Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[piperazinediium [aquabis(μ-pyridine-2,5-dicarboxylato)zincate] dihydrate]

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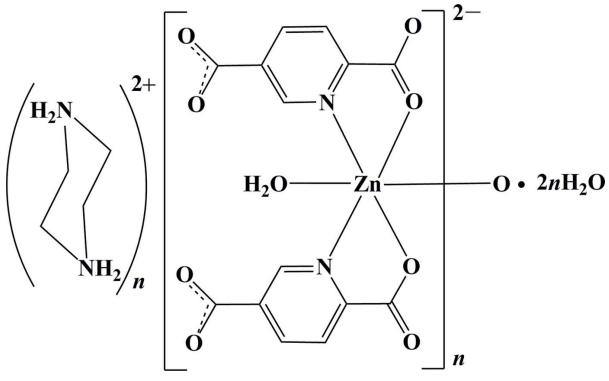
Received 21 November 2007; accepted 27 November 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.025; wR factor = 0.069; data-to-parameter ratio = 20.0.

The polymeric title compound, $\{(C_4H_{12}N_2)[Zn(C_7H_3NO_4)_2(H_2O)]\cdot 2H_2O\}_n$, was obtained by the reaction of zinc(II) nitrate hexahydrate with the proton-transfer compound $(pipzH_2)(py\text{-}2,5\text{-}dc)$ (where pipz is piperazine and py-2,5-dcH_2 is pyridine-2,5-dicarboxylic acid) in aqueous solution. Each Zn^{II} atom is coordinated in a distorted octahedral geometry by four O atoms and two N atoms from one water molecule and two $(py\text{-}2,5\text{-}dc)^{2-}$ ligands, which also act as bridging ligands between Zn^{II} atoms. π–π Stacking interactions between two aromatic rings of $(py\text{-}2,5\text{-}dc)^{2-}$ fragments, with centroid–centroid distances of 3.4747 (7) and 3.7081 (7) Å are observed. The crystal structure is stabilized by O—H···O and N—H···O hydrogen bonds.

Related literature

For related literature, see: Aghabozorg *et al.* (2007, 2007*a*,*b*); Sheshmani *et al.* (2007).



Experimental

Crystal data

$(C_4H_{12}N_2)[Zn(C_7H_3NO_4)_2(H_2O)]\cdot 2H_2O$
M_r = 537.78
Monoclinic, $P2_1/c$
a = 13.1752 (5) Å
b = 11.9066 (5) Å
c = 13.6902 (5) Å
β = 100.567 (1)°
V = 2111.19 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 100 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector' diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.756, T_{max} = 0.808
26339 measured reflections
6148 independent reflections
5458 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.069
S = 1.03
6148 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O3^{i}	0.82	1.93	2.730 (1)	167
O1W—H1WB···O2	0.82	1.86	2.678 (2)	173
O2W—H2WA···O1W	0.82	1.87	2.682 (1)	174
N3—H3B···O8^{ii}	0.92	1.82	2.741 (1)	177
N3—H3C···O1	0.92	2.46	2.912 (1)	111
N3—H3C···O5	0.92	1.94	2.818 (1)	158
O2W—H2WB···O5^{iii}	0.82	1.99	2.805 (1)	170
N4—H4A···O2W^{iv}	0.92	1.78	2.679 (2)	164
N4—H4B···O3^{v}	0.92	1.79	2.714 (1)	179
O9—H9A···O8^{vi}	0.82	1.86	2.678 (1)	173
O9—H9B···O4^{vi}	0.82	1.83	2.640 (1)	172

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2642).

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supporting information

Acta Cryst. (2008). E**64**, m111 [https://doi.org/10.1107/S1600536807063787]

Poly[piperazinediium [aquabis(*μ*-pyridine-2,5-dicarboxylato)zincate] dihydrate]

Hossein Aghabozorg, Zohreh Derikvand, Andya Nemati, Zohreh Bahrami and Jafar Attar Gharamaleki

S1. Comment

Our research group has recently focused on one-pot synthesis of water soluble self-assembly systems that can function as suitable ligands in the synthesis of metal complexes (Aghabozorg *et al.*, 2007, 2007*a*, 2007*b*).

The molecular structure of the title compound is shown in Fig. 1. The negative charge of the anionic complex is neutralized by dicationic piperazinediium species.

