Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Pentaaqua[2-(5-carboxylato-2-oxido-1-pyridinio)acetato]zinc(II) monohydrate

Jing Chen and Yun-Long Feng*

Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, Zhejiang 321004, People's Republic of China
Correspondence e-mail: sky37@zjnu.cn

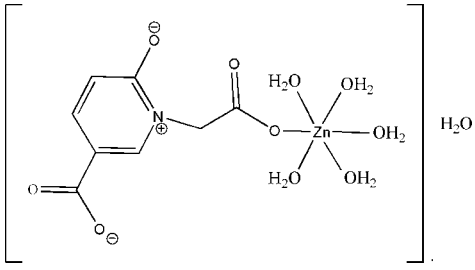
Received 20 April 2010; accepted 12 May 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.084; data-to-parameter ratio = 13.7.

In the title compound, $[Zn(C_8H_5NO_5)(H_2O)_5]\cdot H_2O$, the Zn^{II} atom is coordinated by one O atom from the 2-(5-carboxylato-2-oxidopyridinium-1-yl)acetate ligand and by five water molecules, forming a distorted octahedral geometry. Coordinated and uncoordinated water molecules form O—H···O hydrogen bonds, leading to a three-dimensional framework.

Related literature

For related structures, see: Jiang *et al.* (2009); Szafran *et al.* (2006); Yang *et al.* (2010); Zhang *et al.* (2003); He & Feng (2007).



Experimental

Crystal data

$[Zn(C_8H_5NO_5)(H_2O)_5]\cdot H_2O$
M_r = 368.60
Monoclinic, $P2_1/c$
a = 10.9584 (4) Å
b = 7.5548 (4) Å
c = 16.6510 (7) Å
β = 103.498 (3)°
V = 1340.43 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 293 K
0.36 × 0.09 × 0.05 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.824, T_{max} = 0.918
19343 measured reflections
3086 independent reflections
2233 reflections with $I > 2\sigma(I)$
R_{int} = 0.100

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.084
S = 1.00
3086 reflections
226 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2^{i}	0.83 (2)	2.25 (2)	2.972 (3)	145 (3)
O1W—H1WB···O2W^{ii}	0.81 (2)	2.58 (3)	3.118 (3)	125 (3)
O2W—H2WA···O4^{iii}	0.83 (2)	1.89 (2)	2.716 (2)	169 (3)
O2W—H2WB···O2^{i}	0.80 (2)	1.96 (2)	2.742 (2)	163 (2)
O3W—H3WA···O2^{iv}	0.81 (2)	1.89 (2)	2.701 (2)	173 (2)
O3W—H3WB···O4^{v}	0.82 (2)	2.04 (2)	2.849 (2)	170 (3)
O4W—H4WA···O5^{vi}	0.82 (2)	2.02 (2)	2.810 (2)	160 (3)
O5W—H5WA···O1^{iii}	0.82 (2)	1.90 (2)	2.705 (2)	166 (3)
O5W—H5WB···O1^{iv}	0.81 (2)	1.95 (2)	2.742 (2)	164 (3)
O6W—H6WB···O3^{v}	0.82 (2)	1.89 (2)	2.697 (3)	171 (3)

Symmetry codes: (i) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x, -y, -z+1$; (iii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (vi) $-x, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2541).

References

Bruker (2006). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
He, Y.-H. & Feng, Y.-L. (2007). *Acta Cryst.* E**63**, o3422.
Jiang, M.-X., Feng, Y.-L., He, Y.-H. & Su, H. (2009). *Inorg. Chim. Acta*, **362**, 2856–2860.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Szafran, M., Katrusiak, A., Koput, J. & Dega, S. Z. (2006). *J. Mol. Struct.* **784**, 98–108.
Yang, Q., Zhao, J.-P., Hu, B.-W., Zhang, X.-F. & Bu, X.-H. (2010). *Inorg. Chem.* **49**, 3746–3751.
Zhang, B., Zhu, X.-Q., Lu, J.-Y., He, J., Wang, P. & Cheng, J.-P. (2003). *J. Org. Chem.* **68**, 3295–3298.

supporting information

Acta Cryst. (2010). E**66**, m759 [doi:10.1107/S1600536810017538]

