Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis{2-[5-(2-pyridyl)-2*H*-tetrazol-2-yl]acetato-κ^2N^4,N^5}zinc(II)

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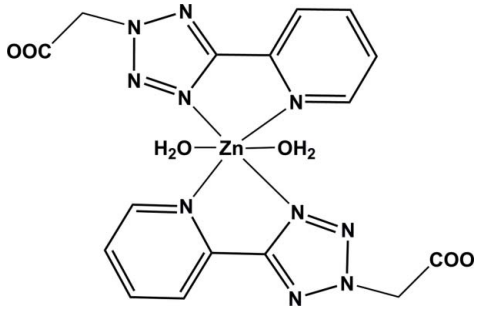
Received 18 June 2009; accepted 22 June 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.027; wR factor = 0.075; data-to-parameter ratio = 14.4.

The title compound, $[Zn(C_8H_6N_5O_2)_2(H_2O)_2]$, was synthesized by hydrothermal reaction of $ZnBr_2$ with 2-[5-(2-pyridyl)-2*H*-tetrazol-2-yl]acetic acid. The Zn^{II} atom lies on an inversion center in a distorted octahedral environment with two planar *trans*-related *N*,*N*′-chelating 2-[5-(2-pyridyl)-2*H*-tetrazol-2-yl]acetic acid ligands in the equatorial plane and two water molecules in the axial positions. In the crystal, O—H···O hydrogen bonds generate an infinite three-dimensional network.

Related literature

For the chemisty of tetrazoles, see: Fu *et al.* (2008); Dai & Fu (2008); Wang *et al.* (2005); Wen (2008); Wittenberger & Donner (1993).



Experimental

Crystal data

$[Zn(C_8H_6N_5O_2)_2(H_2O)_2]$ M_r = 509.76
Monoclinic, $P2_1/c$
a = 7.6407 (15) Å
b = 8.2583 (17) Å
c = 15.155 (3) Å
β = 97.17 (3)°
V = 948.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.36 mm^{-1}
T = 298 K
0.35 × 0.25 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.762, T_{max} = 0.841
(expected range = 0.690–0.762)
9600 measured reflections
2177 independent reflections
1984 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.075
S = 1.11
2177 reflections
151 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WB···O1^{i}	0.85	1.85	2.6891 (19)	172
O1W—H1WA···O2^{ii}	0.85	1.80	2.6365 (17)	169

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by a start-up grant from Southeast University to Professor Ren-Gen Xiong.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2467).

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supporting information

Acta Cryst. (2009). E**65**, m831 [doi:10.1107/S1600536809023940]

Diaquabis{2-[5-(2-pyridyl)-2*H*-tetrazol-2-yl]acetato-κ^2N^4,N^5}zinc(II)

Bo Wang

S1. Comment

The tetrazole functional group has found a wide range of applications in coordination chemistry as ligands, in medicinal chemistry as a metabolically stable surrogate for a carboxylic acid group, and in materials science as high density energy materials(Wang *et al.*, 2005; Fu *et al.*, 2008; Wittenberger *et al.*,1993). We report here the crystal structure of the title compound, Bis[2-(5-(pyridin-2-yl)-2*H*-tetrazol-2-yl)acetic-K^2N^1,N^2]Zinc(II).

In the title compound, the Zn^{II} atom lies on an inversion center. The distorted octahedral Zn^{II} environment contains two planar trans-related N,N-chelating 2-(5-(pyridin-2-yl)-2*H*-tetrazol-2-yl)acetic acid ligands in the equatorial plane and two water ligands in the axial positions. The pyridine and tetrazole rings are nearly coplanar and only twisted from each other by a dihedral angle of 7.06 (1)°. The geometric parameters of the tetrazole rings are comparable to those in related molecules (Wittenberger *et al.*, 1993; Dai & Fu 2008; Wen 2008).

The O atoms from water molecules are involved in intermolecular O—H···O hydrogen bonds building up an infinite three-dimensional network (Table 1 and Fig.2).

S2. Experimental

A mixture of 2-(5-(pyridin-2-yl)-2*H*-tetrazol-2-yl)acetic acid (0.2 mmol), $ZnBr_2$ (0.4 mmol), distilled water (1 ml) and a few drops of ethanol sealed in a glass tube was maintained at 110 °C. Colorless block crystals suitable for X-ray analysis were obtained after 3 days.

S3. Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C-H = 0.93 Å (aromatic) and 0.97 Å (methylene) with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of water molecule located in difference Fourier maps and freely refined using restraints (O-H= 0.85Å and H···H= 1.39Å with *U*ĩso~(H) = 1.5*U*~eq~(O). In the last stage of refinement they were treated as riding on the O atom.

