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Aquabis(3′-hydroxy-2,2′-bipyridine-3-olato-κ^2N,N')zinc(II)

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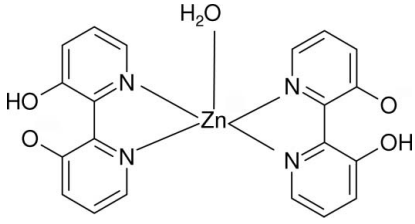
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.030; wR factor = 0.083; data-to-parameter ratio = 11.8.

In the title complex, $[Zn(C_{10}H_7N_2O_2)_2(H_2O)]$, the Zn^{II} ion and water O atom are located on a crystallographic twofold rotation axis and the metal atom assumes a distorted trigonal-bipyramidal ZnN_4O coordination geometry. An intramolecular O—H···O hydrogen bond occurs within the ligand and intermolecular O—H···O hydrogen bonds involving the water molecule result in a sheet structure in the crystal structure. In addition, a short C—O···π contact between the O atom of the deprotonated hydroxyl group and a nearby pyridine ring [O···Cg = 3.977 (2) Å, where Cg is the centroid of the pyridine ring] is observed.

Related literature

For related structures, see: Cargill Thompson *et al.* (1996); Stephenson & Hardie (2007).



Experimental

Crystal data

$[Zn(C_{10}H_7N_2O_2)_2(H_2O)]$
M_r = 457.74
Orthorhombic, *Pbcn*
a = 13.931 (2) Å
b = 9.1685 (16) Å
c = 14.364 (3) Å
V = 1834.7 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.38 mm^{-1}
T = 298 (2) K
0.40 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.608, T_{max} = 0.770
8883 measured reflections
1621 independent reflections
1293 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.083
S = 1.05
1621 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.081 (2)	O3—Zn1	2.002 (2)
Zn1—N2	2.0716 (18)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H5···O2	0.82	1.61	2.410 (3)	165
O3—H1···O2^{i}	0.80	1.83	2.630 (2)	174

Symmetry code: (i) $x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2736).

References

Bruker (1997). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cargill Thompson, A. M. W., Jeffery, J. C., Liard, D. J. & Ward, M. D. (1996). *J. Chem. Soc. Dalton Trans.* pp. 879–884.
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Stephenson, M. D. & Hardie, M. J. (2007). *CrystEngComm.* **9**, 496–502.

supporting information

Acta Cryst. (2008). E**64**, m1131 [doi:10.1107/S1600536808024495]

Aquabis(3′-hydroxy-2,2′-bipyridine-3-olato-κ^2N,N')zinc(II)

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S1. Comment

2,2′-Bipyridine-3,3′-diol (bpd) has the potential to be a useful multi-dentate ligand and may act as a bridging ligand due to coordination of its N and O atoms. A few multi-nuclear complexes have been synthesized with mono-deprotonated bpd as a bridging ligand (Cargill Thompson *et al.* 1996; Stephenson & Hardie, 2007). We attempted to prepare a similar compound, but instead we obtained the mono-nuclear title complex, (I), (Fig. 1) and report its structure herein.

The Zn1 atom in (I) lies in a twofold axis and is in a distorted trigonal bipyramidal geometry (Table 1). The dihedral angle between the N1 and N2 ring mean planes is 13.08 (12)°. An intramolecular O—H···O hydrogen bond between O atom of deprotonated hydroxyl and hydroxyl group (Table 2) occcurs within the ligand. The water molecule (O atom site symmetry 2) makes an intermolecular O—H···.O hydrogen bond to result in a supramolecular sheet structure in the *ab* plane (Fig. 2). In addition to the hydrogen bonds there is weak interaction between C—O bond and pyridine ring and the relevant distances are as follows: C4—O2···$Cg1^{i}$ = 3.977 (2) Å and C4—O2···$Cg1^{i}_{perp}$ = 3.635 Å [$Cg1$ is the centroid of N1/C1—C5 ring, C4—O2···$Cg1^{i}_{perp}$ is the perpendicular distance from O2 atom to ring $Cg1^{i}$; symmetry code: (i) 1/2-*x*, 1/2+*y*, *z*].