Pentaaqua[2-(5-carboxylato-2-oxido-1-pyridinio)acetato]zinc(II) monohydrate

Jing Chen and Yun-Long Feng

S1. Comment

The pyridinium carboxylate ligands, containing both of carboxylate and quaternary ammonium groups, have been extensively employed to design and construct novel complexes due to its versatile coordination behavior to metal ions (Zhang *et al.*, 2003; Szafran *et al.*, 2006; Yang *et al.*, 2010). Herein, we report the synthesis and crystal structure of a new complex, $[ZnL(H_2O)_5].H_2O$ (LH_2 = 5-carboxy-1-carboxymethyl-2-oxidopyridinium; He & Feng, 2007).

As shown in Fig. 1, the metal center Zn^{II} atom is six-coordinated by one O atom from one L^{2-} ligand [Zn—O 2.1039 (16) Å] and five water molecules [Zn—O 2.0554 (17)–2.0988 (19) Å], to form a distorted octahdral geometry. Notably, only one O atom from the flexible carboxylic groups of L^{2-} ligand coordinates to the Zn^{II} ion. As shown in Fig. 2, the complexes connected with each other by the O—H···O hydrogen bonds generate a three-dimensional structure.

S2. Experimental

All the starting materials and solvents were obtained commercially and were used without further purification. A mixture of *N*-carboxymethyl-2-oxo-pyridine-5-carboxylic acid (0.1972 g, 1 mmol), $ZnNO_3$ (0.1901 g, 1 mmol), and purified water (15 ml) was sealed in a 25 ml stainless steel reactor and kept at 393 K for 3 d. Then, the reactor was cooled to room temperature at a speed of 5 K/h. A large quantity of colorless single crystals were filtered out of the mixture with the yield of 85%.

S3. Refinement

The C-bound H atoms were positioned geometrically and included in the refinement using a riding model, with C—H = 0.93 or 0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C). The O-bound H atoms was located in a difference Fourier map and refined, with the distance restraint of O—H = 0.82 (2) Å, and with U_{iso}(H) = 1.2U_{eq}(O).

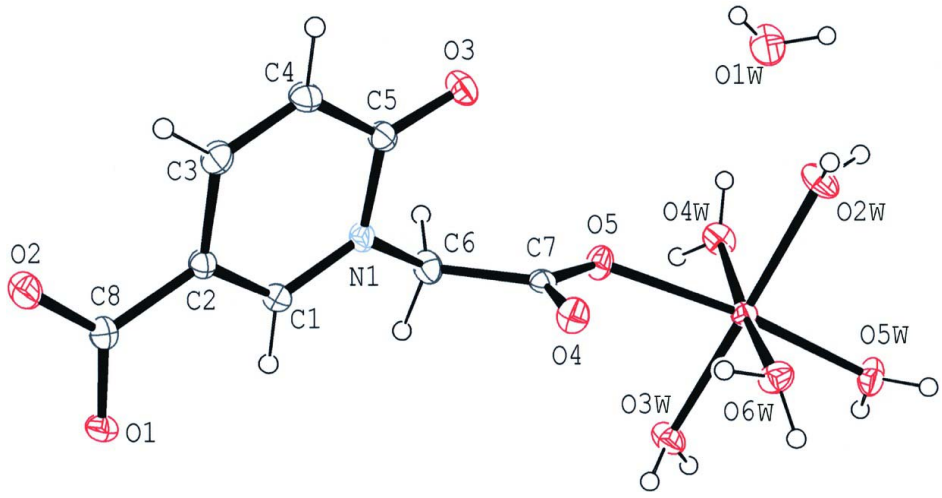


Figure 1

The molecular structure of the title compound, with 30% probability displacement ellipsoids.