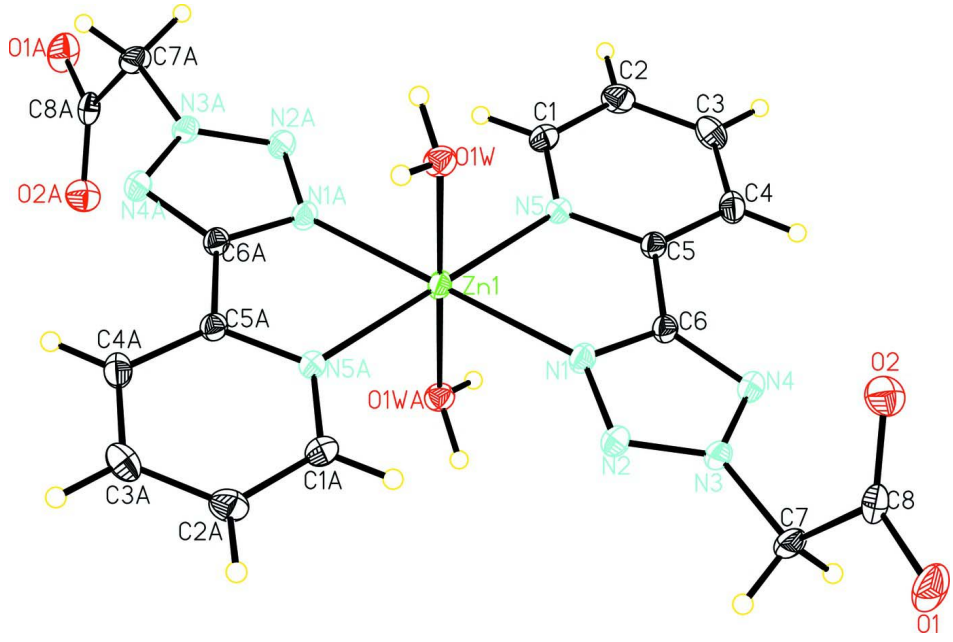

Figure 1

Molecular view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.[Symmetry codes: (i) -x+1, -y+1, -z+1]

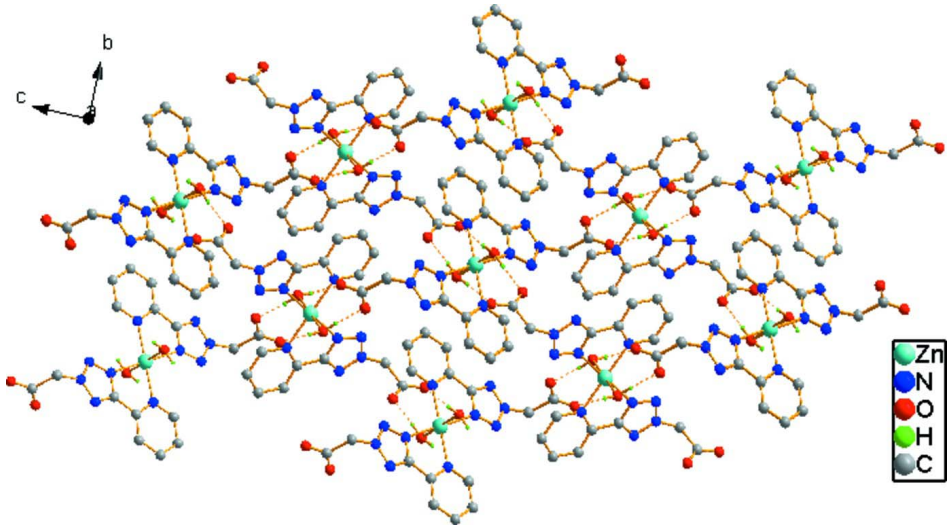

Figure 2

The crystal packing of the title compound viewed along the *a* axis showing the three dimensionnal hydrogen bondings network (dashed line). Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

Diaquabis{2-[5-(2-pyridyl)-2*H*-tetrazol-2-yl]acetato- κ^2N^4,N^5}zinc(II)

Crystal data

$[Zn(C_8H_6N_5O_2)_2(H_2O)_2]$	a = 7.6407 (15) Å
M_r = 509.76	b = 8.2583 (17) Å
Monoclinic, $P2_1/c$	c = 15.155 (3) Å
Hall symbol: -P 2ybc	β = 97.17 (3)°

V = 948.8 (3) Å^3
Z = 2
F(000) = 520
D_x = 1.784 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1984 reflections

θ = 3.6–27.5°
μ = 1.36 mm^{-1}
T = 298 K
Block, colorless
0.35 × 0.25 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.762, T_{max} = 0.841

9600 measured reflections
2177 independent reflections
1984 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.5°, θ_{min} = 3.6°
h = −9→9
k = −10→10
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.075
S = 1.11
2177 reflections
151 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
$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 0.3221P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.5000	0.5000	0.5000	0.02160 (10)
N1	0.32018 (18)	0.61053 (17)	0.39557 (9)	0.0230 (3)
O1W	0.72023 (15)	0.59206 (14)	0.44676 (8)	0.0267 (3)
H1WA	0.7564	0.5199	0.4135	0.040*
H1WB	0.8013	0.6233	0.4865	0.040*
N5	0.45085 (17)	0.73160 (16)	0.55431 (9)	0.0212 (3)
O1	−0.0465 (2)	0.79027 (18)	0.07872 (9)	0.0417 (3)
N2	0.22867 (19)	0.57379 (18)	0.31894 (9)	0.0253 (3)
O2	0.16960 (18)	0.89846 (16)	0.17318 (8)	0.0353 (3)
N3	0.11283 (18)	0.68988 (17)	0.30393 (9)	0.0238 (3)

