

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## Hexaaquazinc(II) bis[tris(3-carboxypyridine-2-carboxylato)zincate(II)]

Mehrnaz Gharagozlou,<sup>a\*</sup> Vratislav Langer<sup>b</sup> and Andya Nemati<sup>c</sup>

<sup>a</sup>Department of Nanotechnology and Nanomaterials, Institute for Color Science and Technology, PO Box 16765-654 Tehran, Iran, <sup>b</sup>Environmental Inorganic Chemistry, Department of Chemical and Biological Engineering, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden, and <sup>c</sup>Iran Compiling Encyclopedia Foundation, Tajrish, Tehran, Iran

Correspondence e-mail: gharagozlou@icrc.ac.ir

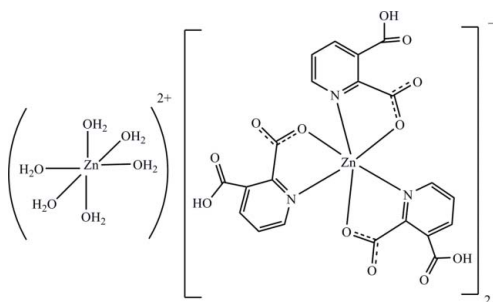
Received 18 October 2010; accepted 15 November 2010

Key indicators: single-crystal X-ray study;  $T = 153$  K; mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å;  $R$  factor = 0.061;  $wR$  factor = 0.158; data-to-parameter ratio = 10.2.

The title compound,  $[\text{Zn}(\text{H}_2\text{O})_6][\text{Zn}(\text{C}_7\text{H}_4\text{NO}_4)_3]_2$ , consists of two  $[\text{Zn}(\text{py}-2,3\text{-dcH})_3]^-$  anions (py-2,3-dcH is 3-carboxypyridine-2-carboxylate) and one  $[\text{Zn}(\text{H}_2\text{O})_6]^{2+}$  cation. The anion is a six-coordinate complex located on a threefold rotation axis with a slightly distorted octahedral geometry around  $\text{Zn}^{2+}$  ion. The cation is also six-coordinate with an octahedral geometry around the Zn atom, located at a  $\bar{3}$  axis. Non-covalent interactions such as  $\pi$ - $\pi$  stacking [centroid-centroid distance = 3.828 (4) Å] and O—H...O hydrogen bonds play important roles in stabilizing the supramolecular structure.

## Related literature

For first-row transition metal complexes of pyridine-2,3-dicarboxylic acid and various bases and for Zn—O distances, see: Aghabozorg, Daneshvar *et al.* (2007); Aghabozorg, Sadrkhanlou *et al.* (2007); Goher *et al.* (1993); Kang *et al.* (2006); Li *et al.* (2006); Prior & Rosseinsky (2001); Swiegers & Malefetse (2000); Yin & Liu (2009). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



## Experimental

## Crystal data

$[\text{Zn}(\text{H}_2\text{O})_6][\text{Zn}(\text{C}_7\text{H}_4\text{NO}_4)_3]_2$   
 $M_r = 1300.88$   
 Trigonal,  $P\bar{3}$   
 $a = 14.470$  (4) Å  
 $c = 6.284$  (2) Å  
 $V = 1139.4$  (6) Å<sup>3</sup>

$Z = 1$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.68$  mm<sup>-1</sup>  
 $T = 153$  K  
 $1.20 \times 0.44 \times 0.42$  mm

## Data collection

Siemens SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.237$ ,  $T_{\max} = 0.538$

10776 measured reflections  
 1356 independent reflections  
 1009 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.154$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$   
 $wR(F^2) = 0.158$   
 $S = 1.00$   
 1356 reflections  
 133 parameters  
 4 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.86$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.82$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Zn1—O1	2.083 (4)	Zn2—O5	2.095 (5)
Zn1—N1	2.157 (5)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3...O2 <sup>v</sup>	0.83 (5)	1.72 (2)	2.547 (5)	169 (7)
O5—H52...O4	0.83 (5)	2.38 (4)	3.157 (7)	156 (7)
O5—H51...O4 <sup>v</sup>	0.82 (6)	2.02 (3)	2.795 (6)	158 (6)

Symmetry codes: (iv)  $y, -x + y, -z$ ; (v)  $-y, x - y, z$ .