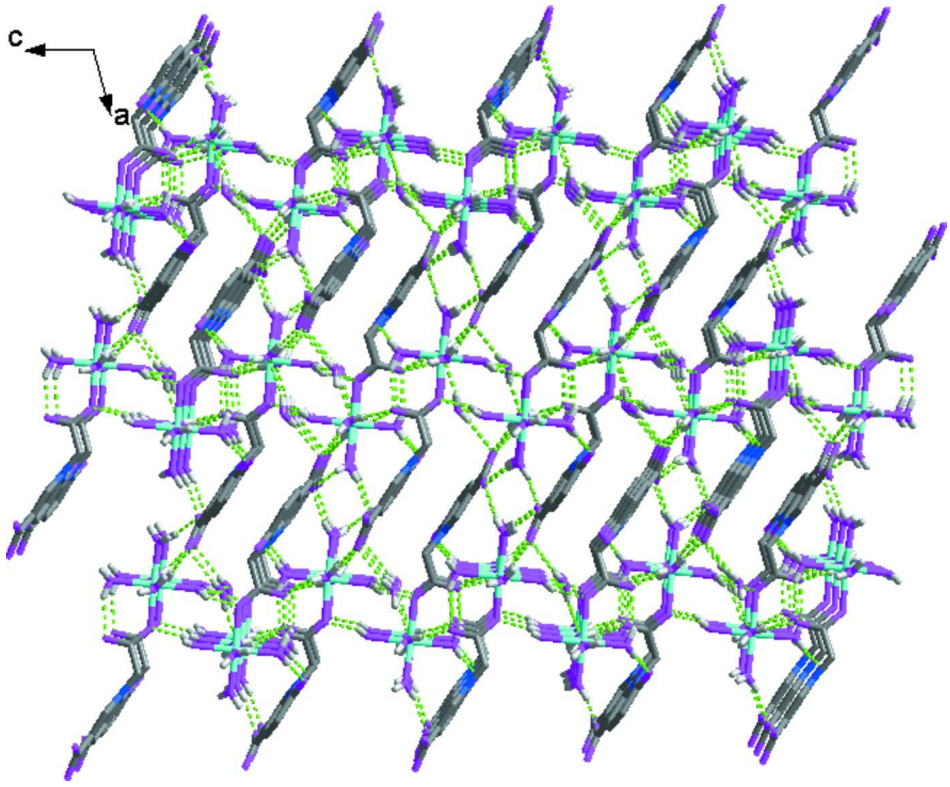


Figure 2

Three-dimensional framework with hydrogen bonding interactions.

Pentaaqua[2-(5-carboxylato-2-oxido-1-pyridinio)acetato]zinc(II) monohydrate

Crystal data

$[Zn(C_8H_5NO_5)(H_2O)_5]\cdot H_2O$
$M_r = 368.60$

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 10.9584 (4) Å
b = 7.5548 (4) Å
c = 16.6510 (7) Å
β = 103.498 (3)°
V = 1340.43 (10) Å^3
Z = 4
F(000) = 760
D_x = 1.826 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6642 reflections
θ = 1.9–27.6°
μ = 1.89 mm^{-1}
T = 293 K
Prism, colourless
0.36 × 0.09 × 0.05 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.824, T_{max} = 0.918

19343 measured reflections
3086 independent reflections
2233 reflections with $I > 2\sigma(I)$
R_{int} = 0.100
θ_{max} = 27.6°, θ_{min} = 1.9°
h = −14→14
k = −9→8
l = −21→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.084
S = 1.00
3086 reflections
226 parameters
18 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
$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 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. 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.14951 (2)	0.39964 (4)	0.404996 (17)	0.02275 (11)
O1	−0.56142 (14)	0.8182 (2)	0.07024 (11)	0.0314 (4)
O1W	0.0969 (2)	0.0417 (3)	0.59084 (15)	0.0564 (6)
H1WA	0.1593 (19)	−0.021 (4)	0.592 (2)	0.068*
H1WB	0.038 (2)	−0.002 (4)	0.5579 (17)	0.068*
O2	−0.70407 (16)	0.6153 (2)	0.01860 (11)	0.0357 (5)
O2W	0.16338 (18)	0.1231 (2)	0.40753 (11)	0.0324 (5)
H2WA	0.149 (2)	0.061 (3)	0.3650 (11)	0.039*