S2. Experimental

A 10-ml H_2O solution of $ZnCl_2$ (0.1214 g, 0.891 mmol) was added to a 10-ml hot ethanol solution containing 2,2′-bi-pyridine-3,3′-diol (0.1664 g, 0.884 mmol), and the mixed solution was stirred for a few minutes. Yellow blocks of (I) were obtained after the solution had been allowed to stand at room temperature for two weeks.

S3. Refinement

The water H atom was located in a difference Fourier map and refined as riding in its as found relative position with U_{iso}(H) = 1.5U_{eq}(O). The other H atoms geometrically placed (C—H = 0.93-0.96Å, O—H = 0.82Å) and refined as riding with with U_{iso} = U_{iso} = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C, O).

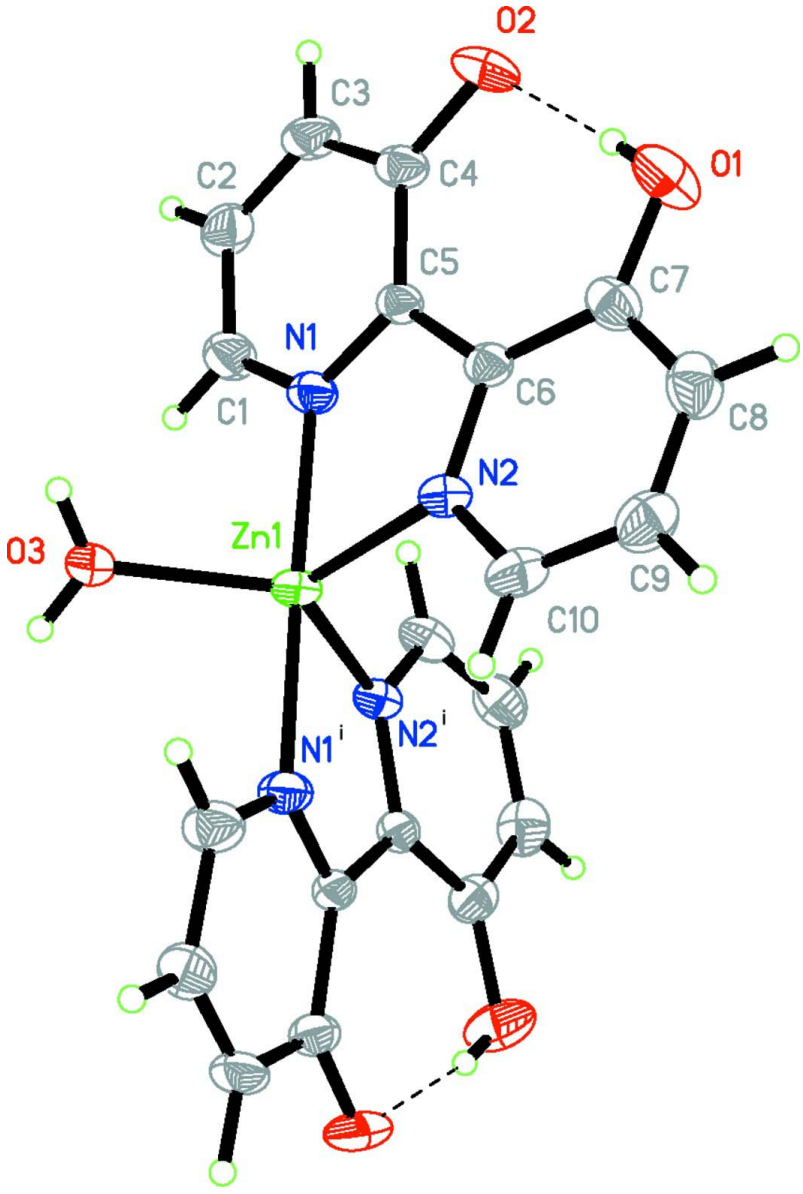

Figure 1

View of (I), showing displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level. The hydrogen bond is indicated by a dashed line. Symmetry code: (i) -1/2 + *x*, -1/2 + *y*, 3/2 - *z*