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2010); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

We acknowledge financial support of this work by the Nation Elite Foundation. We are also grateful to the Institute for Color Science and Technology.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2373).

## References

- Aghabozorg, H., Daneshvar, S., Motyeian, E., Ghadermazi, M. & Attar Gharamaleki, J. (2007). *Acta Cryst.* **E63**, m2468–m2469.  
 Aghabozorg, H., Sadrkhanlou, E., Soleimannejad, J. & Adams, H. (2007). *Acta Cryst.* **E63**, m1769.  
 Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.  
 Brandenburg, K. (2010). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

- Bruker (2003). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Goher, M. A. S., Youssef, A. A., Zhou, Z.-Y. & Mak, T. C. W. (1993). *Polyhedron*, **12**, 1871–1878.
- Kang, Y., Zhang, J., Li, Z.-J., Cheng, J.-K. & Yao, Y.-G. (2006). *Inorg. Chim. Acta*, **359**, 2201–2209.
- Li, M., Xiang, J., Yuan, L., Wu, S., Chen, S. & Sun, J. (2006). *Cryst. Growth Des.* **6**, 2036–2040.
- Prior, T. J. & Rosseinsky, M. J. (2001). *Chem. Commun.* pp. 495–496.
- Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Swiegers, G. F. & Malefetse, T. J. (2000). *Chem. Rev.* **100**, 3483–3537.
- Yin, H. & Liu, S.-X. (2009). *J. Mol. Struct.* **918**, 165–173.

## supporting information

*Acta Cryst.* (2010). E66, m1606–m1607 [https://doi.org/10.1107/S1600536810047252]

## Hexaaquazinc(II) bis[tris(3-carboxypyridine-2-carboxylato)zincate(II)]

Mehrnaz Gharagozlou, Vratislav Langer and Andya Nemati

### S1. Comment

Metal-organic coordination complexes with one-, two- or three-dimensional structures have attracted attentions for their potential applications as photoelectric materials, catalysis, carriers, sensors, *etc.* (Prior & Rosseinsky, 2001; Swiegers & Malefetse, 2000). From a chemical point of view, L-lysine, a base, contains two amino groups and one carboxylic acid group, these amino groups often participate in hydrogen bonding and as a general base in catalysis. There are previously reported compounds containing pyridine-2,3-dicarboxylic acid, (py-2,3-dcH<sub>2</sub>), (Goher *et al.*, 1993; Yin & Liu 2009; Aghabozorg, Daneshvar *et al.*, 2007, Kang *et al.*, 2006, Li *et al.*, 2006).

The title compound consists of two [Zn(py-2,3-dcH)<sub>3</sub>]<sup>−</sup> anions and one Zn(H<sub>2</sub>O)<sub>6</sub><sup>2+</sup> cation. The anion is a six-coordinate complex located at a 3-fold crystallographic axis around Zn1 atom by three chelating (py-2,3-dcH)<sup>−</sup> ligands *via* one N and one O atom from carboxylate groups (Fig. 1). The cation is also six-coordinate with an octahedral geometry around Zn2 atom, located at a 3-bar axis. L-lysine, even it was included during the synthesis, is not part of this crystal structure and we were surprised that the product material contains Zn atoms in both form of cation and anion units. In anionic complex the three O—Zn1—N angles indicate that there is a distorted octahedral geometry around Zn1 atoms (for selected bond distances and angles see Table 1), but in cationic unit there are three O—Zn2—O angles exactly 180° as imposed by the crystallographic symmetry and good octahedral geometry environment around Zn2 atom (Table 1). The anionic Zn—O distances (Table 1) fall within the range of those found in related Zn complexes, 2.031–2.117 Å (Aghabozorg, Daneshvar *et al.*, 2007; Aghabozorg, Sadr-khanlou *et al.*, 2007; Kang, *et al.*, 2006; Li, *et al.*, 2006; Yin, *et al.*, 2009).