H2WB	0.207 (2)	0.071 (3)	0.4456 (11)	0.039*
O3	−0.30374 (16)	0.1584 (2)	0.26291 (11)	0.0322 (4)
O3W	0.13340 (17)	0.6755 (3)	0.41312 (11)	0.0331 (5)
H3WA	0.183 (2)	0.732 (3)	0.4479 (12)	0.040*
H3WB	0.120 (2)	0.730 (3)	0.3697 (10)	0.040*
O4	−0.08994 (16)	0.4075 (2)	0.22554 (10)	0.0290 (4)
O4W	0.12338 (18)	0.3724 (2)	0.52419 (11)	0.0306 (4)
H4WA	0.092 (2)	0.452 (2)	0.5466 (16)	0.037*
H4WB	0.103 (2)	0.276 (2)	0.5380 (16)	0.037*
O5	−0.04711 (15)	0.3999 (2)	0.36330 (10)	0.0263 (4)
O5W	0.33859 (16)	0.4349 (3)	0.45253 (12)	0.0348 (5)
H5WA	0.400 (2)	0.396 (3)	0.4376 (16)	0.042*
H5WB	0.357 (2)	0.520 (3)	0.4830 (15)	0.042*
O6W	0.17072 (18)	0.3938 (2)	0.28435 (11)	0.0302 (4)
H6WB	0.2178 (19)	0.467 (3)	0.2718 (16)	0.036*
H6WA	0.1020 (16)	0.399 (3)	0.2526 (15)	0.036*
N1	−0.34860 (18)	0.4432 (3)	0.22449 (12)	0.0223 (5)
C1	−0.4197 (2)	0.5668 (3)	0.17514 (15)	0.0233 (6)
H1A	−0.3972	0.6854	0.1826	0.028*
C2	−0.5222 (2)	0.5226 (3)	0.11561 (14)	0.0224 (5)
C3	−0.5541 (2)	0.3417 (3)	0.10731 (15)	0.0287 (6)
H3A	−0.6260	0.3074	0.0687	0.034*
C4	−0.4824 (2)	0.2166 (3)	0.15441 (15)	0.0279 (6)
H4A	−0.5046	0.0981	0.1462	0.033*
C5	−0.3744 (2)	0.2628 (3)	0.21590 (15)	0.0248 (6)
C6	−0.2487 (2)	0.4933 (3)	0.29580 (14)	0.0269 (6)
H6A	−0.2699	0.4489	0.3455	0.032*
H6B	−0.2454	0.6214	0.2996	0.032*
C7	−0.1195 (2)	0.4249 (3)	0.29292 (15)	0.0216 (5)
C8	−0.6009 (2)	0.6622 (3)	0.06435 (14)	0.0240 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02172 (18)	0.0210 (2)	0.02425 (17)	0.00083 (12)	0.00280 (12)	−0.00019 (12)
O1	0.0270 (10)	0.0199 (11)	0.0432 (11)	−0.0037 (8)	−0.0001 (8)	0.0073 (9)
O1W	0.0464 (15)	0.0551 (16)	0.0705 (17)	0.0124 (12)	0.0194 (12)	0.0136 (13)
O2	0.0303 (11)	0.0272 (11)	0.0393 (11)	−0.0024 (8)	−0.0125 (8)	−0.0002 (8)
O2W	0.0466 (13)	0.0209 (11)	0.0242 (10)	0.0051 (8)	−0.0032 (9)	−0.0027 (8)
O3	0.0332 (10)	0.0268 (11)	0.0346 (10)	0.0082 (8)	0.0040 (8)	0.0064 (8)
O3W	0.0361 (11)	0.0223 (11)	0.0341 (11)	0.0003 (8)	−0.0053 (9)	−0.0004 (8)
O4	0.0275 (10)	0.0371 (11)	0.0215 (9)	0.0010 (8)	0.0042 (8)	0.0006 (8)
O4W	0.0394 (12)	0.0296 (12)	0.0237 (10)	0.0038 (9)	0.0093 (8)	−0.0017 (8)
O5	0.0196 (9)	0.0366 (11)	0.0205 (9)	0.0013 (7)	0.0003 (7)	0.0007 (8)
O5W	0.0203 (10)	0.0372 (13)	0.0448 (12)	0.0009 (8)	0.0036 (9)	−0.0134 (9)
O6W	0.0278 (11)	0.0356 (12)	0.0258 (10)	−0.0059 (8)	0.0035 (8)	0.0019 (8)
N1	0.0183 (11)	0.0221 (13)	0.0242 (11)	0.0009 (9)	0.0002 (8)	−0.0009 (9)
C1	0.0237 (14)	0.0203 (15)	0.0260 (13)	0.0004 (10)	0.0058 (11)	0.0006 (11)

