

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Aquabis(5-butylpyridine-2-carboxylato)-zinc monohydrate

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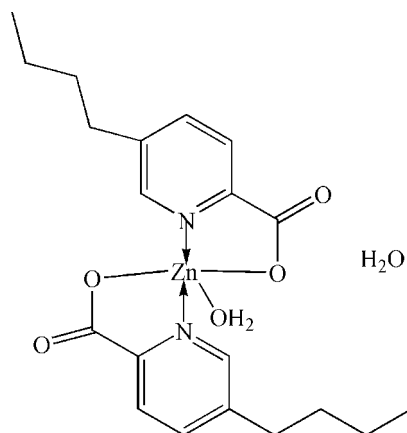
Received 26 May 2011; accepted 5 June 2011

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.027; wR factor = 0.075; data-to-parameter ratio = 14.6.

In the title complex, $[\text{Zn}(\text{C}_{10}\text{H}_{12}\text{NO}_2)_2(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$, the Zn^{II} ion is coordinated by two N and two O atoms from two 5-*n*-butylpyridine-2-carboxylato ligands and one O atom from a water molecule in a distorted square-pyramidal geometry. In the crystal, intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds link molecules into a two-dimensional supramolecular structure parallel to (001).

Related literature

For related structures, see: Pons *et al.* (2004); Yoshikawa *et al.* (2002); Qin *et al.* (2007); He *et al.* (2007).



Experimental

Crystal data

$[\text{Zn}(\text{C}_{10}\text{H}_{12}\text{NO}_2)_2(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$
 $M_r = 457.81$
 Triclinic, $P\bar{1}$
 $a = 9.6949$ (13) Å
 $b = 10.0054$ (14) Å
 $c = 11.9249$ (17) Å
 $\alpha = 97.799$ (2)°
 $\beta = 91.533$ (2)°
 $\gamma = 113.464$ (2)°
 $V = 1047.1$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.21$ mm⁻¹
 $T = 293$ K
 $0.48 \times 0.42 \times 0.15$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2008a)
 $T_{\min} = 0.594$, $T_{\max} = 0.839$
 7770 measured reflections
 3847 independent reflections
 3410 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.075$
 $S = 1.06$
 3847 reflections
 264 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.47$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O2W}-\text{H2B} \cdots \text{O4}$	0.85	1.94	2.780 (2)	172
$\text{O2W}-\text{H2A} \cdots \text{O4}^{\text{i}}$	0.85	2.02	2.849 (2)	165
$\text{O1W}-\text{H1B} \cdots \text{O2W}^{\text{ii}}$	0.84	1.80	2.638 (2)	175
$\text{O1W}-\text{H1A} \cdots \text{O2}^{\text{iii}}$	0.85	1.79	2.636 (2)	174

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008b); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008b); molecular graphics: SHELXTL (Sheldrick, 2008b); software used to prepare material for publication: SHELXTL.

This work was supported by the Guangzhou Science and Technology Projects Fund (2010Y1-C371), the Guangzhou Municipal Bureau of Education Projects Fund (10 A168) and the doctoral startup fund of Guangzhou Medical College (2008 C25).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5046).

References

- Bruker (2001). SAINT-Plus. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2004). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
 He, L., Yan, J.-B., Guo, X.-X. & Song, W.-D. (2007). *Acta Cryst.* **E63**, m1649.
 Pons, J., March, R., Rius, J. & Ros, J. (2004). *Inorg. Chim. Acta*, **357**, 3789–3792.
 Qin, L., Guo, H.-F., Li, X., Ma, D.-Y. & Song, W.-D. (2007). *Acta Cryst.* **E63**, m2853.
 Sheldrick, G. M. (2008a). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008b). *Acta Cryst.* **A64**, 112–122.
 Yoshikawa, Y., Ueda, E., Kawabe, K., Miyake, H., Takino, T., Sakurai, H. & Kojima, Y. (2002). *J. Biol. Inorg. Chem.* **7**, 68–73.

supporting information

Acta Cryst. (2011). E67, m908 [doi:10.1107/S1600536811021623]

Aquabis(5-butylpyridine-2-carboxylato)zinc monohydrate**Yi-Wen Tao and Yun Wang****S1. Comment**

As known for a long time, pyridine-2-carboxylato ion and its derivatives are good chelating ligands for many transition metals (Pons, *et al.*, 2004; Yoshikawa, *et al.*, 2002; Qin *et al.*, 2007; He *et al.*, 2007). Here, we report a new zinc complex based on 5-n-butylpyridine-2-carboxylate.