The Zn^{II} atom is hexacoordinated by two nitrogen atoms, two O atoms from carboxylate groups of two $(py\text{-}2,5\text{-}dc)^{2-}$ fragments, one O atom from a bridging $(py\text{-}2,5\text{-}dc)^{2-}$ ligand and one O atom from a coordinated water molecule. O7 and O9 atoms occupy the axial positions, while N1, N2, O1 and O5 atoms form the equatorial plane. The O9—Zn1—$O7^{i}$ (i: -*x* + 1, *y* - 1/2, -*z* + 1/2) bond angle revealed ~7.6° deviation from linearity. There are two uncoordinated water molecules and one piperazinediium ion as counter-ion, with some hydrogen bonds to water molecules and coordinated COO^{-} groups of $(py\text{-}2,5\text{-}dc)^{2-}$ fragments.

The $(py\text{-}2,5\text{-}dc)^{2-}$ fragments are bridging *via* carboxylate group, connecting the Zn^{II} atoms together into a layered structure in which the space between the $[Zn(H_2O)(py\text{-}2,5\text{-}dc)_2]^{2-}$ species is filled by piperazinediium ions and water molecules (Fig. 2).

The dihedral angle between the aromatic rings of $(py\text{-}2,5\text{-}dc)^{2-}$ groups connected to the same Zn atom is 6.82 (6)°, indicating that these fragments are almost coparallel.

π-*π* stacking interactions between two aromatic rings of $(py\text{-}2,5\text{-}dc)^{2-}$, with centroid-centroid distances of 3.4747 (7) Å (symmetry code: -*x*, 1/2 + *y*, 1/2 - *z*) and 3.7081 (7) Å (symmetry code: -*x*, -1 - *y*, -*z*) are observed in the title compound (Fig. 3).

S2. Experimental

The proton transfer compound was prepared by a reaction between piperazineand pyridine-2,5-dicarboxylicacid (Sheshmani, *et al.*, 2007). A solution of $Zn(NO_3)_2.6H_2O$ (130 mg, 0.5 mmol) in water (15 ml) was added to an aqueous solution of $(pipzH_2)(py\text{-}2,5\text{-}dc)$ (253 mg, 1.0 mmol) in water (15 ml) in a 1:2 molar ratio. Colorless crystals were obtained after a few days at room temperature.

S3. Refinement

The hydrogen atoms of NH_2 groups and water molecules were found in difference Fourier synthesis. Nevertheless, all hydrogen atoms were refined using a riding model with with the U_{iso}(H) parameters equal to 1.2 U_{eq}(C,*N*,*O*) and $C_{aromatic}$—H = 0.95 Å, $C_{methylene}$—H = 0.99 Å, O—H = 0.82Å and N—H = 0.92 Å.

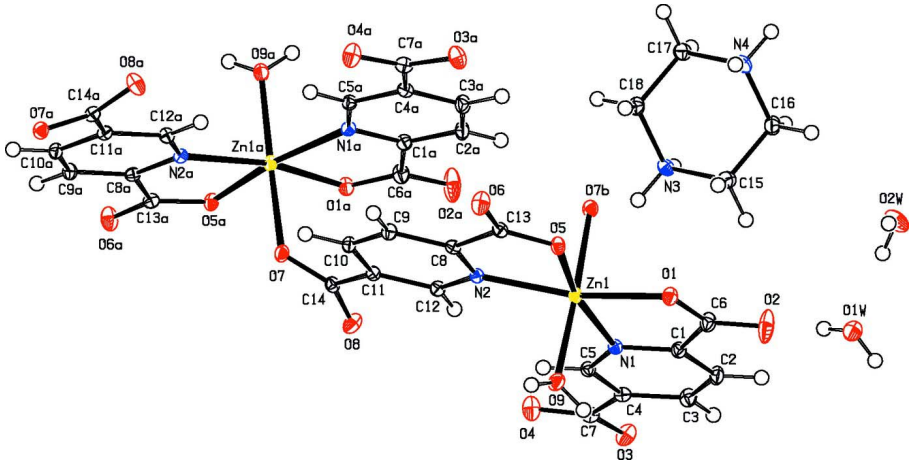

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.Atoms marked with *a* are related by the symmetry code: -*x* + 1, *y* - 1/2, -*z* + 1/2.

