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Aquabis(5-methylpyrazine-2-carboxylato)zinc(II) trihydrate

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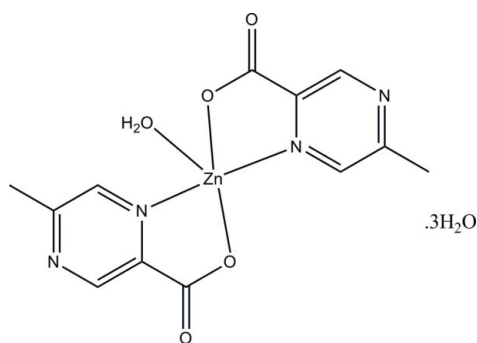
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.038; wR factor = 0.109; data-to-parameter ratio = 11.2.

In the title compound, $[\text{Zn}(\text{C}_6\text{H}_5\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O}$, the Zn^{II} centre is five-coordinated by two *O,N*-bidentate Schiff base ligands and one O atom from a water molecule in a slightly distorted square-pyramidal geometry. In the crystal, the complex and uncoordinated water molecules are linked by $\text{O}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{N}$ and $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds, forming a three-dimensional network.

Related literature

For background to the molecular architecture and biological activity of benzoic acid–metal complexes, see: Cheng *et al.* (2006); Yang *et al.* (2004). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $[\text{Zn}(\text{C}_6\text{H}_5\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O}$
 $M_r = 411.67$

 Triclinic, $P\bar{1}$
 $a = 8.134$ (4) Å

 $b = 10.492$ (5) Å

 $c = 10.982$ (5) Å

 $\alpha = 66.61$ (2)°

 $\beta = 81.85$ (2)°

 $\gamma = 78.33$ (2)°

 $V = 840.3$ (7) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 1.51$ mm⁻¹
 $T = 296$ K

 $0.32 \times 0.28 \times 0.23$ mm

Data collection

 Enraf–Nonius CAD-4 diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\text{min}} = 0.644$, $T_{\text{max}} = 0.723$
 4392 measured reflections

 2923 independent reflections
 2539 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$
 3 standard reflections every 200 reflections
 intensity decay: 1%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.109$
 $S = 1.05$

2923 reflections

260 parameters

12 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.43$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.68$ e Å⁻³

Table 1

Selected bond lengths (Å).

Zn1–N1	1.989 (2)	Zn1–O4	1.957 (2)
Zn1–N3	1.985 (2)	Zn1–O5	2.245 (3)
Zn1–O2	1.951 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

<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>
C9–H9 \cdots O1 ⁱ	0.93	2.35	3.204 (4)	153
C3–H3 \cdots O3 ⁱⁱ	0.93	2.36	3.255 (4)	162
O8–H8B \cdots N4 ⁱⁱⁱ	0.832 (10)	2.30 (2)	3.044 (4)	150 (3)
O6–H6E \cdots O7	0.841 (10)	2.092 (11)	2.932 (4)	177 (4)
O6–H6D \cdots O8	0.839 (10)	1.924 (14)	2.755 (4)	171 (4)
O8–H8A \cdots O1	0.835 (10)	1.953 (13)	2.781 (4)	171 (4)
O7–H7B \cdots O3 ⁱⁱⁱ	0.836 (10)	1.996 (18)	2.797 (3)	160 (4)
O7–H7A \cdots N2 ^{iv}	0.839 (10)	2.185 (18)	2.977 (4)	157 (3)
O5–H5B \cdots O6 ^v	0.835 (10)	1.924 (11)	2.754 (4)	172 (3)
O5–H5A \cdots O7 ^{vi}	0.830 (10)	2.034 (11)	2.861 (4)	175 (4)

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5038).

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supporting information

Acta Cryst. (2009). E65, m1083–m1084 [doi:10.1107/S1600536809031778]

Aquabis(5-methylpyrazine-2-carboxylato)zinc(II) trihydrate**Yong-Ming Cui, Jin Li, Xian Zhang and Qing-Fu Zeng****S1. Comment**