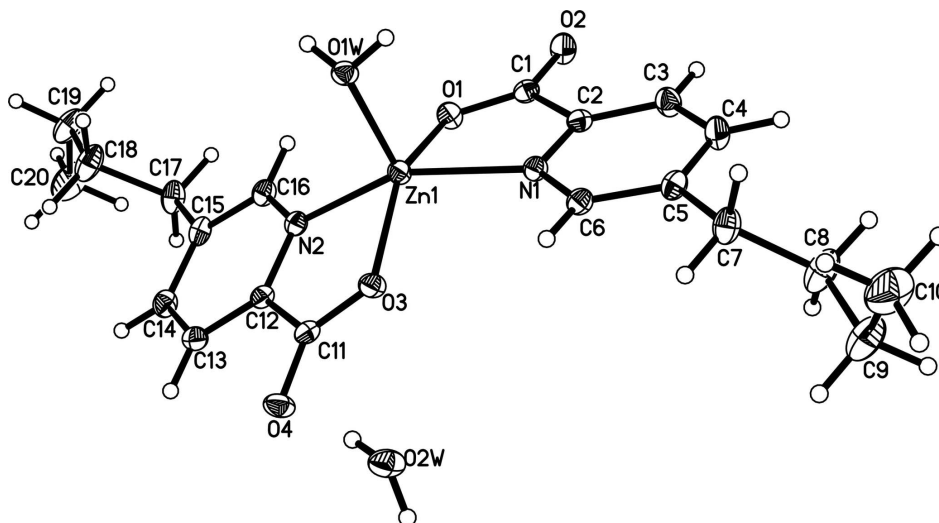
The crystal structure of the title compound, (I), is shown in Fig. 1. The coordination sphere of the Zn^{II} ion should be described as a distorted square-pyramidal, in which the four basal positions are occupied by two N atoms and two O atoms from two 5-n-butylpyridine-2-carboxylato ligands, and the fifth apical site is occupied by the O atom of the coordinated solvent water molecule. The Zn(II) ion is out of the plane formed by N₂O₂ unit 0.504 (8) Å towards the Zn—O_{water} bond. The average Zn—N, Zn—O_{ligand}, and the Zn—O_{water} are 2.094, 2.043, and 2.044 Å, respectively, in agreement with the corresponding distances found in other Zn complexes containing similar ligands (Qin *et al.*, 2007; He *et al.*, 2007). It was noting that the title complex was linked into a two-dimensional supermolecular structure under the help of the intermolecular O—H...O hydrogen bonds interactions.

S2. Experimental

The title complex was prepared by the addition of a stoichiometric amount to zinc acetate dehydrate (0.054 mmol) to a hot aqueous solution (5 ml) of fusaric acid (30 mmol) which was extracted from the endophytic fungus *phomopsis sp.* from the mangrove tree on the South China Sea coast. The resulting solution was filtered, and colorless crystals were obtained by slow evaporation of a methanol-water solution (90:10 v/v) at room temperature over several days.

S3. Refinement

All the H atoms bonded to the C atoms were placed using the HFIX commands in *SHELXL-97*, with C—H distances of 0.95, 0.98 and 0.99 Å, and were allowed for as riding atoms with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$. For the H atom of the water molecule, they were found from difference Fourier maps with the O—H bond length restrained to 0.85 Å.