There are three principal hydrogen bonds of O—H<sup>⋯</sup>O type (see Table 2) forming a complicated and extensive hydrogen bonding pattern. Graph-set analysis (Bernstein *et al.*, 1995) on the first level is indicating chains with symbols C<sup>2</sup><sub>2</sub>(20) and C<sup>2</sup><sub>2</sub>(16) for hydrogen bond with donor atoms O3 and O5, respectively, as well as ring R<sup>2</sup><sub>2</sub>(20) for hydrogen bond with O3 as a donor. On second level graph-set, most important are ring R<sup>1</sup><sub>2</sub>(6) and chains C<sup>2</sup><sub>2</sub>(14) and C<sup>2</sup><sub>2</sub>(16) between hexa-aqua zinc cations, as well as rings R<sup>3</sup><sub>3</sub>(15) formed between anions and cations.

There are  $\pi$ - $\pi$  stacking interactions between anions proved by short distance Cg4<sup>⋯</sup>Cg4 3.828 (4) Å [Cg4 is centroid of N1/C2—C6 ring. Symmetry code:  $I - x, I - y, I - z$ ]. These  $\pi$ - $\pi$  stacking interactions and O—H<sup>⋯</sup>O hydrogen bonds have important roles in stabilizing the structure. Crystal packing is depicted in Fig. 2.

### S2. Experimental

The title compound was prepared by the reaction of pyridine-2,3-dicarboxylic acid (py-2,3-dcH<sub>2</sub>) (167 mg, 1 mmol), L-Lysine (L-Lys) (164 mg, 1 mmol) and with zinc(II) nitrate hexahydrate Zn(NO<sub>3</sub>)<sub>2</sub> · 6H<sub>2</sub>O (148.7 mg, 0.5 mmol), which were dissolved in distilled water (30 ml) as solvent in 2:2:1 molar ratio. The crystals were obtained by slow evaporation of solvent at room temperature.

### S3. Refinement

Aromatic hydrogen atoms were refined isotropically with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and their positions were constrained to ideal geometry using an appropriate riding model, with  $\text{C}-\text{H} = 0.95$ . The carboxylate and water H atoms were located at the difference Fourier map and refined isotropically with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ , and restrained to ideal geometry with  $\text{O}-\text{H}$  distances  $0.84(2)\text{Å}$  and  $\text{H}\cdots\text{H}$  distance  $1.34(2)\text{Å}$  for the water molecule.

