

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

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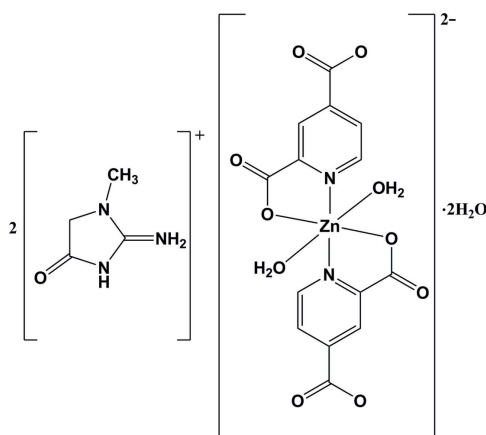
Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.002$ Å;

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 $N-H \cdots O$, $O-H \cdots O$ and weak $C-H \cdots O$ 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

$(C_4H_8N_3O)_2[Zn(C_7H_3NO_4)_2 \cdot (H_2O)_2] \cdot 2H_2O$

$M_r = 695.93$

Triclinic, $P\bar{1}$

$a = 5.3209$ (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) Å³

$Z = 1$

Mo $K\alpha$ radiation

$\mu = 0.96$ mm⁻¹

$T = 298$ K

$0.30 \times 0.20 \times 0.15$ 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, °).

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

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

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supplementary materials

Acta Cryst. (2011). E67, m435-m436 [doi:10.1107/S1600536811008452]

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

diaquabis(pyridine-2,4-dicarboxylato-

H. Aghabozorg, F. Jafarbak, M. Mirzaei and B. Notash

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 (pydcH₂) and various metals, such as (creatH)(pydcH).H₂O (Moghimi *et al.*, 2004), (creatH)₂[Bi(pydc)₂]₂.4H₂O (Moghimi *et al.*, 2005), (creatH)[Zn(pydc)(pydcH)].4H₂O (Aghabozorg *et al.*, 2008*c*), (creatH)[Cr(pydc)₂](pydcH₂).6H₂O (Aghabozorg *et al.*, 2008*a*) and (H₃O)(creatH)[Ni(pydc)₂].3H₂O (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(H₂O)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 \cdots O, O—H \cdots O, and weak C—H \cdots O hydrogen bonds play an important role in the stabilization of the crystal structure (Fig. 2 and Table 1).

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(NO₃)₂.4H₂O (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.

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 NH₂ group were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH), 0.97 (CH₂) and 0.96 (CH₃) Å and N—H = 0.86 Å and with $U_{iso}(H) = 1.2(1.5 \text{ for methyl})U_{eq}(C, N)$.

Figures

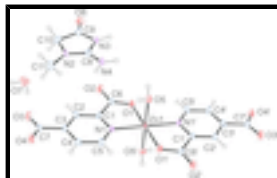


Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i) $-x+1, -y, -z+1$.]

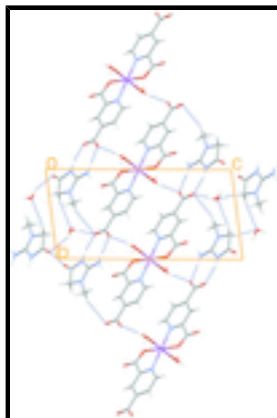


Fig. 2. The packing diagram of the title compound. Intermolecular hydrogen bonds are shown as blue dashed lines.

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

Crystal data

$(C_4H_8N_3O)_2[Zn(C_7H_3NO_4)_2(H_2O)_2] \cdot 2H_2O$

$M_r = 695.93$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 5.3209\ (11)\ \text{\AA}$

$b = 8.3893\ (17)\ \text{\AA}$

$c = 16.621\ (3)\ \text{\AA}$

$\alpha = 81.58\ (3)^\circ$

$\beta = 85.26\ (3)^\circ$

$\gamma = 74.09\ (3)^\circ$

$V = 705.1\ (3)\ \text{\AA}^3$

$Z = 1$

$F(000) = 360.0$

$D_x = 1.639\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3787 reflections