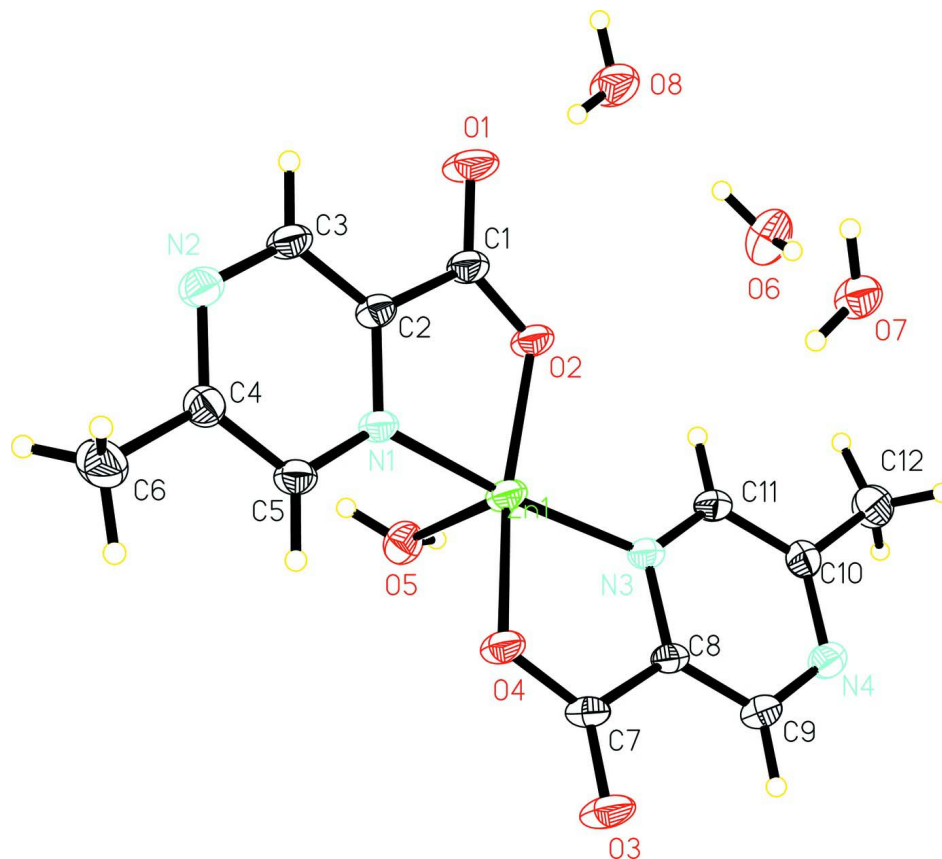
There has been much research interest in benzoic acid metal complexes due to their molecular architectures and biological activities (Cheng *et al.*, 2006; Yang *et al.*, 2004). In this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The Zn^{II} atom is five-coordinated by two O and two N atoms from the two Schiff base ligands and one O from the water molecule, forming a slightly distorted square pyramid coordination (Table 1). The mononuclear complex interacts with the solvent water molecules to form a three-dimensional network (Table 2).

S2. Experimental

A mixture of 5-methylpyrazine-2-carboxylic acid (276 mg, 2 mmol) and Zn(NO₃)₂·6H₂O (1 mmol, 271 mg) in methanol (10 ml) was stirred for 3 h. After keeping the filtrate in air for 7 d, colourless blocks of (I) were formed.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å for the aromatic H atoms and C—H = 0.96 Å for the aliphatic H atoms) and were refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

**Figure 1**

The molecular structure of (I) showing 30% probability displacement ellipsoids.

Aquabis(5-methylpyrazine-2-carboxylato)zinc(II) trihydrate

Crystal data

$[\text{Zn}(\text{C}_6\text{H}_5\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O}$

$M_r = 411.67$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.134 (4) \text{ \AA}$

$b = 10.492 (5) \text{ \AA}$

$c = 10.982 (5) \text{ \AA}$

$\alpha = 66.61 (2)^\circ$

$\beta = 81.85 (2)^\circ$

$\gamma = 78.33 (2)^\circ$

$V = 840.3 (7) \text{ \AA}^3$

$Z = 2$

$F(000) = 424$

$D_x = 1.627 \text{ Mg m}^{-3}$

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

Cell parameters from 25 reflections

$\theta = 9\text{--}12^\circ$

$\mu = 1.51 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colourless

$0.32 \times 0.28 \times 0.23 \text{ mm}$

Data collection

Enraf–Nonius CAD-4

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega/2\theta$ scans

Absorption correction: ψ scan

(North *et al.*, 1968)