C2	0.0210 (13)	0.0208 (14)	0.0239 (13)	0.0004 (11)	0.0026 (10)	−0.0001 (11)
C3	0.0243 (14)	0.0286 (16)	0.0298 (14)	−0.0037 (11)	−0.0004 (11)	−0.0039 (12)
C4	0.0286 (14)	0.0187 (14)	0.0339 (14)	−0.0023 (11)	0.0025 (11)	−0.0032 (12)
C5	0.0255 (13)	0.0245 (16)	0.0262 (13)	0.0031 (11)	0.0096 (11)	0.0031 (11)
C6	0.0263 (14)	0.0267 (16)	0.0247 (13)	0.0027 (12)	−0.0002 (11)	−0.0034 (11)
C7	0.0221 (13)	0.0142 (14)	0.0267 (13)	−0.0036 (10)	0.0021 (10)	−0.0005 (10)
C8	0.0225 (13)	0.0264 (16)	0.0223 (13)	0.0027 (11)	0.0034 (10)	0.0002 (11)

Geometric parameters (Å, º)

Zn1—O5W	2.0554 (17)	O5W—H5WA	0.821 (16)
Zn1—O6W	2.0759 (18)	O5W—H5WB	0.812 (16)
Zn1—O4W	2.0805 (18)	O6W—H6WB	0.816 (15)
Zn1—O2W	2.0945 (18)	O6W—H6WA	0.814 (16)
Zn1—O3W	2.0988 (19)	N1—C1	1.362 (3)
Zn1—O5	2.1039 (16)	N1—C5	1.392 (3)
O1—C8	1.251 (3)	N1—C6	1.464 (3)
O1W—H1WA	0.829 (17)	C1—C2	1.355 (3)
O1W—H1WB	0.812 (17)	C1—H1A	0.9300
O2—C8	1.257 (3)	C2—C3	1.409 (4)
O2W—H2WA	0.832 (15)	C2—C8	1.498 (3)
O2W—H2WB	0.802 (15)	C3—C4	1.356 (3)
O3—C5	1.246 (3)	C3—H3A	0.9300
O3W—H3WA	0.813 (15)	C4—C5	1.416 (3)
O3W—H3WB	0.816 (15)	C4—H4A	0.9300
O4—C7	1.245 (3)	C6—C7	1.518 (3)
O4W—H4WA	0.823 (15)	C6—H6A	0.9700
O4W—H4WB	0.809 (15)	C6—H6B	0.9700
O5—C7	1.267 (3)		
O5W—Zn1—O6W	92.57 (8)	H6WB—O6W—H6WA	110 (2)
O5W—Zn1—O4W	89.79 (8)	C1—N1—C5	122.35 (19)
O6W—Zn1—O4W	172.96 (8)	C1—N1—C6	121.7 (2)
O5W—Zn1—O2W	93.41 (8)	C5—N1—C6	115.59 (19)
O6W—Zn1—O2W	88.53 (7)	C2—C1—N1	122.1 (2)
O4W—Zn1—O2W	84.70 (7)	C2—C1—H1A	118.9
O5W—Zn1—O3W	86.50 (7)	N1—C1—H1A	118.9
O6W—Zn1—O3W	96.52 (7)	C1—C2—C3	117.1 (2)
O4W—Zn1—O3W	90.25 (7)	C1—C2—C8	120.8 (2)
O2W—Zn1—O3W	174.95 (8)	C3—C2—C8	122.0 (2)
O5W—Zn1—O5	171.74 (7)	C4—C3—C2	121.5 (2)
O6W—Zn1—O5	91.03 (7)	C4—C3—H3A	119.3
O4W—Zn1—O5	87.51 (7)	C2—C3—H3A	119.3
O2W—Zn1—O5	94.10 (7)	C3—C4—C5	121.4 (2)
O3W—Zn1—O5	85.71 (6)	C3—C4—H4A	119.3
H1WA—O1W—H1WB	107 (3)	C5—C4—H4A	119.3
Zn1—O2W—H2WA	123.1 (17)	O3—C5—N1	118.3 (2)
Zn1—O2W—H2WB	122.1 (18)	O3—C5—C4	126.2 (2)