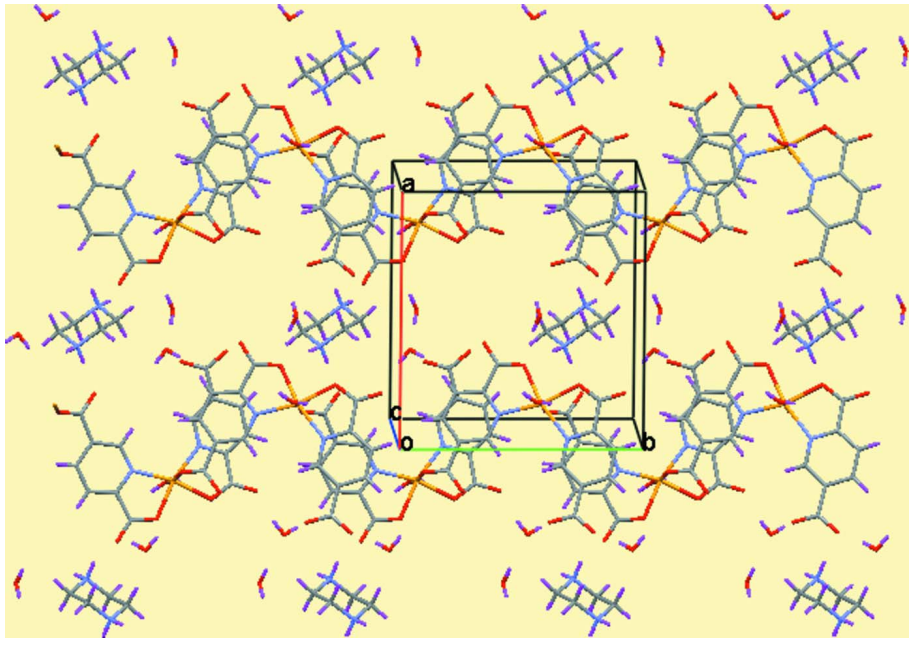

Figure 2

Packing diagram of the title compound, the space between $[Zn(H_2O)(py\text{-}2,5\text{-}dc)_2]^{2-}$ layers, is filled by piperazinediium ions and water molecules.

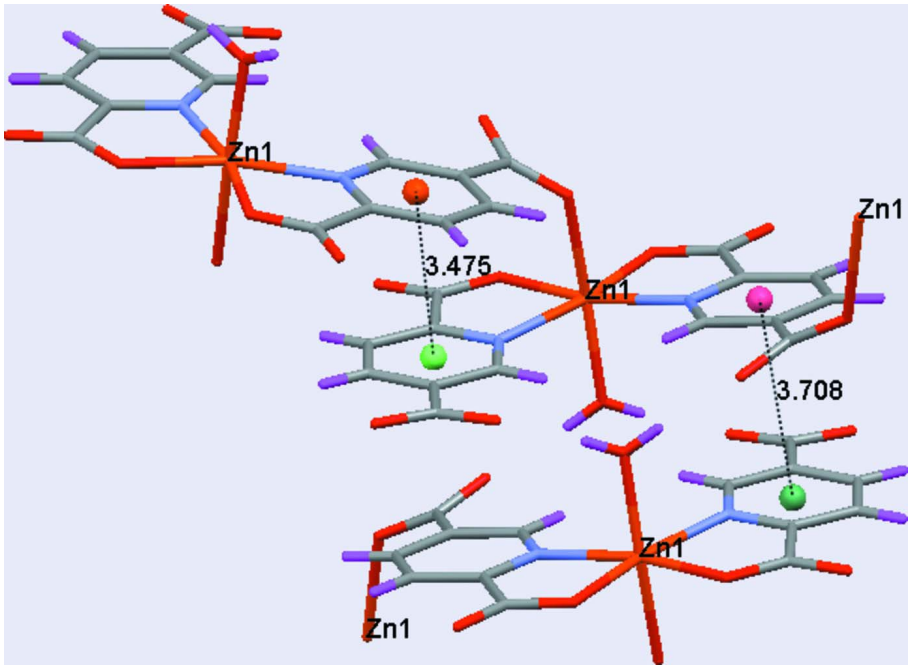

Figure 3

π-π Stacking interactions between aromatic rings of pyridine-2,5-dicarboxylate fragments with centroid-centroid distances of 3.4747 (7) Å (symmetry code: -*x*, 1/2 + *y*, 1/2 - *z*) and 3.7081 (7) Å (symmetry code: -*x*, -1 - *y*, -*z*).