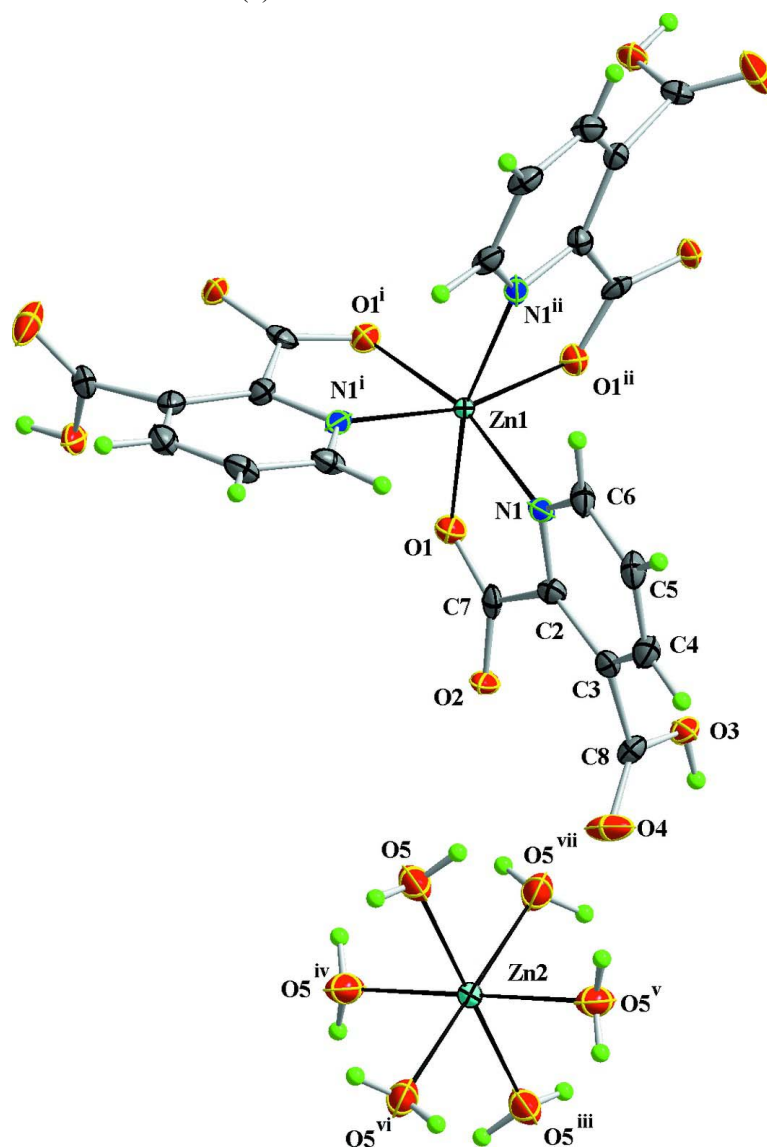
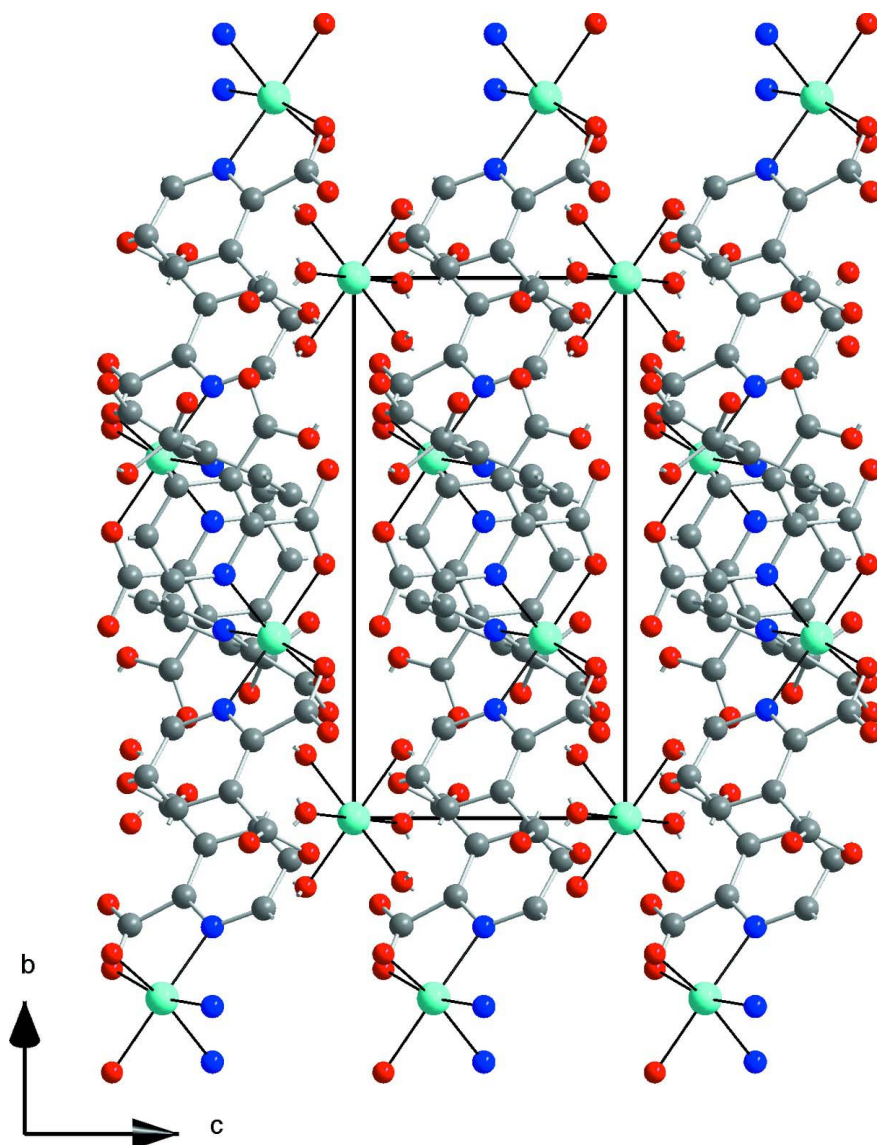