$T_{\min} = 0.644$, $T_{\max} = 0.723$

4392 measured reflections

2923 independent reflections

2539 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.0^\circ$

$h = -9 \rightarrow 9$

$k = -12 \rightarrow 12$
 $l = -13 \rightarrow 13$

3 standard reflections every 200 reflections
 intensity decay: 1%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.109$
 $S = 1.05$
 2923 reflections
 260 parameters
 12 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
 $w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.6023P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.016$
 $\Delta\rho_{\max} = 0.43 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.68 \text{ e } \text{\AA}^{-3}$

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6126 (4)	0.8388 (3)	0.6598 (3)	0.0398 (8)
C2	0.7345 (4)	0.8625 (3)	0.5379 (3)	0.0328 (7)
C3	0.7920 (4)	0.9875 (3)	0.4653 (3)	0.0402 (8)
H3	0.7551	1.0635	0.4912	0.048*
C4	0.9502 (4)	0.8932 (3)	0.3229 (3)	0.0371 (7)
C5	0.8939 (4)	0.7652 (3)	0.3960 (3)	0.0358 (7)
H5	0.9310	0.6891	0.3703	0.043*
C6	1.0683 (5)	0.9107 (4)	0.2018 (4)	0.0555 (10)
H6A	1.0163	0.9832	0.1257	0.083*
H6B	1.0947	0.8237	0.1881	0.083*
H6C	1.1699	0.9363	0.2139	0.083*
C7	0.6723 (4)	0.3717 (3)	0.5483 (3)	0.0350 (7)
C8	0.5573 (4)	0.3445 (3)	0.6745 (3)	0.0315 (7)
C9	0.4702 (4)	0.2334 (3)	0.7297 (3)	0.0387 (7)
H9	0.4846	0.1673	0.6908	0.046*
C10	0.3477 (4)	0.3130 (4)	0.8926 (3)	0.0381 (7)
C11	0.4392 (4)	0.4242 (3)	0.8389 (3)	0.0362 (7)
H11	0.4281	0.4886	0.8793	0.043*
C12	0.2293 (5)	0.2978 (4)	1.0126 (4)	0.0533 (10)
H12A	0.1158	0.3146	0.9883	0.080*
H12B	0.2421	0.3647	1.0487	0.080*
H12C	0.2539	0.2042	1.0781	0.080*

