 (15)
C6—O1—Zn1	114.83 (9)	O3—C7—C3	118.71 (14)
Zn1—O5—H5B	116.8 (17)	O4—C7—C3	115.32 (14)
Zn1—O5—H5A	121 (2)	N4—C8—N2	127.93 (15)
H5B—O5—H5A	106 (3)	N4—C8—N3	121.60 (14)
H7A—O7—H7B	103 (4)	N2—C8—N3	110.47 (13)
C5—N1—C1	118.96 (13)	O6—C9—N3	126.13 (17)
C5—N1—Zn1	127.89 (10)	O6—C9—C10	127.74 (16)
C1—N1—Zn1	113.12 (10)	N3—C9—C10	106.12 (14)
C8—N2—C10	110.12 (14)	N2—C10—C9	102.65 (13)
C8—N2—C11	127.22 (14)	N2—C10—H10A	111.2
C10—N2—C11	122.56 (14)	C9—C10—H10A	111.2
C9—N3—C8	110.51 (14)	N2—C10—H10B	111.2
C9—N3—H3	118 (2)	C9—C10—H10B	111.2
C8—N3—H3	131 (2)	H10A—C10—H10B	109.2
C8—N4—H4B	120.0	N2—C11—H11A	109.5

C8—N4—H4A	120.0	N2—C11—H11B	109.5
H4B—N4—H4A	120.0	H11A—C11—H11B	109.5
N1—C1—C2	122.12 (13)	N2—C11—H11C	109.5
N1—C1—C6	116.08 (12)	H11A—C11—H11C	109.5
C2—C1—C6	121.80 (13)	H11B—C11—H11C	109.5
C1—C2—C3	118.85 (13)		

N1—Zn1—O1—C6	3.82 (11)	C3—C4—C5—N1	1.5 (3)
N1^{i}—Zn1—O1—C6	−176.18 (11)	Zn1—O1—C6—O2	175.35 (14)
O5—Zn1—O1—C6	−85.11 (12)	Zn1—O1—C6—C1	−5.02 (18)
O5^{i}—Zn1—O1—C6	94.89 (12)	N1—C1—C6—O2	−176.70 (15)
O1—Zn1—N1—C5	−179.66 (15)	C2—C1—C6—O2	2.4 (2)
O1^{i}—Zn1—N1—C5	0.34 (15)	N1—C1—C6—O1	3.6 (2)
O5—Zn1—N1—C5	−87.80 (14)	C2—C1—C6—O1	−177.22 (14)
O5^{i}—Zn1—N1—C5	92.20 (14)	C4—C3—C7—O3	−175.83 (16)
O1—Zn1—N1—C1	−1.69 (11)	C2—C3—C7—O3	6.3 (3)
O1^{i}—Zn1—N1—C1	178.31 (11)	C4—C3—C7—O4	5.8 (2)
O5—Zn1—N1—C1	90.17 (11)	C2—C3—C7—O4	−172.14 (17)
O5^{i}—Zn1—N1—C1	−89.83 (11)	C10—N2—C8—N4	176.19 (18)
C5—N1—C1—C2	−1.2 (2)	C11—N2—C8—N4	−0.2 (3)
Zn1—N1—C1—C2	−179.41 (12)	C10—N2—C8—N3	−3.2 (2)
C5—N1—C1—C6	177.91 (14)	C11—N2—C8—N3	−179.64 (17)
Zn1—N1—C1—C6	−0.26 (17)	C9—N3—C8—N4	−178.09 (16)
N1—C1—C2—C3	1.9 (2)	C9—N3—C8—N2	1.4 (2)
C6—C1—C2—C3	−177.24 (14)	C8—N3—C9—O6	−179.20 (18)
C1—C2—C3—C4	−0.8 (2)	C8—N3—C9—C10	1.0 (2)
C1—C2—C3—C7	177.16 (15)	C8—N2—C10—C9	3.57 (19)
C2—C3—C4—C5	−0.8 (2)	C11—N2—C10—C9	−179.80 (16)
C7—C3—C4—C5	−178.81 (15)	O6—C9—C10—N2	177.51 (19)
C1—N1—C5—C4	−0.5 (2)	N3—C9—C10—N2	−2.67 (19)
Zn1—N1—C5—C4	177.40 (12)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O3^{ii}	0.91 (3)	1.87 (3)	2.764 (2)	165 (3)
N4—H4*A*···O4^{ii}	0.86	1.86	2.706 (2)	168
N4—H4*B*···O2^{iii}	0.86	1.92	2.771 (2)	169
O5—H5*A*···O4^{ii}	0.79 (2)	1.95 (3)	2.729 (2)	171 (3)
O5—H5*B*···O1^{iii}	0.85 (3)	1.98 (3)	2.8088 (17)	165 (2)
O7—H7*A*···O3	0.73 (4)	2.32 (4)	2.968 (3)	148 (4)
O7—H7*B*···O6^{iv}	0.82 (4)	2.26 (4)	2.993 (3)	149 (4)
C5—H5···O5^{v}	0.93	2.46	3.308 (2)	152
C11—H11*A*···O2^{iii}	0.96	2.48	3.425 (3)	167

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