Figure 1

The molecular structure of the title compound, with the displacement ellipsoids drawn at 50% probability level.



**Figure 2**

A view of along the *a* axis of the crystal packing in the title compounds. Layers perpendicular to *c*-directions are connected *via* hydrogen bonds.

**Hexaaquazinc(II) bis[tris(3-carboxypyridine-2-carboxylato)zincate(II)]**

*Crystal data*

$[\text{Zn}(\text{H}_2\text{O})_6][\text{Zn}(\text{C}_7\text{H}_4\text{NO}_4)_3]_2$

$M_r = 1300.88$

Trigonal,  $P\bar{3}$

Hall symbol:  $-P\ 3$

$a = 14.470\ (4)\ \text{\AA}$

$c = 6.284\ (2)\ \text{\AA}$

$V = 1139.4\ (6)\ \text{\AA}^3$

$Z = 1$

$F(000) = 660$

$D_x = 1.896\ \text{Mg m}^{-3}$

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

Cell parameters from 1491 reflections

$\theta = 2.8\text{--}22.5^\circ$

$\mu = 1.68\ \text{mm}^{-1}$

$T = 153\ \text{K}$

Block, colourless

$1.20 \times 0.44 \times 0.42\ \text{mm}$

*Data collection*

Siemens SMART CCD area-detector  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
 $\omega$  scans  
Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 2003)  
 $T_{\min} = 0.237$ ,  $T_{\max} = 0.538$

10776 measured reflections  
1356 independent reflections  
1009 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.154$   
 $\theta_{\max} = 25.1^\circ$ ,  $\theta_{\min} = 2.8^\circ$   
 $h = -17 \rightarrow 17$   
 $k = -17 \rightarrow 17$   
 $l = -7 \rightarrow 7$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.061$   
 $wR(F^2) = 0.158$   
 $S = 1.00$   
1356 reflections  
133 parameters  
4 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0993P)^2 + 0.9035P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.86 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.82 \text{ e } \text{\AA}^{-3}$   
Extinction correction: *SHELXL97* (Sheldrick,  
2008),  $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$   
Extinction coefficient: 0.035 (5)

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.3333	0.6667	0.29441 (18)	0.0155 (4)
O1	0.2510 (3)	0.5298 (3)	0.1090 (6)	0.0193 (9)
O2	0.1958 (3)	0.3552 (3)	0.0954 (6)	0.0194 (10)
O3	0.3623 (3)	0.2972 (3)	0.1662 (6)	0.0213 (10)
H3	0.352 (5)	0.247 (4)	0.086 (9)	0.032*
O4	0.2312 (4)	0.1865 (3)	0.3858 (7)	0.0322 (11)
N1	0.3482 (4)	0.5491 (4)	0.4789 (7)	0.0161 (11)
C2	0.3119 (4)	0.4565 (4)	0.3746 (8)	0.0155 (12)
C3	0.3237 (4)	0.3729 (4)	0.4533 (9)	0.0167 (13)
C4	0.3667 (5)	0.3851 (5)	0.6543 (10)	0.0216 (14)
H4	0.3725	0.3283	0.7164	0.026*
C5	0.4011 (4)	0.4781 (5)	0.7648 (9)	0.0200 (13)
H5	0.4294	0.4863	0.9044	0.024*
C6	0.3935 (4)	0.5601 (5)	0.6677 (9)	0.0183 (13)
H6	0.4219	0.6267	0.7391	0.022*