Poly[piperazinediium [aquabis(*μ*-pyridine-2,5-dicarboxylato)zincate] dihydrate]

Crystal data

$(C_4H_{12}N_2)[Zn(C_7H_3NO_4)_2(H_2O)]\cdot 2H_2O$
$M_r = 537.78$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.1752\ (5)$ Å
$b = 11.9066\ (5)$ Å
$c = 13.6902\ (5)$ Å
$\beta = 100.567\ (1)°$
$V = 2111.19\ (14)$ Å^3
$Z = 4$
$F(000) = 1112$
$D_x = 1.692$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 583 reflections
$\theta = 3$–$30°$
$\mu = 1.24$ mm^{-1}
$T = 100$ K
Prism, colourless
0.24 × 0.20 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector′ diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.756$, $T_{max} = 0.808$
26339 measured reflections
6148 independent reflections
5458 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 30.0°$, $\theta_{min} = 1.6°$
$h = -18\rightarrow18$
$k = -16\rightarrow16$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.069$
$S = 1.03$
6148 reflections
307 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 1.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.83$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.157893 (10)	−0.413714 (11)	0.162746 (10)	0.00887 (5)
O1	0.22982 (7)	−0.25877 (8)	0.17492 (7)	0.01233 (17)
O2	0.20008 (9)	−0.07463 (9)	0.15203 (11)	0.0298 (3)
O3	−0.32052 (7)	−0.19745 (8)	0.00316 (8)	0.01648 (19)
O4	−0.28405 (7)	−0.37980 (8)	0.01990 (8)	0.01749 (19)
O5	0.30053 (7)	−0.48325 (7)	0.22242 (7)	0.01115 (17)
O6	0.38201 (7)	−0.64637 (8)	0.26384 (8)	0.0179 (2)
O7	−0.11016 (7)	−0.88980 (8)	0.19126 (7)	0.01188 (17)
O8	−0.17065 (7)	−0.73902 (8)	0.10247 (7)	0.01579 (19)
O9	0.18192 (7)	−0.43941 (8)	0.01814 (7)	0.01400 (18)
H9A	0.1826	−0.3867	−0.0203	0.017*
H9B	0.2171	−0.4917	0.0041	0.017*
N1	0.03069 (8)	−0.30642 (9)	0.10358 (8)	0.00939 (19)
N2	0.11783 (8)	−0.58497 (8)	0.17585 (8)	0.00904 (19)
C1	0.05938 (9)	−0.19776 (10)	0.10974 (9)	0.0110 (2)
C2	−0.01048 (10)	−0.11078 (11)	0.08528 (10)	0.0135 (2)
H2A	0.0123	−0.0349	0.0895	0.016*
C3	−0.11439 (10)	−0.13610 (11)	0.05445 (10)	0.0134 (2)
H3A	−0.1637	−0.0777	0.0380	0.016*
C4	−0.14516 (9)	−0.24797 (10)	0.04793 (9)	0.0103 (2)
C5	−0.06942 (9)	−0.33022 (10)	0.07249 (9)	0.0099 (2)
H5A	−0.0898	−0.4068	0.0669	0.012*
C6	0.17291 (10)	−0.17423 (11)	0.14852 (10)	0.0141 (2)
C7	−0.25825 (9)	−0.27880 (11)	0.02066 (9)	0.0116 (2)
C8	0.20087 (9)	−0.65035 (10)	0.20725 (9)	0.0093 (2)