**Figure 1**

The molecular structure of the title complex with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Aquabis(5-butylpyridine-2-carboxylato)zinc monohydrate

Crystal data

$[\text{Zn}(\text{C}_{20}\text{H}_{12}\text{NO}_2)_2(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$

$M_r = 457.81$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.6949\ (13)\ \text{\AA}$

$b = 10.0054\ (14)\ \text{\AA}$

$c = 11.9249\ (17)\ \text{\AA}$

$\alpha = 97.799\ (2)^\circ$

$\beta = 91.533\ (2)^\circ$

$\gamma = 113.464\ (2)^\circ$

$V = 1047.1\ (3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 480$

$D_x = 1.452\ \text{Mg m}^{-3}$

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

Cell parameters from 5809 reflections

$\theta = 2.3\text{--}27.0^\circ$

$\mu = 1.21\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, colorless

$0.48 \times 0.42 \times 0.15\ \text{mm}$

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 2008a)

$T_{\min} = 0.594$, $T_{\max} = 0.839$

7770 measured reflections

3847 independent reflections

3410 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 1.7^\circ$

$h = -11 \rightarrow 11$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.075$

$S = 1.06$

3847 reflections

264 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.5567P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.008$
 $\Delta\rho_{\max} = 0.47 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.9784 (2)	0.0833 (2)	0.17910 (17)	0.0249 (4)
C2	1.0361 (2)	0.2469 (2)	0.22551 (17)	0.0239 (4)
C3	1.1290 (3)	0.3107 (2)	0.32451 (18)	0.0311 (5)
H3	1.1603	0.2528	0.3674	0.037*
C4	1.1761 (3)	0.4611 (2)	0.36059 (19)	0.0341 (5)
H4	1.2413	0.5071	0.4282	0.041*
C5	1.1283 (2)	0.5447 (2)	0.29835 (17)	0.0275 (4)
C6	1.0337 (2)	0.4707 (2)	0.19940 (17)	0.0250 (4)
H6	0.9991	0.5254	0.1555	0.030*
C7	1.1750 (3)	0.7081 (2)	0.33348 (18)	0.0336 (5)
H7A	1.1100	0.7396	0.2878	0.040*
H7B	1.2801	0.7601	0.3147	0.040*
C8	1.1666 (4)	0.7566 (3)	0.4578 (2)	0.0496 (7)
H8A	1.2515	0.7516	0.5025	0.059*
H8B	1.0716	0.6866	0.4823	0.059*
C9	1.1725 (4)	0.9123 (3)	0.4849 (2)	0.0544 (7)
H9A	1.0839	0.9153	0.4439	0.065*
H9B	1.1639	0.9341	0.5673	0.065*
C10	1.3102 (4)	1.0292 (3)	0.4550 (3)	0.0681 (9)
H10A	1.3987	1.0303	0.4976	0.102*
H10B	1.3044	1.1251	0.4743	0.102*
H10C	1.3193	1.0100	0.3734	0.102*
C11	0.6412 (2)	0.2796 (2)	-0.07353 (16)	0.0238 (4)
C12	0.5820 (2)	0.1149 (2)	-0.11734 (16)	0.0225 (4)
C13	0.4469 (2)	0.0367 (2)	-0.18239 (18)	0.0285 (5)
H13	0.3866	0.0852	-0.2049	0.034*
C14	0.4004 (2)	-0.1145 (2)	-0.21448 (18)	0.0303 (5)
H14	0.3074	-0.1704	-0.2593	0.036*
C15	0.4900 (3)	-0.1841 (2)	-0.18108 (17)	0.0281 (5)
C16	0.6254 (2)	-0.0962 (2)	-0.11735 (17)	0.0264 (4)
H16	0.6890	-0.1414	-0.0949	0.032*
C17	0.4419 (3)	-0.3486 (2)	-0.21017 (18)	0.0348 (5)

