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 Aquabis(3'-hydroxy-2,2'-bipyridine-3-olato- $\kappa^2N,N'$ )zinc(II)

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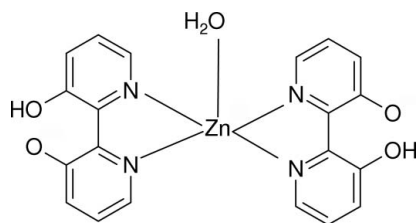
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 Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.030;  $wR$  factor = 0.083; data-to-parameter ratio = 11.8.

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  $O-H \cdots O$  hydrogen bond occurs within the ligand and intermolecular  $O-H \cdots O$  hydrogen bonds involving the water molecule result in a sheet structure in the crystal structure. In addition, a short  $C-O \cdots \pi$  contact between the O atom of the deprotonated hydroxyl group and a nearby pyridine ring [ $O \cdots Cg = 3.977$  (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<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 1.38$  mm<sup>-1</sup>
 $T = 298$  (2) K

 $0.40 \times 0.21 \times 0.20$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.035$ 

## 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  
 $\Delta\rho_{\text{max}} = 0.24$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.22$  e Å<sup>-3</sup>

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, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H5 $\cdots$ O2	0.82	1.61	2.410 (3)	165
O3—H1 $\cdots$ O2 <sup>i</sup>	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.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Stephenson, M. D. & Hardie, M. J. (2007). *CrystEngComm.* **9**, 496–502.

**supplementary materials**

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## Aquabis(3'-hydroxy-2,2'-bipyridine-3-olato- $\kappa^2N,N'$ )zinc(II)

S. G. Zhang and C. Hou

### 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) occurs 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<sup>i</sup> = 3.977 (2) Å and C4—O2...Cg1<sup>i</sup><sub>perp</sub> = 3.635 Å [Cg1 is the centroid of N1/C1—C5 ring, C4—O2...Cg1<sup>i</sup><sub>perp</sub> is the perpendicular distance from O2 atom to ring Cg1<sup>i</sup>; symmetry code: (i) 1/2-*x*, 1/2+*y*, *z*].

### Experimental

A 10-ml H<sub>2</sub>O solution of ZnCl<sub>2</sub> (0.1214 g, 0.891 mmol) was added to a 10-ml hot ethanol solution containing 2,2'-bipyridine-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.

### Refinement

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

Figures

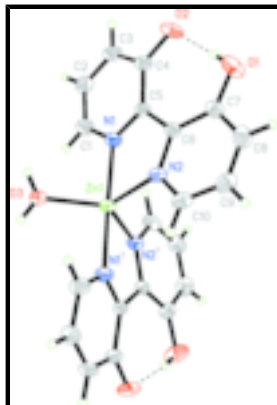


Fig. 1. View of (I), showing displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level. The hydrogen bond is indicated by a dashed line. Symmetry code: (i)  $-1/2 + x, -1/2 + y, 3/2 - z$

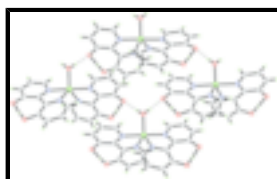


Fig. 2. Intermolecular hydrogen bonds (dashed line) in the crystal of (I).

**Aquabis(3'-hydroxy-2,2'-bipyridine-3-olato- $\kappa^2$ N,N')**zinc(II)

*Crystal data*

[Zn(C<sub>10</sub>H<sub>7</sub>N<sub>2</sub>O<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)]

$M_r = 457.74$

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<sup>3</sup>

$Z = 4$

$F_{000} = 936$

$D_x = 1.657$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 2299 reflections

$\theta = 2.7$ – $24.6^\circ$

$\mu = 1.38$  mm<sup>-1</sup>

$T = 298$  (2) K

Block, yellow

$0.40 \times 0.21 \times 0.20$  mm

*Data collection*

Bruker SMART APEX CCD  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$  (2) K

$\varphi$  and  $\omega$  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  $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\text{max}} = 25.0^\circ$

$\theta_{\text{min}} = 2.7^\circ$

$h = -15 \rightarrow 16$

$k = -9 \rightarrow 10$

$l = -17 \rightarrow 17$

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)] = 0.030$	H-atom parameters constrained
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.4048P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
1621 reflections	$(\Delta/\sigma)_{\max} < 0.001$
137 parameters	$\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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)

## supplementary materials

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 ( $\text{\AA}$ , $^\circ$ )

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 <sup>i</sup>	2.0716 (18)
C6—C7	1.407 (3)	Zn1—N1 <sup>i</sup>	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 <sup>i</sup>	122.79 (5)
N2—C6—C5	114.11 (18)	N2—Zn1—N2 <sup>i</sup>	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 <sup>i</sup> —Zn1—N1	101.58 (7)
C8—C7—C6	118.1 (2)	O3—Zn1—N1 <sup>i</sup>	90.73 (5)
C9—C8—C7	121.6 (2)	N2—Zn1—N1 <sup>i</sup>	101.58 (7)
C9—C8—H4	119.2	N2 <sup>i</sup> —Zn1—N1 <sup>i</sup>	77.61 (7)
C7—C8—H4	119.2	N1—Zn1—N1 <sup>i</sup>	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 <sup>i</sup>	-77.43 (17)
C4—C5—C6—C7	-14.4 (3)	C6—N2—Zn1—N2 <sup>i</sup>	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 <sup>i</sup>	4.08 (19)
C5—C6—C7—C8	-176.6 (2)	C6—N2—Zn1—N1 <sup>i</sup>	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 <sup>i</sup>	75.4 (2)
C2—C1—N1—Zn1	171.39 (19)	C5—N1—Zn1—N2 <sup>i</sup>	-112.72 (16)
C4—C5—N1—C1	-0.7 (3)	C1—N1—Zn1—N1 <sup>i</sup>	131.69 (18)
C6—C5—N1—C1	177.6 (2)	C5—N1—Zn1—N1 <sup>i</sup>	-56.46 (16)

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

## supplementary materials

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### Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H5 $\cdots$ O2	0.82	1.61	2.410 (3)	165
O3—H1 $\cdots$ O2 <sup>ii</sup>	0.80	1.83	2.630 (2)	174

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



Fig. 2