C9	0.19325 (9)	−0.76566 (10)	0.21772 (9)	0.0109 (2)
H9C	0.2534	−0.8101	0.2377	0.013*
C10	0.09628 (9)	−0.81510 (10)	0.19858 (9)	0.0108 (2)
H10A	0.0892	−0.8938	0.2064	0.013*
C11	0.00939 (9)	−0.74839 (10)	0.16771 (9)	0.0094 (2)
C12	0.02468 (9)	−0.63331 (10)	0.15639 (9)	0.0100 (2)
H12A	−0.0338	−0.5873	0.1338	0.012*
C13	0.30435 (9)	−0.59080 (10)	0.23404 (9)	0.0104 (2)
C14	−0.09852 (9)	−0.79664 (10)	0.15208 (9)	0.0101 (2)
N3	0.35861 (8)	−0.31370 (9)	0.36536 (8)	0.0119 (2)
H3B	0.2960	−0.2863	0.3754	0.014*
H3C	0.3469	−0.3564	0.3084	0.014*
N4	0.49509 (8)	−0.22071 (9)	0.53234 (8)	0.0123 (2)
H4A	0.5059	−0.1777	0.5892	0.015*
H4B	0.5580	−0.2480	0.5233	0.015*
C15	0.42751 (10)	−0.21754 (11)	0.35168 (10)	0.0149 (2)
H15A	0.3933	−0.1696	0.2962	0.018*
H15B	0.4926	−0.2463	0.3347	0.018*
C16	0.45104 (10)	−0.14881 (11)	0.44632 (10)	0.0150 (2)
H16A	0.5008	−0.0886	0.4384	0.018*
H16B	0.3869	−0.1129	0.4588	0.018*
C17	0.42647 (10)	−0.31659 (11)	0.54554 (10)	0.0136 (2)
H17A	0.3609	−0.2879	0.5616	0.016*
H17B	0.4602	−0.3642	0.6014	0.016*
C18	0.40415 (10)	−0.38587 (11)	0.45105 (10)	0.0135 (2)
H18A	0.4689	−0.4202	0.4384	0.016*
H18B	0.3555	−0.4471	0.4589	0.016*
O1W	0.37141 (7)	0.04431 (8)	0.14623 (7)	0.01687 (19)
H1WA	0.3491	0.0939	0.1065	0.020*
H1WB	0.3222	0.0028	0.1486	0.020*
O2W	0.50510 (8)	0.07757 (9)	0.31667 (8)	0.0206 (2)
H2WA	0.4610	0.0668	0.2669	0.025*
H2WB	0.5594	0.0516	0.3052	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.00708 (7)	0.00737 (7)	0.01160 (7)	−0.00038 (5)	0.00023 (5)	−0.00018 (5)
O1	0.0093 (4)	0.0106 (4)	0.0159 (4)	−0.0009 (3)	−0.0006 (3)	0.0007 (3)
O2	0.0161 (5)	0.0113 (5)	0.0573 (8)	−0.0044 (4)	−0.0058 (5)	0.0039 (5)
O3	0.0096 (4)	0.0164 (5)	0.0234 (5)	0.0031 (3)	0.0029 (4)	0.0053 (4)
O4	0.0101 (4)	0.0143 (4)	0.0279 (5)	0.0001 (3)	0.0030 (4)	−0.0020 (4)
O5	0.0089 (4)	0.0092 (4)	0.0148 (4)	−0.0007 (3)	0.0008 (3)	−0.0009 (3)
O6	0.0098 (4)	0.0143 (4)	0.0277 (5)	0.0015 (3)	−0.0013 (4)	0.0024 (4)
O7	0.0132 (4)	0.0094 (4)	0.0134 (4)	−0.0020 (3)	0.0035 (3)	0.0006 (3)
O8	0.0097 (4)	0.0159 (5)	0.0209 (5)	−0.0020 (3)	0.0001 (3)	0.0068 (4)
O9	0.0179 (5)	0.0108 (4)	0.0140 (4)	0.0025 (3)	0.0045 (3)	0.0017 (3)
N1	0.0086 (4)	0.0095 (5)	0.0100 (5)	0.0000 (3)	0.0015 (4)	−0.0007 (4)

N2	0.0090 (5)	0.0088 (4)	0.0094 (4)	−0.0001 (3)	0.0019 (4)	−0.0004 (3)
C1	0.0103 (5)	0.0105 (5)	0.0118 (5)	−0.0009 (4)	0.0010 (4)	0.0002 (4)
C2	0.0144 (6)	0.0083 (5)	0.0169 (6)	0.0002 (4)	0.0005 (5)	0.0005 (4)
C3	0.0124 (5)	0.0114 (6)	0.0161 (6)	0.0030 (4)	0.0014 (4)	0.0003 (4)
C4	0.0091 (5)	0.0126 (5)	0.0095 (5)	0.0014 (4)	0.0022 (4)	0.0006 (4)
C5	0.0096 (5)	0.0097 (5)	0.0103 (5)	0.0000 (4)	0.0014 (4)	−0.0003 (4)
C6	0.0115 (5)	0.0118 (5)	0.0182 (6)	−0.0019 (4)	0.0002 (5)	0.0011 (5)
C7	0.0083 (5)	0.0156 (6)	0.0110 (5)	0.0009 (4)	0.0024 (4)	0.0002 (4)
C8	0.0082 (5)	0.0110 (5)	0.0087 (5)	0.0000 (4)	0.0020 (4)	−0.0009 (4)
C9	0.0097 (5)	0.0103 (5)	0.0126 (5)	0.0016 (4)	0.0021 (4)	0.0002 (4)
C10	0.0127 (5)	0.0082 (5)	0.0117 (5)	−0.0003 (4)	0.0025 (4)	−0.0001 (4)
C11	0.0093 (5)	0.0098 (5)	0.0093 (5)	−0.0011 (4)	0.0027 (4)	−0.0007 (4)
C12	0.0085 (5)	0.0105 (5)	0.0108 (5)	−0.0003 (4)	0.0014 (4)	0.0003 (4)
C13	0.0093 (5)	0.0116 (5)	0.0103 (5)	−0.0007 (4)	0.0019 (4)	−0.0011 (4)
C14	0.0099 (5)	0.0102 (5)	0.0107 (5)	−0.0019 (4)	0.0034 (4)	−0.0014 (4)
N3	0.0084 (4)	0.0138 (5)	0.0125 (5)	0.0001 (4)	−0.0004 (4)	−0.0021 (4)
N4	0.0085 (4)	0.0145 (5)	0.0134 (5)	−0.0015 (4)	0.0008 (4)	−0.0031 (4)
C15	0.0136 (6)	0.0173 (6)	0.0134 (6)	−0.0029 (5)	0.0013 (5)	0.0012 (5)
C16	0.0150 (6)	0.0116 (6)	0.0175 (6)	−0.0013 (4)	0.0007 (5)	0.0000 (5)
C17	0.0116 (5)	0.0161 (6)	0.0130 (6)	−0.0028 (4)	0.0019 (4)	0.0001 (5)
C18	0.0123 (5)	0.0111 (5)	0.0161 (6)	−0.0005 (4)	0.0001 (4)	0.0000 (4)
O1W	0.0133 (4)	0.0167 (5)	0.0195 (5)	−0.0004 (4)	0.0002 (4)	0.0024 (4)
O2W	0.0142 (5)	0.0265 (5)	0.0203 (5)	0.0045 (4)	0.0007 (4)	−0.0099 (4)