H17A	0.5116	-0.3770	-0.1667	0.042*
H17B	0.3397	-0.3986	-0.1853	0.042*
C18	0.4389 (4)	-0.4036 (3)	-0.3335 (2)	0.0471 (7)
H18A	0.5387	-0.3483	-0.3602	0.057*
H18B	0.3629	-0.3829	-0.3767	0.057*
C19	0.4019 (3)	-0.5685 (3)	-0.3597 (2)	0.0483 (7)
H19A	0.4110	-0.5946	-0.4414	0.058*
H19B	0.4777	-0.5890	-0.3161	0.058*
C20	0.2495 (4)	-0.6646 (3)	-0.3326 (3)	0.0684 (10)
H20A	0.2403	-0.6422	-0.2512	0.103*
H20B	0.2340	-0.7682	-0.3520	0.103*
H20C	0.1733	-0.6469	-0.3765	0.103*
N1	0.98977 (19)	0.32660 (18)	0.16371 (14)	0.0230 (4)
N2	0.67075 (19)	0.04994 (18)	-0.08590 (13)	0.0228 (3)
O1	0.88860 (16)	0.03799 (15)	0.09036 (12)	0.0277 (3)
O2	1.02181 (19)	0.00693 (17)	0.23255 (13)	0.0351 (4)
O3	0.76689 (16)	0.33710 (15)	-0.01438 (12)	0.0262 (3)
O4	0.56258 (16)	0.34586 (16)	-0.09763 (13)	0.0319 (3)
O1W	1.02425 (16)	0.24272 (15)	-0.09978 (12)	0.0253 (3)
H1A	1.0153	0.1655	-0.1447	0.038*
H1B	1.1118	0.2841	-0.0657	0.038*
O2W	0.69815 (17)	0.64141 (17)	0.00070 (14)	0.0364 (4)
H2A	0.6306	0.6516	0.0409	0.055*
H2B	0.6653	0.5519	-0.0315	0.055*
Zn1	0.86873 (3)	0.19830 (2)	0.010473 (19)	0.02289 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0274 (11)	0.0232 (10)	0.0270 (10)	0.0130 (9)	0.0052 (9)	0.0040 (8)
C2	0.0226 (10)	0.0245 (10)	0.0262 (10)	0.0113 (9)	0.0042 (8)	0.0036 (8)
C3	0.0358 (12)	0.0285 (11)	0.0303 (11)	0.0154 (10)	-0.0039 (9)	0.0032 (9)
C4	0.0394 (13)	0.0308 (12)	0.0278 (11)	0.0121 (10)	-0.0068 (10)	-0.0004 (9)
C5	0.0316 (11)	0.0231 (10)	0.0253 (10)	0.0090 (9)	0.0039 (9)	0.0015 (8)
C6	0.0281 (11)	0.0225 (10)	0.0252 (10)	0.0110 (9)	0.0035 (8)	0.0035 (8)
C7	0.0424 (13)	0.0221 (11)	0.0295 (11)	0.0072 (10)	-0.0006 (10)	0.0013 (9)
C8	0.085 (2)	0.0331 (13)	0.0338 (13)	0.0273 (14)	0.0130 (13)	0.0042 (10)
C9	0.085 (2)	0.0381 (15)	0.0421 (15)	0.0281 (15)	0.0152 (14)	0.0021 (11)
C10	0.073 (2)	0.0339 (15)	0.089 (2)	0.0174 (15)	0.0115 (18)	-0.0066 (15)
C11	0.0247 (10)	0.0241 (10)	0.0238 (10)	0.0115 (9)	0.0061 (8)	0.0019 (8)
C12	0.0224 (10)	0.0227 (10)	0.0220 (10)	0.0088 (8)	0.0053 (8)	0.0025 (8)
C13	0.0252 (11)	0.0319 (12)	0.0285 (11)	0.0128 (9)	0.0025 (9)	0.0013 (9)
C14	0.0246 (11)	0.0301 (11)	0.0272 (11)	0.0037 (9)	0.0008 (9)	-0.0017 (9)
C15	0.0349 (12)	0.0232 (10)	0.0208 (10)	0.0065 (9)	0.0046 (9)	0.0014 (8)
C16	0.0320 (11)	0.0230 (10)	0.0236 (10)	0.0105 (9)	0.0039 (9)	0.0039 (8)
C17	0.0450 (14)	0.0218 (11)	0.0283 (11)	0.0055 (10)	-0.0014 (10)	0.0005 (9)
C18	0.077 (2)	0.0301 (13)	0.0324 (13)	0.0203 (13)	0.0135 (12)	0.0027 (10)
C19	0.0670 (18)	0.0298 (13)	0.0418 (14)	0.0143 (13)	0.0186 (13)	-0.0012 (10)