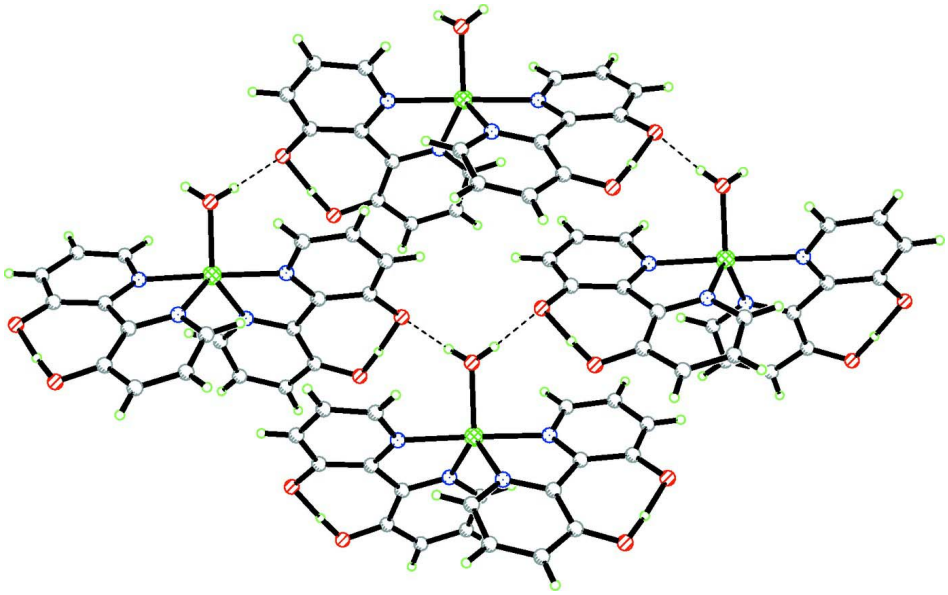

Figure 2

Intermolecular hydrogen bonds (dashed line) in the crystal of (I).

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Crystal data

$[Zn(C_{10}H_7N_2O_2)_2(H_2O)]$
$M_r = 457.74$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 13.931\ (2)$ Å
$b = 9.1685\ (16)$ Å
$c = 14.364\ (3)$ Å
$V = 1834.7\ (6)$ Å^3
$Z = 4$
$F(000) = 936$
$D_x = 1.657$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2299 reflections
$\theta = 2.7–24.6°$
$\mu = 1.38$ mm^{-1}
$T = 298$ K
Block, yellow
0.40 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.608$, $T_{max} = 0.770$
8883 measured reflections
1621 independent reflections
1293 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -15\rightarrow16$
$k = -9\rightarrow10$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.083$
$S = 1.05$
1621 reflections
137 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difmap and geom
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.4048P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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}
C1	0.18495 (17)	−0.0831 (3)	0.84200 (18)	0.0497 (6)
H8A	0.1443	−0.1318	0.8829	0.060*
C2	0.28226 (18)	−0.0979 (3)	0.85235 (18)	0.0505 (6)
H7	0.3078	−0.1560	0.8993	0.061*
C3	0.34041 (17)	−0.0251 (3)	0.7919 (2)	0.0484 (6)
H6A	0.4066	−0.0346	0.7980	0.058*
C4	0.30414 (16)	0.0627 (3)	0.72164 (17)	0.0405 (6)
C5	0.20250 (14)	0.0718 (2)	0.71420 (15)	0.0328 (5)
C6	0.14629 (15)	0.1528 (2)	0.64177 (14)	0.0335 (5)
C7	0.18121 (17)	0.2589 (3)	0.57966 (15)	0.0433 (6)
C8	0.1158 (2)	0.3273 (3)	0.52075 (16)	0.0532 (7)
H4	0.1371	0.4013	0.4816	0.064*
C9	0.0216 (2)	0.2884 (3)	0.51908 (18)	0.0530 (7)
H3	−0.0212	0.3329	0.4783	0.064*
C10	−0.00846 (16)	0.1818 (3)	0.57930 (17)	0.0482 (6)
H2	−0.0724	0.1528	0.5782	0.058*
N1	0.14707 (14)	−0.00122 (19)	0.77522 (15)	0.0401 (5)
N2	0.05150 (12)	0.11824 (19)	0.63953 (12)	0.0379 (5)
O1	0.27183 (13)	0.3017 (2)	0.57387 (13)	0.0673 (6)
H5	0.3044	0.2553	0.6111	0.101*
O2	0.36348 (11)	0.1306 (2)	0.66513 (12)	0.0574 (5)
O3	0.0000	−0.2225 (3)	0.7500	0.0640 (8)
H1	−0.0443	−0.2657	0.7730	0.096*
Zn1	0.0000	−0.00413 (4)	0.7500	0.03787 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0382 (14)	0.0538 (16)	0.0571 (16)	−0.0007 (11)	−0.0022 (12)	0.0162 (12)
C2	0.0420 (14)	0.0485 (15)	0.0610 (16)	0.0054 (11)	−0.0147 (12)	0.0037 (12)
C3	0.0248 (12)	0.0561 (16)	0.0644 (16)	0.0022 (11)	−0.0092 (13)	−0.0119 (13)
C4	0.0291 (12)	0.0451 (13)	0.0474 (13)	−0.0045 (11)	0.0016 (11)	−0.0133 (11)
C5	0.0264 (11)	0.0330 (12)	0.0389 (12)	−0.0026 (9)	0.0007 (9)	−0.0086 (10)