Geometric parameters (Å, º)

Zn1—O1	2.0668 (9)	C8—C13	1.5208 (17)
Zn1—O5	2.0788 (9)	C9—C10	1.3874 (17)
Zn1—O9	2.0840 (9)	C9—H9C	0.9500
Zn1—N2	2.1222 (10)	C10—C11	1.3938 (17)
Zn1—N1	2.1445 (10)	C10—H10A	0.9500
Zn1—O7^{i}	2.2209 (9)	C11—C12	1.3976 (16)
O1—C6	1.2675 (16)	C11—C14	1.5119 (16)
O2—C6	1.2372 (16)	C12—H12A	0.9500
O3—C7	1.2636 (15)	N3—C18	1.4888 (17)
O4—C7	1.2492 (16)	N3—C15	1.4941 (17)
O5—C13	1.2903 (15)	N3—H3B	0.9201
O6—C13	1.2239 (15)	N3—H3C	0.9200
O7—C14	1.2536 (15)	N4—C16	1.4852 (17)
O7—Zn1^{ii}	2.2209 (9)	N4—C17	1.4877 (16)
O8—C14	1.2643 (15)	N4—H4A	0.9200
O9—H9A	0.8200	N4—H4B	0.9199
O9—H9B	0.8199	C15—C16	1.5156 (18)
N1—C5	1.3399 (15)	C15—H15A	0.9900
N1—C1	1.3461 (16)	C15—H15B	0.9900
N2—C12	1.3374 (15)	C16—H16A	0.9900
N2—C8	1.3472 (15)	C16—H16B	0.9900
C1—C2	1.3852 (17)	C17—C18	1.5167 (18)

C1—C6	1.5187 (17)	C17—H17A	0.9900
C2—C3	1.3898 (18)	C17—H17B	0.9900
C2—H2A	0.9500	C18—H18A	0.9900
C3—C4	1.3904 (17)	C18—H18B	0.9900
C3—H3A	0.9500	O1W—H1WA	0.8200
C4—C5	1.3946 (16)	O1W—H1WB	0.8200
C4—C7	1.5133 (17)	O2W—H2WA	0.8200
C5—H5A	0.9500	O2W—H2WB	0.8199
C8—C9	1.3859 (17)		