C20	0.068 (2)	0.0414 (16)	0.069 (2)	0.0008 (15)	0.0174 (17)	-0.0152 (14)
N1	0.0237 (9)	0.0204 (8)	0.0241 (8)	0.0085 (7)	0.0012 (7)	0.0018 (7)
N2	0.0255 (9)	0.0207 (8)	0.0210 (8)	0.0085 (7)	0.0021 (7)	0.0018 (6)
O1	0.0304 (8)	0.0211 (7)	0.0310 (8)	0.0107 (6)	-0.0030 (6)	0.0020 (6)
O2	0.0506 (10)	0.0279 (8)	0.0316 (8)	0.0223 (8)	-0.0051 (7)	0.0020 (6)
O3	0.0234 (7)	0.0208 (7)	0.0327 (8)	0.0098 (6)	-0.0020 (6)	-0.0023 (6)
O4	0.0277 (8)	0.0270 (8)	0.0431 (9)	0.0161 (7)	-0.0029 (7)	-0.0016 (7)
O1W	0.0243 (7)	0.0229 (7)	0.0296 (7)	0.0116 (6)	0.0011 (6)	0.0012 (6)
O2W	0.0281 (8)	0.0241 (8)	0.0546 (10)	0.0112 (7)	-0.0004 (7)	-0.0025 (7)
Zn1	0.02298 (14)	0.01954 (13)	0.02499 (14)	0.00872 (10)	-0.00164 (9)	0.00013 (9)

Geometric parameters (Å, °)

C1—O2	1.241 (2)	C13—C14	1.389 (3)
C1—O1	1.261 (3)	C13—H13	0.9500
C1—C2	1.519 (3)	C14—C15	1.391 (3)
C2—N1	1.345 (3)	C14—H14	0.9500
C2—C3	1.376 (3)	C15—C16	1.386 (3)
C3—C4	1.388 (3)	C15—C17	1.508 (3)
C3—H3	0.9500	C16—N2	1.342 (3)
C4—C5	1.387 (3)	C16—H16	0.9500
C4—H4	0.9500	C17—C18	1.494 (3)
C5—C6	1.395 (3)	C17—H17A	0.9900
C5—C7	1.506 (3)	C17—H17B	0.9900
C6—N1	1.332 (3)	C18—C19	1.528 (3)
C6—H6	0.9500	C18—H18A	0.9900
C7—C8	1.511 (3)	C18—H18B	0.9900
C7—H7A	0.9900	C19—C20	1.480 (4)
C7—H7B	0.9900	C19—H19A	0.9900
C8—C9	1.525 (3)	C19—H19B	0.9900
C8—H8A	0.9900	C20—H20A	0.9800
C8—H8B	0.9900	C20—H20B	0.9800
C9—C10	1.474 (4)	C20—H20C	0.9800
C9—H9A	0.9900	N1—Zn1	2.1007 (16)
C9—H9B	0.9900	N2—Zn1	2.0877 (17)
C10—H10A	0.9800	O1—Zn1	2.0416 (14)
C10—H10B	0.9800	O3—Zn1	2.0443 (14)
C10—H10C	0.9800	O1W—Zn1	1.9825 (14)
C11—O4	1.243 (2)	O1W—H1A	0.8498
C11—O3	1.264 (2)	O1W—H1B	0.8440
C11—C12	1.521 (3)	O2W—H2A	0.8514
C12—N2	1.341 (3)	O2W—H2B	0.8510
C12—C13	1.377 (3)		
O2—C1—O1	126.36 (19)	C15—C14—H14	120.0
O2—C1—C2	117.37 (18)	C16—C15—C14	117.25 (19)
O1—C1—C2	116.27 (17)	C16—C15—C17	120.7 (2)
N1—C2—C3	121.57 (19)	C14—C15—C17	122.0 (2)