C6	0.0311 (12)	0.0340 (11)	0.0353 (11)	0.0003 (9)	0.0039 (9)	−0.0069 (9)
C7	0.0451 (14)	0.0455 (14)	0.0393 (13)	−0.0082 (11)	0.0066 (11)	−0.0059 (11)
C8	0.0669 (19)	0.0496 (16)	0.0432 (14)	−0.0014 (13)	0.0054 (13)	0.0075 (12)
C9	0.0555 (16)	0.0570 (17)	0.0464 (15)	0.0136 (14)	−0.0026 (12)	0.0049 (13)
C10	0.0356 (14)	0.0567 (16)	0.0525 (15)	0.0114 (11)	−0.0028 (11)	0.0013 (13)
N1	0.0276 (11)	0.0446 (12)	0.0482 (11)	0.0002 (8)	0.0001 (9)	0.0067 (9)
N2	0.0272 (10)	0.0421 (11)	0.0444 (11)	0.0025 (8)	0.0014 (8)	0.0001 (8)
O1	0.0538 (12)	0.0821 (14)	0.0661 (12)	−0.0260 (10)	0.0022 (9)	0.0184 (11)
O2	0.0277 (9)	0.0776 (13)	0.0669 (11)	−0.0141 (8)	0.0075 (8)	−0.0009 (10)
O3	0.0353 (14)	0.0391 (14)	0.118 (2)	0.000	0.0278 (13)	0.000
Zn1	0.0232 (2)	0.0418 (3)	0.0487 (3)	0.000	0.00383 (15)	0.000

Geometric parameters (Å, º)

C1—N1	1.328 (3)	C7—C8	1.392 (3)
C1—C2	1.370 (3)	C8—C9	1.361 (4)
C1—H8A	0.9300	C8—H4	0.9300
C2—C3	1.362 (4)	C9—C10	1.371 (4)
C2—H7	0.9300	C9—H3	0.9300
C3—C4	1.386 (4)	C10—N2	1.336 (3)
C3—H6A	0.9300	C10—H2	0.9300
C4—O2	1.315 (3)	O1—H5	0.8200
C4—C5	1.422 (3)	O3—H1	0.8042
C5—N1	1.346 (3)	Zn1—N1	2.081 (2)
C5—C6	1.499 (3)	Zn1—N2	2.0716 (18)
C6—N2	1.359 (3)	Zn1—N2^{i}	2.0716 (18)
C6—C7	1.407 (3)	Zn1—N1^{i}	2.081 (2)
C7—O1	1.324 (3)	O3—Zn1	2.002 (2)
N1—C1—C2	121.8 (2)	C8—C9—C10	118.0 (2)
N1—C1—H8A	119.1	C8—C9—H3	121.0
C2—C1—H8A	119.1	C10—C9—H3	121.0
C3—C2—C1	118.1 (2)	N2—C10—C9	121.9 (2)
C3—C2—H7	121.0	N2—C10—H2	119.0
C1—C2—H7	121.0	C9—C10—H2	119.0
C2—C3—C4	122.1 (2)	C1—N1—C5	121.6 (2)
C2—C3—H6A	118.9	C1—N1—Zn1	120.67 (16)
C4—C3—H6A	118.9	C5—N1—Zn1	117.24 (15)
O2—C4—C3	119.7 (2)	C10—N2—C6	121.4 (2)
O2—C4—C5	123.5 (2)	C10—N2—Zn1	121.03 (15)
C3—C4—C5	116.8 (2)	C6—N2—Zn1	116.41 (14)
N1—C5—C4	119.5 (2)	C7—O1—H5	109.5
N1—C5—C6	113.49 (18)	Zn1—O3—H1	119.5
C4—C5—C6	126.9 (2)	O3—Zn1—N2	122.79 (5)
N2—C6—C7	118.8 (2)	O3—Zn1—N2^{i}	122.79 (5)
N2—C6—C5	114.11 (18)	N2—Zn1—N2^{i}	114.42 (10)
C7—C6—C5	127.03 (19)	O3—Zn1—N1	90.73 (5)
O1—C7—C8	116.9 (2)	N2—Zn1—N1	77.61 (7)