H2WA—O2W—H2WB	111 (2)	N1—C5—C4	115.5 (2)
Zn1—O3W—H3WA	120.8 (18)	N1—C6—C7	114.4 (2)
Zn1—O3W—H3WB	116.6 (19)	N1—C6—H6A	108.7
H3WA—O3W—H3WB	109 (2)	C7—C6—H6A	108.7
Zn1—O4W—H4WA	121.7 (18)	N1—C6—H6B	108.7
Zn1—O4W—H4WB	118.0 (19)	C7—C6—H6B	108.7
H4WA—O4W—H4WB	111 (2)	H6A—C6—H6B	107.6
C7—O5—Zn1	132.66 (16)	O4—C7—O5	125.4 (2)
Zn1—O5W—H5WA	131.2 (19)	O4—C7—C6	120.3 (2)
Zn1—O5W—H5WB	114.9 (18)	O5—C7—C6	114.1 (2)
H5WA—O5W—H5WB	112 (2)	O1—C8—O2	124.0 (2)
Zn1—O6W—H6WB	117.0 (19)	O1—C8—C2	118.4 (2)
Zn1—O6W—H6WA	109.4 (19)	O2—C8—C2	117.6 (2)
O5W—Zn1—O5—C7	103.1 (5)	C1—N1—C5—C4	−2.3 (3)
O6W—Zn1—O5—C7	−12.8 (2)	C6—N1—C5—C4	171.2 (2)
O4W—Zn1—O5—C7	174.1 (2)	C3—C4—C5—O3	178.9 (2)
O2W—Zn1—O5—C7	−101.4 (2)	C3—C4—C5—N1	0.5 (4)
O3W—Zn1—O5—C7	83.6 (2)	C1—N1—C6—C7	−121.4 (2)
C5—N1—C1—C2	1.6 (4)	C5—N1—C6—C7	65.1 (3)
C6—N1—C1—C2	−171.5 (2)	Zn1—O5—C7—O4	21.6 (4)
N1—C1—C2—C3	1.0 (3)	Zn1—O5—C7—C6	−154.06 (16)
N1—C1—C2—C8	177.9 (2)	N1—C6—C7—O4	32.4 (3)
C1—C2—C3—C4	−2.8 (4)	N1—C6—C7—O5	−151.6 (2)
C8—C2—C3—C4	−179.6 (2)	C1—C2—C8—O1	9.1 (3)
C2—C3—C4—C5	2.1 (4)	C3—C2—C8—O1	−174.2 (2)
C1—N1—C5—O3	179.1 (2)	C1—C2—C8—O2	−170.0 (2)
C6—N1—C5—O3	−7.4 (3)	C3—C2—C8—O2	6.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2^{i}	0.83 (2)	2.25 (2)	2.972 (3)	145 (3)
O1*W*—H1*WB*···O2*W*^{ii}	0.81 (2)	2.58 (3)	3.118 (3)	125 (3)
O2*W*—H2*WA*···O4^{iii}	0.83 (2)	1.89 (2)	2.716 (2)	169 (3)
O2*W*—H2*WB*···O2^{i}	0.80 (2)	1.96 (2)	2.742 (2)	163 (2)
O3*W*—H3*WA*···O2^{iv}	0.81 (2)	1.89 (2)	2.701 (2)	173 (2)
O3*W*—H3*WB*···O4^{v}	0.82 (2)	2.04 (2)	2.849 (2)	170 (3)
O4*W*—H4*WA*···O5^{vi}	0.82 (2)	2.02 (2)	2.810 (2)	160 (3)
O5*W*—H5*WA*···O1^{iii}	0.82 (2)	1.90 (2)	2.705 (2)	166 (3)
O5*W*—H5*WB*···O1^{iv}	0.81 (2)	1.95 (2)	2.742 (2)	164 (3)
O6*W*—H6*WB*···O3^{v}	0.82 (2)	1.89 (2)	2.697 (3)	171 (3)

Symmetry codes: (i) *x*+1, −*y*+1/2, *z*+1/2; (ii) −*x*, −*y*, −*z*+1; (iii) −*x*, *y*−1/2, −*z*+1/2; (iv) *x*+1, −*y*+3/2, *z*+1/2; (v) −*x*, *y*+1/2, −*z*+1/2; (vi) −*x*, −*y*+1, −*z*+1.