C7	0.2490 (4)	0.4467 (4)	0.1750 (9)	0.0168 (13)
C8	0.2983 (5)	0.2751 (4)	0.3263 (9)	0.0187 (13)
Zn2	0.0000	0.0000	0.0000	0.0226 (5)
O5	0.0098 (3)	0.1271 (4)	0.1776 (7)	0.0305 (11)
H51	−0.038 (3)	0.109 (5)	0.267 (8)	0.046*
H52	0.069 (2)	0.161 (5)	0.238 (9)	0.046*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn1	0.0124 (5)	0.0124 (5)	0.0217 (7)	0.0062 (2)	0.000	0.000
O1	0.017 (2)	0.016 (2)	0.024 (2)	0.0074 (18)	−0.0023 (17)	−0.0024 (17)
O2	0.016 (2)	0.011 (2)	0.031 (2)	0.0056 (18)	−0.0076 (17)	−0.0055 (17)
O3	0.019 (2)	0.016 (2)	0.029 (3)	0.0096 (19)	0.0048 (19)	−0.0047 (18)
O4	0.040 (3)	0.013 (2)	0.035 (3)	0.007 (2)	0.012 (2)	0.0014 (19)
N1	0.012 (2)	0.012 (2)	0.020 (3)	0.003 (2)	0.0024 (19)	−0.003 (2)
C2	0.013 (3)	0.013 (3)	0.018 (3)	0.005 (2)	0.001 (2)	0.002 (2)
C3	0.011 (3)	0.013 (3)	0.025 (3)	0.005 (2)	0.003 (2)	0.000 (2)
C4	0.021 (3)	0.021 (3)	0.027 (3)	0.014 (3)	0.003 (3)	0.001 (3)
C5	0.015 (3)	0.027 (3)	0.021 (3)	0.013 (3)	−0.002 (2)	−0.002 (3)
C6	0.014 (3)	0.025 (3)	0.018 (3)	0.012 (3)	−0.002 (2)	−0.005 (2)
C7	0.009 (3)	0.022 (3)	0.022 (3)	0.010 (3)	0.003 (2)	0.000 (3)
C8	0.020 (3)	0.015 (3)	0.026 (3)	0.012 (3)	−0.001 (3)	0.001 (2)
Zn2	0.0185 (6)	0.0185 (6)	0.0307 (11)	0.0092 (3)	0.000	0.000
O5	0.018 (2)	0.029 (3)	0.038 (3)	0.008 (2)	0.001 (2)	−0.004 (2)

*Geometric parameters (Å, °)*

Zn1—O1	2.083 (4)	C3—C4	1.380 (8)
Zn1—N1	2.157 (5)	C3—C8	1.502 (8)
O1—C7	1.259 (7)	C4—C5	1.369 (8)
O2—C7	1.256 (7)	C4—H4	0.9500
O3—C8	1.294 (7)	C5—C6	1.386 (8)
O3—H3	0.83 (5)	C5—H5	0.9500
O4—C8	1.217 (7)	C6—H6	0.9500
N1—C6	1.327 (7)	Zn2—O5	2.095 (5)
N1—C2	1.340 (7)	O5—H51	0.82 (5)
C2—C3	1.393 (8)	O5—H52	0.83 (6)
C2—C7	1.514 (8)		
O1—Zn1—O1 <sup>i</sup>	91.76 (15)	C5—C4—H4	119.7
O1—Zn1—N1 <sup>i</sup>	165.35 (16)	C6—C5—C4	118.2 (5)
O1—Zn1—N1	77.62 (16)	C6—C5—H5	120.9
O1 <sup>i</sup> —Zn1—N1	98.55 (15)	C4—C5—H5	120.9
N1 <sup>i</sup> —Zn1—N1	93.83 (16)	N1—C6—C5	122.5 (5)
C7—O1—Zn1	116.9 (4)	N1—C6—H6	118.8
C8—O3—H3	117 (5)	C5—C6—H6	118.8
C6—N1—C2	118.7 (5)	O2—C7—O1	125.8 (5)