O1—C7—C6	125.0 (2)	N2^{i}—Zn1—N1	101.58 (7)
C8—C7—C6	118.1 (2)	O3—Zn1—N1^{i}	90.73 (5)
C9—C8—C7	121.6 (2)	N2—Zn1—N1^{i}	101.58 (7)
C9—C8—H4	119.2	N2^{i}—Zn1—N1^{i}	77.61 (7)
C7—C8—H4	119.2	N1—Zn1—N1^{i}	178.53 (10)
N1—C1—C2—C3	0.3 (4)	C4—C5—N1—Zn1	−172.45 (15)
C1—C2—C3—C4	0.3 (4)	C6—C5—N1—Zn1	5.8 (2)
C2—C3—C4—O2	−180.0 (2)	C9—C10—N2—C6	−2.3 (4)
C2—C3—C4—C5	−1.0 (4)	C9—C10—N2—Zn1	165.07 (19)
O2—C4—C5—N1	−179.9 (2)	C7—C6—N2—C10	0.6 (3)
C3—C4—C5—N1	1.2 (3)	C5—C6—N2—C10	179.53 (19)
O2—C4—C5—C6	2.1 (4)	C7—C6—N2—Zn1	−167.35 (15)
C3—C4—C5—C6	−176.8 (2)	C5—C6—N2—Zn1	11.6 (2)
N1—C5—C6—N2	−11.3 (3)	C10—N2—Zn1—O3	102.57 (17)
C4—C5—C6—N2	166.8 (2)	C6—N2—Zn1—O3	−89.42 (15)
N1—C5—C6—C7	167.5 (2)	C10—N2—Zn1—N2^{i}	−77.43 (17)
C4—C5—C6—C7	−14.4 (3)	C6—N2—Zn1—N2^{i}	90.58 (15)
N2—C6—C7—O1	−179.3 (2)	C10—N2—Zn1—N1	−174.67 (19)
C5—C6—C7—O1	1.9 (4)	C6—N2—Zn1—N1	−6.65 (14)
N2—C6—C7—C8	2.2 (3)	C10—N2—Zn1—N1^{i}	4.08 (19)
C5—C6—C7—C8	−176.6 (2)	C6—N2—Zn1—N1^{i}	172.10 (14)
O1—C7—C8—C9	178.0 (2)	C1—N1—Zn1—O3	−48.31 (19)
C6—C7—C8—C9	−3.4 (4)	C5—N1—Zn1—O3	123.54 (16)
C7—C8—C9—C10	1.8 (4)	C1—N1—Zn1—N2	−171.8 (2)
C8—C9—C10—N2	1.1 (4)	C5—N1—Zn1—N2	0.05 (16)
C2—C1—N1—C5	−0.1 (4)	C1—N1—Zn1—N2^{i}	75.4 (2)
C2—C1—N1—Zn1	171.39 (19)	C5—N1—Zn1—N2^{i}	−112.72 (16)
C4—C5—N1—C1	−0.7 (3)	C1—N1—Zn1—N1^{i}	131.69 (18)
C6—C5—N1—C1	177.6 (2)	C5—N1—Zn1—N1^{i}	−56.46 (16)

Symmetry code: (i) $-x, y, -z+3/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H5···O2	0.82	1.61	2.410 (3)	165
O3—H1···O2^{ii}	0.80	1.83	2.630 (2)	174

Symmetry code: (ii) $x-1/2, y-1/2, -z+3/2$.