$\theta = 2.5\text{--}29.2^\circ$

$\mu = 0.96\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Block, colorless

$0.30 \times 0.20 \times 0.15\ \text{mm}$

Data collection

Stoe IPDS-2
diffractometer

Radiation source: fine-focus sealed tube
graphite

ω scans

Absorption correction: numerical
(*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)

$T_{\min} = 0.793$, $T_{\max} = 0.862$

3787 independent reflections

3206 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 29.2^\circ$, $\theta_{\min} = 2.5^\circ$

$h = -7 \rightarrow 7$

$k = -11 \rightarrow 11$

7743 measured reflections

$l = -18 \rightarrow 22$

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.033$

Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.090$

H atoms treated by a mixture of independent and constrained refinement

$S = 1.05$

$w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

3787 reflections

$(\Delta/\sigma)_{\max} = 0.001$

226 parameters

$\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$

1 restraint

$\Delta\rho_{\min} = -0.48 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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*

supplementary materials

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 (\AA^2)

	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 (\AA , $^\circ$)

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)		

supplementary materials

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 codes: (i) $-x+1, -y, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N3—H3 \cdots O3 ⁱⁱ	0.91 (3)	1.87 (3)	2.764 (2)	165 (3)
N4—H4A \cdots O4 ⁱⁱ	0.86	1.86	2.706 (2)	168
N4—H4B \cdots O2 ⁱⁱⁱ	0.86	1.92	2.771 (2)	169
O5—H5A \cdots O4 ⁱⁱ	0.79 (2)	1.95 (3)	2.729 (2)	171 (3)
O5—H5B \cdots O1 ⁱⁱⁱ	0.85 (3)	1.98 (3)	2.8088 (17)	165 (2)
O7—H7A \cdots O3	0.73 (4)	2.32 (4)	2.968 (3)	148 (4)
O7—H7B \cdots O6 ^{iv}	0.82 (4)	2.26 (4)	2.993 (3)	149 (4)
C5—H5 \cdots O5 ^v	0.93	2.46	3.308 (2)	152
C11—H11A \cdots 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) $-x+2, -y, -z+1$.

Fig. 1

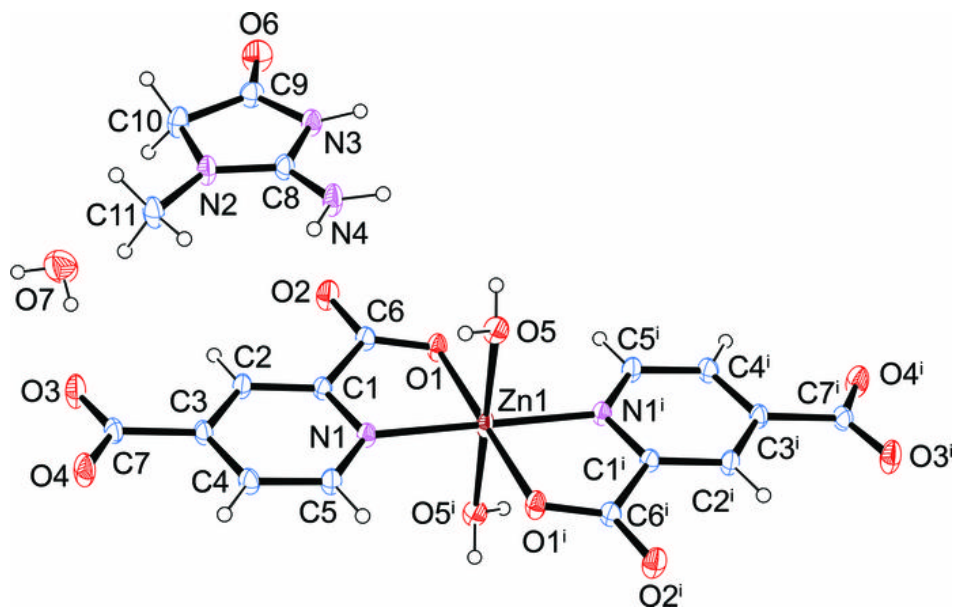


Fig. 2