N1—C2—C1	115.64 (17)	N2—C16—C15	122.97 (19)
C3—C2—C1	122.79 (18)	N2—C16—H16	118.5
C2—C3—C4	118.9 (2)	C15—C16—H16	118.5
C2—C3—H3	120.6	C18—C17—C15	114.50 (19)
C4—C3—H3	120.6	C18—C17—H17A	108.6
C5—C4—C3	120.3 (2)	C15—C17—H17A	108.6
C5—C4—H4	119.9	C18—C17—H17B	108.6
C3—C4—H4	119.9	C15—C17—H17B	108.6
C4—C5—C6	116.93 (19)	H17A—C17—H17B	107.6
C4—C5—C7	122.71 (19)	C17—C18—C19	113.5 (2)
C6—C5—C7	120.36 (19)	C17—C18—H18A	108.9
N1—C6—C5	122.96 (19)	C19—C18—H18A	108.9
N1—C6—H6	118.5	C17—C18—H18B	108.9
C5—C6—H6	118.5	C19—C18—H18B	108.9
C5—C7—C8	115.23 (19)	H18A—C18—H18B	107.7
C5—C7—H7A	108.5	C20—C19—C18	114.3 (2)
C8—C7—H7A	108.5	C20—C19—H19A	108.7
C5—C7—H7B	108.5	C18—C19—H19A	108.7
C8—C7—H7B	108.5	C20—C19—H19B	108.7
H7A—C7—H7B	107.5	C18—C19—H19B	108.7
C7—C8—C9	113.9 (2)	H19A—C19—H19B	107.6
C7—C8—H8A	108.8	C19—C20—H20A	109.5
C9—C8—H8A	108.8	C19—C20—H20B	109.5
C7—C8—H8B	108.8	H20A—C20—H20B	109.5
C9—C8—H8B	108.8	C19—C20—H20C	109.5
H8A—C8—H8B	107.7	H20A—C20—H20C	109.5
C10—C9—C8	114.8 (3)	H20B—C20—H20C	109.5
C10—C9—H9A	108.6	C6—N1—C2	119.38 (17)
C8—C9—H9A	108.6	C6—N1—Zn1	129.26 (14)
C10—C9—H9B	108.6	C2—N1—Zn1	111.10 (13)
C8—C9—H9B	108.6	C12—N2—C16	119.00 (17)
H9A—C9—H9B	107.6	C12—N2—Zn1	112.83 (13)
C9—C10—H10A	109.5	C16—N2—Zn1	128.17 (14)
C9—C10—H10B	109.5	C1—O1—Zn1	115.66 (13)
H10A—C10—H10B	109.5	C11—O3—Zn1	116.22 (12)
C9—C10—H10C	109.5	Zn1—O1W—H1A	111.6
H10A—C10—H10C	109.5	Zn1—O1W—H1B	110.8
H10B—C10—H10C	109.5	H1A—O1W—H1B	110.4
O4—C11—O3	125.56 (18)	H2A—O2W—H2B	108.2
O4—C11—C12	117.92 (17)	O1W—Zn1—O1	106.09 (6)
O3—C11—C12	116.52 (17)	O1W—Zn1—O3	102.80 (6)
N2—C12—C13	122.02 (18)	O1—Zn1—O3	151.11 (6)
N2—C12—C11	114.71 (17)	O1W—Zn1—N2	104.39 (6)
C13—C12—C11	123.26 (18)	O1—Zn1—N2	92.68 (6)
C12—C13—C14	118.69 (19)	O3—Zn1—N2	79.70 (6)
C12—C13—H13	120.7	O1W—Zn1—N1	103.25 (6)
C14—C13—H13	120.7	O1—Zn1—N1	79.91 (6)
C13—C14—C15	120.04 (19)	O3—Zn1—N1	93.96 (6)