O1—Zn1—O5	87.46 (3)	C9—C10—C11	119.48 (11)
O1—Zn1—O9	93.46 (4)	C9—C10—H10A	120.3
O5—Zn1—O9	91.78 (4)	C11—C10—H10A	120.3
O1—Zn1—N2	165.55 (4)	C10—C11—C12	117.73 (11)
O5—Zn1—N2	78.76 (4)	C10—C11—C14	121.67 (11)
O9—Zn1—N2	91.30 (4)	C12—C11—C14	120.52 (11)
O1—Zn1—N1	79.27 (4)	N2—C12—C11	123.05 (11)
O5—Zn1—N1	166.71 (4)	N2—C12—H12A	118.5
O9—Zn1—N1	88.45 (4)	C11—C12—H12A	118.5
N2—Zn1—N1	114.52 (4)	O6—C13—O5	126.08 (12)
O1—Zn1—O7^{i}	90.82 (4)	O6—C13—C8	119.08 (11)
O5—Zn1—O7^{i}	94.71 (3)	O5—C13—C8	114.84 (10)
O9—Zn1—O7^{i}	172.38 (4)	O7—C14—O8	124.83 (11)
N2—Zn1—O7^{i}	86.06 (4)	O7—C14—C11	117.47 (11)
N1—Zn1—O7^{i}	86.15 (4)	O8—C14—C11	117.67 (11)
C6—O1—Zn1	116.57 (8)	C18—N3—C15	112.01 (10)
C13—O5—Zn1	117.11 (8)	C18—N3—H3B	109.2
C14—O7—Zn1^{ii}	125.14 (8)	C15—N3—H3B	109.2
Zn1—O9—H9A	121.2	C18—N3—H3C	109.2
Zn1—O9—H9B	121.7	C15—N3—H3C	109.2
H9A—O9—H9B	111.0	H3B—N3—H3C	107.9
C5—N1—C1	118.15 (10)	C16—N4—C17	112.39 (10)
C5—N1—Zn1	130.51 (8)	C16—N4—H4A	109.1
C1—N1—Zn1	110.97 (8)	C17—N4—H4A	109.1
C12—N2—C8	118.47 (10)	C16—N4—H4B	109.1
C12—N2—Zn1	129.05 (8)	C17—N4—H4B	109.1
C8—N2—Zn1	112.47 (8)	H4A—N4—H4B	107.9
N1—C1—C2	122.48 (11)	N3—C15—C16	109.90 (10)
N1—C1—C6	116.52 (11)	N3—C15—H15A	109.7
C2—C1—C6	120.98 (11)	C16—C15—H15A	109.7
C1—C2—C3	119.02 (12)	N3—C15—H15B	109.7
C1—C2—H2A	120.5	C16—C15—H15B	109.7
C3—C2—H2A	120.5	H15A—C15—H15B	108.2
C2—C3—C4	119.13 (11)	N4—C16—C15	110.83 (11)
C2—C3—H3A	120.4	N4—C16—H16A	109.5
C4—C3—H3A	120.4	C15—C16—H16A	109.5
C3—C4—C5	118.03 (11)	N4—C16—H16B	109.5
C3—C4—C7	120.70 (11)	C15—C16—H16B	109.5

C5—C4—C7	121.19 (11)	H16A—C16—H16B	108.1
N1—C5—C4	123.18 (11)	N4—C17—C18	109.93 (10)
N1—C5—H5A	118.4	N4—C17—H17A	109.7
C4—C5—H5A	118.4	C18—C17—H17A	109.7
O2—C6—O1	126.75 (12)	N4—C17—H17B	109.7
O2—C6—C1	116.73 (12)	C18—C17—H17B	109.7
O1—C6—C1	116.51 (11)	H17A—C17—H17B	108.2
O4—C7—O3	124.76 (12)	N3—C18—C17	110.19 (10)
O4—C7—C4	119.32 (11)	N3—C18—H18A	109.6
O3—C7—C4	115.88 (11)	C17—C18—H18A	109.6
N2—C8—C9	122.37 (11)	N3—C18—H18B	109.6
N2—C8—C13	116.57 (10)	C17—C18—H18B	109.6
C9—C8—C13	121.04 (11)	H18A—C18—H18B	108.1
C8—C9—C10	118.85 (11)	H1WA—O1W—H1WB	105.7
C8—C9—H9C	120.6	H2WA—O2W—H2WB	107.0
C10—C9—H9C	120.6		