C6—N1—Zn1	128.6 (4)	O2—C7—C2	116.8 (5)
C2—N1—Zn1	112.5 (3)	O1—C7—C2	117.3 (5)
N1—C2—C3	122.5 (5)	O4—C8—O3	126.5 (5)
N1—C2—C7	114.5 (5)	O4—C8—C3	121.3 (5)
C3—C2—C7	122.8 (5)	O3—C8—C3	111.9 (5)
C4—C3—C2	117.2 (5)	O5—Zn2—O5 <sup>ii</sup>	180.0
C4—C3—C8	119.2 (5)	O5—Zn2—O5 <sup>iii</sup>	85.74 (18)
C2—C3—C8	123.5 (5)	Zn2—O5—H51	114 (5)
C3—C4—C5	120.6 (5)	Zn2—O5—H52	111 (5)
C3—C4—H4	119.7	H51—O5—H52	109 (3)
O1 <sup>iv</sup> —Zn1—O1—C7	-172.0 (4)	C7—C2—C3—C4	-169.1 (5)
O1 <sup>i</sup> —Zn1—O1—C7	96.2 (4)	N1—C2—C3—C8	-170.8 (5)
N1 <sup>iv</sup> —Zn1—O1—C7	-94.3 (4)	C7—C2—C3—C8	14.7 (9)
N1 <sup>i</sup> —Zn1—O1—C7	53.1 (8)	C2—C3—C4—C5	-3.3 (9)
N1—Zn1—O1—C7	-2.2 (4)	C8—C3—C4—C5	173.0 (5)
O1 <sup>iv</sup> —Zn1—N1—C6	-132.6 (6)	C3—C4—C5—C6	-1.3 (9)
O1—Zn1—N1—C6	-176.9 (5)	C2—N1—C6—C5	-2.6 (8)
O1 <sup>i</sup> —Zn1—N1—C6	93.2 (5)	Zn1—N1—C6—C5	-177.4 (4)
N1 <sup>iv</sup> —Zn1—N1—C6	-79.0 (4)	C4—C5—C6—N1	4.5 (9)
N1 <sup>i</sup> —Zn1—N1—C6	15.1 (5)	Zn1—O1—C7—O2	173.2 (4)
O1 <sup>iv</sup> —Zn1—N1—C2	52.4 (8)	Zn1—O1—C7—C2	-3.5 (6)
O1—Zn1—N1—C2	8.0 (4)	N1—C2—C7—O2	-166.2 (5)
O1 <sup>i</sup> —Zn1—N1—C2	-81.9 (4)	C3—C2—C7—O2	8.7 (8)
N1 <sup>iv</sup> —Zn1—N1—C2	105.9 (4)	N1—C2—C7—O1	10.8 (7)
N1 <sup>i</sup> —Zn1—N1—C2	-159.9 (4)	C3—C2—C7—O1	-174.3 (5)
C6—N1—C2—C3	-2.5 (8)	C4—C3—C8—O4	63.8 (8)
Zn1—N1—C2—C3	173.1 (4)	C2—C3—C8—O4	-120.1 (7)
C6—N1—C2—C7	172.4 (5)	C4—C3—C8—O3	-110.0 (6)
Zn1—N1—C2—C7	-12.0 (6)	C2—C3—C8—O3	66.1 (7)
N1—C2—C3—C4	5.4 (8)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 $\cdots$ O2 <sup>v</sup>	0.83 (5)	1.72 (2)	2.547 (5)	169 (7)
O5—H52 $\cdots$ O4	0.83 (5)	2.38 (4)	3.157 (7)	156 (7)
O5—H51 $\cdots$ O4 <sup>vi</sup>	0.82 (6)	2.02 (3)	2.795 (6)	158 (6)

Symmetry codes: (v)  $y, -x+y, -z$ ; (vi)  $-y, x-y, z$ .