C13—C14—H14	120.0	N2—Zn1—N1	152.36 (6)
O2—C1—C2—N1	178.32 (18)	C1—C2—N1—Zn1	-6.2 (2)
O1—C1—C2—N1	-2.8 (3)	C13—C12—N2—C16	-1.0 (3)
O2—C1—C2—C3	-2.0 (3)	C11—C12—N2—C16	177.81 (17)
O1—C1—C2—C3	176.9 (2)	C13—C12—N2—Zn1	179.31 (15)
N1—C2—C3—C4	-0.3 (3)	C11—C12—N2—Zn1	-1.9 (2)
C1—C2—C3—C4	-179.9 (2)	C15—C16—N2—C12	-0.2 (3)
C2—C3—C4—C5	0.8 (3)	C15—C16—N2—Zn1	179.46 (15)
C3—C4—C5—C6	-0.5 (3)	O2—C1—O1—Zn1	-170.40 (17)
C3—C4—C5—C7	179.7 (2)	C2—C1—O1—Zn1	10.8 (2)
C4—C5—C6—N1	-0.3 (3)	O4—C11—O3—Zn1	179.89 (16)
C7—C5—C6—N1	179.44 (19)	C12—C11—O3—Zn1	0.5 (2)
C4—C5—C7—C8	-45.1 (3)	C1—O1—Zn1—O1W	89.95 (15)
C6—C5—C7—C8	135.1 (2)	C1—O1—Zn1—O3	-90.86 (18)
C5—C7—C8—C9	-164.3 (2)	C1—O1—Zn1—N2	-164.24 (14)
C7—C8—C9—C10	-59.7 (4)	C1—O1—Zn1—N1	-11.06 (14)
O4—C11—C12—N2	-178.46 (18)	C11—O3—Zn1—O1W	101.39 (14)
O3—C11—C12—N2	0.9 (3)	C11—O3—Zn1—O1	-77.81 (18)
O4—C11—C12—C13	0.4 (3)	C11—O3—Zn1—N2	-1.18 (14)
O3—C11—C12—C13	179.76 (19)	C11—O3—Zn1—N1	-154.05 (14)
N2—C12—C13—C14	1.1 (3)	C12—N2—Zn1—O1W	-99.05 (13)
C11—C12—C13—C14	-177.59 (18)	C16—N2—Zn1—O1W	81.32 (17)
C12—C13—C14—C15	-0.1 (3)	C12—N2—Zn1—O1	153.59 (13)
C13—C14—C15—C16	-1.0 (3)	C16—N2—Zn1—O1	-26.04 (17)
C13—C14—C15—C17	177.75 (19)	C12—N2—Zn1—O3	1.66 (13)
C14—C15—C16—N2	1.1 (3)	C16—N2—Zn1—O3	-177.97 (17)
C17—C15—C16—N2	-177.61 (19)	C12—N2—Zn1—N1	80.37 (19)
C16—C15—C17—C18	-112.4 (3)	C16—N2—Zn1—N1	-99.3 (2)
C14—C15—C17—C18	68.9 (3)	C6—N1—Zn1—O1W	78.55 (18)
C15—C17—C18—C19	175.5 (2)	C2—N1—Zn1—O1W	-95.41 (14)
C17—C18—C19—C20	63.4 (4)	C6—N1—Zn1—O1	-177.13 (18)
C5—C6—N1—C2	0.9 (3)	C2—N1—Zn1—O1	8.90 (13)
C5—C6—N1—Zn1	-172.66 (15)	C6—N1—Zn1—O3	-25.60 (18)
C3—C2—N1—C6	-0.6 (3)	C2—N1—Zn1—O3	160.44 (13)
C1—C2—N1—C6	179.13 (17)	C6—N1—Zn1—N2	-100.9 (2)
C3—C2—N1—Zn1	174.08 (16)	C2—N1—Zn1—N2	85.17 (19)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2 <i>W</i> —H2 <i>B</i> ...O4	0.85	1.94	2.780 (2)	172
O2 <i>W</i> —H2 <i>A</i> ...O4 ⁱ	0.85	2.02	2.849 (2)	165
O1 <i>W</i> —H1 <i>B</i> ...O2 <i>W</i> ⁱⁱ	0.84	1.80	2.638 (2)	175
O1 <i>W</i> —H1 <i>A</i> ...O2 ⁱⁱⁱ	0.85	1.79	2.636 (2)	174

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