O5—Zn1—O1—C6	−178.14 (10)	C7—C4—C5—N1	−175.31 (11)
O9—Zn1—O1—C6	90.24 (10)	Zn1—O1—C6—O2	178.27 (13)
N2—Zn1—O1—C6	−160.74 (14)	Zn1—O1—C6—C1	−0.95 (15)
N1—Zn1—O1—C6	2.47 (9)	N1—C1—C6—O2	178.30 (13)
O7^{i}—Zn1—O1—C6	−83.46 (9)	C2—C1—C6—O2	−3.7 (2)
O1—Zn1—O5—C13	179.97 (9)	N1—C1—C6—O1	−2.41 (17)
O9—Zn1—O5—C13	−86.64 (9)	C2—C1—C6—O1	175.64 (12)
N2—Zn1—O5—C13	4.33 (9)	C3—C4—C7—O4	−176.67 (12)
N1—Zn1—O5—C13	−177.44 (14)	C5—C4—C7—O4	−0.21 (18)
O7^{i}—Zn1—O5—C13	89.35 (9)	C3—C4—C7—O3	1.13 (17)
O1—Zn1—N1—C5	−176.42 (11)	C5—C4—C7—O3	177.58 (11)
O5—Zn1—N1—C5	−179.05 (13)	C12—N2—C8—C9	1.56 (18)
O9—Zn1—N1—C5	89.77 (11)	Zn1—N2—C8—C9	−177.67 (9)
N2—Zn1—N1—C5	−0.96 (12)	C12—N2—C8—C13	−176.63 (11)
O7^{i}—Zn1—N1—C5	−84.85 (11)	Zn1—N2—C8—C13	4.14 (13)
O1—Zn1—N1—C1	−3.59 (8)	N2—C8—C9—C10	−2.33 (18)
O5—Zn1—N1—C1	−6.2 (2)	C13—C8—C9—C10	175.78 (11)
O9—Zn1—N1—C1	−97.41 (9)	C8—C9—C10—C11	1.14 (18)
N2—Zn1—N1—C1	171.87 (8)	C9—C10—C11—C12	0.67 (18)
O7^{i}—Zn1—N1—C1	87.97 (8)	C9—C10—C11—C14	−176.08 (11)
O1—Zn1—N2—C12	158.72 (13)	C8—N2—C12—C11	0.41 (18)
O5—Zn1—N2—C12	176.45 (11)	Zn1—N2—C12—C11	179.49 (9)
O9—Zn1—N2—C12	−92.00 (11)	C10—C11—C12—N2	−1.51 (18)
N1—Zn1—N2—C12	−3.11 (12)	C14—C11—C12—N2	175.29 (11)
O7^{i}—Zn1—N2—C12	80.84 (11)	Zn1—O5—C13—O6	176.62 (11)
O1—Zn1—N2—C8	−22.2 (2)	Zn1—O5—C13—C8	−3.37 (13)
O5—Zn1—N2—C8	−4.43 (8)	N2—C8—C13—O6	179.33 (12)
O9—Zn1—N2—C8	87.12 (8)	C9—C8—C13—O6	1.12 (18)
N1—Zn1—N2—C8	176.02 (8)	N2—C8—C13—O5	−0.67 (16)
O7^{i}—Zn1—N2—C8	−100.03 (8)	C9—C8—C13—O5	−178.89 (11)
C5—N1—C1—C2	0.03 (18)	Zn1^{ii}—O7—C14—O8	−82.76 (15)

Zn1—N1—C1—C2	−173.79 (10)	Zn1^{ii}—O7—C14—C11	95.54 (12)
C5—N1—C1—C6	178.04 (11)	C10—C11—C14—O7	18.00 (17)
Zn1—N1—C1—C6	4.23 (13)	C12—C11—C14—O7	−158.66 (11)
N1—C1—C2—C3	0.9 (2)	C10—C11—C14—O8	−163.58 (12)
C6—C1—C2—C3	−177.05 (12)	C12—C11—C14—O8	19.76 (17)
C1—C2—C3—C4	−0.72 (19)	C18—N3—C15—C16	−56.65 (14)
C2—C3—C4—C5	−0.27 (18)	C17—N4—C16—C15	−56.30 (14)
C2—C3—C4—C7	176.29 (12)	N3—C15—C16—N4	55.00 (14)
C1—N1—C5—C4	−1.11 (18)	C16—N4—C17—C18	56.56 (14)
Zn1—N1—C5—C4	171.29 (9)	C15—N3—C18—C17	57.58 (13)
C3—C4—C5—N1	1.24 (18)	N4—C17—C18—N3	−56.24 (13)

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) −*x*, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O3^{iii}	0.82	1.93	2.730 (1)	167
O1*W*—H1*WB*···O2	0.82	1.86	2.678 (2)	173
O2*W*—H2*WA*···O1*W*	0.82	1.87	2.682 (1)	174
N3—H3*B*···O8^{i}	0.92	1.82	2.741 (1)	177
N3—H3*C*···O1	0.92	2.46	2.912 (1)	111
N3—H3*C*···O5	0.92	1.94	2.818 (1)	158
O2*W*—H2*WB*···O5^{iv}	0.82	1.99	2.805 (1)	170
N4—H4*A*···O2*W*^{v}	0.92	1.78	2.679 (2)	164
N4—H4*B*···O3^{vi}	0.92	1.79	2.714 (1)	179
O9—H9*A*···O8^{vii}	0.82	1.86	2.678 (1)	173
O9—H9*B*···O4^{vii}	0.82	1.83	2.640 (1)	172

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