H5A	0.964 (4)	0.540 (3)	0.750 (3)	0.040 (10)*
H7A	0.070 (5)	0.7757 (14)	0.720 (4)	0.056 (12)*
H8A	0.406 (6)	0.908 (4)	0.855 (3)	0.090 (18)*
H5B	0.875 (4)	0.438 (3)	0.8366 (14)	0.048 (11)*
H7B	0.175 (4)	0.675 (4)	0.683 (3)	0.076 (15)*
H8B	0.329 (5)	0.985 (2)	0.929 (3)	0.049 (12)*
H6D	0.259 (6)	0.734 (3)	0.977 (4)	0.088 (18)*
H6E	0.183 (5)	0.674 (4)	0.915 (2)	0.065 (14)*
N1	0.7865 (3)	0.7518 (3)	0.5033 (2)	0.0317 (6)
N2	0.9005 (4)	1.0029 (3)	0.3579 (3)	0.0417 (7)
N3	0.5426 (3)	0.4391 (3)	0.7298 (2)	0.0318 (6)
N4	0.3644 (4)	0.2175 (3)	0.8390 (3)	0.0405 (7)
O1	0.5584 (4)	0.9371 (3)	0.6954 (3)	0.0624 (8)
O2	0.5775 (3)	0.7154 (2)	0.7156 (2)	0.0423 (6)
O3	0.6850 (4)	0.2940 (2)	0.4880 (2)	0.0514 (7)
O4	0.7438 (3)	0.4786 (2)	0.5142 (2)	0.0394 (5)
O5	0.9020 (3)	0.4833 (3)	0.7568 (2)	0.0449 (6)
O6	0.2178 (4)	0.6625 (3)	0.9876 (3)	0.0635 (8)
O7	0.0982 (4)	0.6891 (3)	0.7377 (3)	0.0494 (6)
O8	0.3459 (4)	0.9068 (3)	0.9238 (3)	0.0654 (8)
Zn1	0.68363 (5)	0.58672 (4)	0.62838 (4)	0.03747 (16)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0472 (19)	0.0338 (17)	0.0442 (18)	-0.0088 (14)	0.0072 (15)	-0.0233 (15)
C2	0.0402 (17)	0.0294 (15)	0.0330 (15)	-0.0068 (13)	-0.0022 (13)	-0.0157 (13)
C3	0.051 (2)	0.0308 (16)	0.0444 (18)	-0.0087 (14)	0.0016 (15)	-0.0211 (15)
C4	0.0361 (17)	0.0369 (17)	0.0363 (16)	-0.0046 (13)	-0.0006 (13)	-0.0131 (14)
C5	0.0402 (18)	0.0325 (16)	0.0380 (17)	-0.0037 (13)	-0.0005 (14)	-0.0187 (14)
C6	0.059 (2)	0.048 (2)	0.050 (2)	-0.0061 (18)	0.0150 (18)	-0.0161 (18)
C7	0.0468 (18)	0.0249 (15)	0.0339 (16)	-0.0017 (13)	-0.0005 (14)	-0.0146 (13)
C8	0.0359 (16)	0.0247 (14)	0.0368 (16)	-0.0031 (12)	-0.0015 (13)	-0.0158 (13)
C9	0.0465 (19)	0.0318 (16)	0.0431 (18)	-0.0077 (14)	-0.0030 (15)	-0.0190 (15)
C10	0.0327 (17)	0.0417 (18)	0.0410 (17)	-0.0068 (13)	0.0010 (13)	-0.0178 (15)
C11	0.0392 (17)	0.0352 (16)	0.0406 (17)	-0.0054 (13)	0.0015 (14)	-0.0226 (14)
C12	0.053 (2)	0.062 (2)	0.050 (2)	-0.0182 (18)	0.0151 (17)	-0.0278 (19)
N1	0.0369 (14)	0.0270 (12)	0.0339 (13)	-0.0041 (10)	-0.0003 (11)	-0.0158 (11)
N2	0.0494 (17)	0.0327 (14)	0.0427 (15)	-0.0095 (12)	0.0032 (13)	-0.0147 (12)
N3	0.0352 (14)	0.0287 (13)	0.0349 (13)	-0.0047 (10)	0.0007 (11)	-0.0169 (11)
N4	0.0444 (16)	0.0356 (14)	0.0450 (16)	-0.0121 (12)	0.0025 (13)	-0.0181 (13)
O1	0.092 (2)	0.0378 (13)	0.0634 (17)	-0.0178 (13)	0.0312 (15)	-0.0344 (13)
O2	0.0563 (14)	0.0331 (12)	0.0444 (13)	-0.0164 (10)	0.0166 (11)	-0.0243 (10)
O3	0.0831 (19)	0.0376 (13)	0.0436 (13)	-0.0201 (12)	0.0148 (13)	-0.0273 (11)
O4	0.0550 (14)	0.0322 (12)	0.0372 (12)	-0.0144 (10)	0.0103 (10)	-0.0205 (10)
O5	0.0494 (15)	0.0442 (14)	0.0403 (14)	-0.0148 (11)	0.0000 (11)	-0.0127 (12)
O6	0.079 (2)	0.071 (2)	0.0412 (15)	-0.0360 (17)	0.0014 (14)	-0.0121 (14)
O7	0.0609 (17)	0.0442 (15)	0.0444 (14)	-0.0189 (12)	0.0128 (12)	-0.0185 (12)

O8	0.080 (2)	0.0525 (18)	0.0684 (19)	-0.0268 (15)	0.0282 (16)	-0.0311 (15)
Zn1	0.0488 (3)	0.0304 (2)	0.0392 (2)	-0.01200 (16)	0.00646 (16)	-0.01988 (17)

Geometric parameters (Å, °)

C1—O1	1.224 (4)	C10—N4	1.327 (4)
C1—O2	1.266 (4)	C10—C11	1.394 (5)
C1—C2	1.516 (4)	C10—C12	1.492 (5)
C2—N1	1.334 (4)	C11—N3	1.336 (4)
C2—C3	1.373 (4)	C11—H11	0.9300
C3—N2	1.345 (4)	C12—H12A	0.9600
C3—H3	0.9300	C12—H12B	0.9600
C4—N2	1.325 (4)	C12—H12C	0.9600
C4—C5	1.395 (5)	Zn1—N1	1.989 (2)
C4—C6	1.497 (5)	Zn1—N3	1.985 (2)
C5—N1	1.341 (4)	Zn1—O2	1.951 (2)
C5—H5	0.9300	Zn1—O4	1.957 (2)
C6—H6A	0.9600	Zn1—O5	2.245 (3)
C6—H6B	0.9600	O5—H5A	0.830 (10)
C6—H6C	0.9600	O5—H5B	0.835 (10)
C7—O3	1.221 (4)	O6—H6D	0.839 (10)
C7—O4	1.267 (4)	O6—H6E	0.841 (10)
C7—C8	1.518 (4)	O7—H7A	0.839 (10)
C8—N3	1.334 (4)	O7—H7B	0.836 (10)
C8—C9	1.370 (4)	O8—H8A	0.835 (10)
C9—N4	1.347 (4)	O8—H8B	0.832 (10)
C9—H9	0.9300		
O1—C1—O2	126.4 (3)	N3—C11—H11	119.7
O1—C1—C2	118.7 (3)	C10—C11—H11	119.7
O2—C1—C2	115.0 (3)	C10—C12—H12A	109.5
N1—C2—C3	120.3 (3)	C10—C12—H12B	109.5
N1—C2—C1	115.6 (3)	H12A—C12—H12B	109.5
C3—C2—C1	124.1 (3)	C10—C12—H12C	109.5
N2—C3—C2	121.7 (3)	H12A—C12—H12C	109.5
N2—C3—H3	119.2	H12B—C12—H12C	109.5
C2—C3—H3	119.2	C2—N1—C5	118.9 (3)
N2—C4—C5	121.2 (3)	C2—N1—Zn1	110.7 (2)
N2—C4—C6	118.0 (3)	C5—N1—Zn1	130.3 (2)
C5—C4—C6	120.8 (3)	C4—N2—C3	117.8 (3)
N1—C5—C4	120.0 (3)	C8—N3—C11	118.4 (3)
N1—C5—H5	120.0	C8—N3—Zn1	111.5 (2)
C4—C5—H5	120.0	C11—N3—Zn1	130.1 (2)
C4—C6—H6A	109.5	C10—N4—C9	117.6 (3)
C4—C6—H6B	109.5	C1—O2—Zn1	115.0 (2)
H6A—C6—H6B	109.5	C7—O4—Zn1	115.3 (2)
C4—C6—H6C	109.5	Zn1—O5—H5A	112 (2)
H6A—C6—H6C	109.5	Zn1—O5—H5B	114 (2)

H6B—C6—H6C	109.5	H5A—O5—H5B	110.6 (17)
O3—C7—O4	126.2 (3)	H6D—O6—H6E	108.5 (17)
O3—C7—C8	119.0 (3)	H7A—O7—H7B	109.8 (17)
O4—C7—C8	114.8 (3)	H8A—O8—H8B	110.3 (18)
N3—C8—C9	120.6 (3)	O2—Zn1—O4	166.16 (10)
N3—C8—C7	115.2 (3)	O2—Zn1—N3	95.36 (10)
C9—C8—C7	124.2 (3)	O4—Zn1—N3	83.22 (9)
N4—C9—C8	121.7 (3)	O2—Zn1—N1	83.64 (9)
N4—C9—H9	119.2	O4—Zn1—N1	95.00 (10)
C8—C9—H9	119.2	N3—Zn1—N1	168.45 (10)
N4—C10—C11	121.0 (3)	O2—Zn1—O5	97.35 (10)
N4—C10—C12	118.2 (3)	O4—Zn1—O5	96.49 (10)
C11—C10—C12	120.8 (3)	N3—Zn1—O5	94.98 (10)
N3—C11—C10	120.6 (3)	N1—Zn1—O5	96.55 (10)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9 \cdots O1 ⁱ	0.93	2.35	3.204 (4)	153
C3—H3 \cdots O3 ⁱⁱ	0.93	2.36	3.255 (4)	162
O8—H8B \cdots N4 ⁱⁱ	0.83 (1)	2.30 (2)	3.044 (4)	150 (3)
O6—H6E \cdots O7	0.84 (1)	2.09 (1)	2.932 (4)	177 (4)
O6—H6D \cdots O8	0.84 (1)	1.92 (1)	2.755 (4)	171 (4)
O8—H8A \cdots O1	0.84 (1)	1.95 (1)	2.781 (4)	171 (4)
O7—H7B \cdots O3 ⁱⁱⁱ	0.84 (1)	2.00 (2)	2.797 (3)	160 (4)
O7—H7A \cdots N2 ^{iv}	0.84 (1)	2.19 (2)	2.977 (4)	157 (3)
O5—H5B \cdots O6 ^v	0.84 (1)	1.92 (1)	2.754 (4)	172 (3)
O5—H5A \cdots O7 ^{vi}	0.83 (1)	2.03 (1)	2.861 (4)	175 (4)

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