C5	0.3275 (2)	0.82286 (19)	0.50739 (10)	0.0211 (3)
C6	0.2532 (2)	0.74873 (19)	0.42345 (10)	0.0213 (3)
N4	0.12076 (19)	0.80232 (17)	0.36653 (9)	0.0260 (3)
C1	0.5300 (2)	0.7902 (2)	0.63096 (11)	0.0275 (4)
H1	0.6149	0.7271	0.6643	0.033*
C4	0.2795 (2)	0.9734 (2)	0.53507 (12)	0.0281 (4)
H4	0.1925	1.0336	0.5013	0.034*
C2	0.4912 (3)	0.9404 (2)	0.66288 (12)	0.0320 (4)
H2	0.5501	0.9787	0.7162	0.038*
C3	0.3640 (3)	1.0324 (2)	0.61438 (13)	0.0330 (4)
H3	0.3349	1.1339	0.6348	0.040*
C7	−0.0122 (2)	0.6946 (2)	0.22339 (11)	0.0303 (4)
H7A	−0.1255	0.7307	0.2384	0.036*
H7B	−0.0273	0.5858	0.1996	0.036*
C8	0.0445 (2)	0.8059 (2)	0.15154 (11)	0.0258 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02190 (16)	0.02041 (15)	0.02109 (15)	0.00495 (9)	−0.00280 (10)	−0.00076 (9)
N1	0.0233 (7)	0.0239 (7)	0.0206 (6)	0.0030 (5)	−0.0022 (5)	0.0012 (5)
O1W	0.0250 (6)	0.0283 (6)	0.0263 (6)	0.0004 (5)	0.0008 (5)	−0.0052 (5)
N5	0.0203 (6)	0.0205 (6)	0.0221 (7)	0.0006 (5)	−0.0002 (5)	0.0001 (5)
O1	0.0499 (8)	0.0481 (9)	0.0238 (6)	0.0109 (7)	−0.0081 (6)	0.0047 (6)
N2	0.0269 (7)	0.0258 (7)	0.0213 (7)	0.0009 (6)	−0.0041 (5)	0.0027 (5)
O2	0.0390 (7)	0.0371 (7)	0.0304 (7)	−0.0054 (6)	0.0071 (5)	0.0062 (6)
N3	0.0234 (7)	0.0250 (7)	0.0211 (7)	−0.0008 (5)	−0.0043 (5)	0.0048 (5)
C5	0.0198 (7)	0.0216 (7)	0.0217 (8)	−0.0003 (6)	0.0018 (6)	0.0029 (6)
C6	0.0211 (7)	0.0211 (7)	0.0214 (8)	0.0005 (6)	0.0012 (6)	0.0044 (6)
N4	0.0254 (7)	0.0257 (7)	0.0253 (7)	0.0031 (6)	−0.0031 (5)	0.0032 (6)
C1	0.0249 (8)	0.0301 (9)	0.0258 (8)	−0.0007 (7)	−0.0034 (7)	−0.0010 (7)
C4	0.0293 (9)	0.0231 (8)	0.0317 (9)	0.0049 (7)	0.0035 (7)	0.0030 (7)
C2	0.0362 (10)	0.0319 (9)	0.0270 (9)	−0.0047 (8)	0.0002 (7)	−0.0069 (7)
C3	0.0430 (11)	0.0229 (8)	0.0342 (10)	0.0004 (7)	0.0089 (8)	−0.0060 (7)
C7	0.0284 (9)	0.0334 (9)	0.0254 (8)	−0.0047 (7)	−0.0109 (7)	0.0067 (7)
C8	0.0292 (8)	0.0260 (8)	0.0217 (8)	0.0103 (7)	0.0012 (6)	0.0034 (6)

Geometric parameters (Å, º)

Zn1—O1W	2.0974 (13)	N3—N4	1.324 (2)
Zn1—O1W^{i}	2.0974 (13)	N3—C7	1.453 (2)
Zn1—N5	2.1340 (14)	C5—C4	1.377 (2)
Zn1—N5^{i}	2.1340 (14)	C5—C6	1.461 (2)
Zn1—N1^{i}	2.1640 (14)	C6—N4	1.321 (2)
Zn1—N1	2.1640 (14)	C1—C2	1.377 (3)
N1—N2	1.3142 (19)	C1—H1	0.9300
N1—C6	1.341 (2)	C4—C3	1.380 (3)
O1W—H1WA	0.8486	C4—H4	0.9300

O1W—H1WB	0.8480	C2—C3	1.373 (3)
N5—C1	1.332 (2)	C2—H2	0.9300
N5—C5	1.339 (2)	C3—H3	0.9300
O1—C8	1.235 (2)	C7—C8	1.529 (2)
N2—N3	1.305 (2)	C7—H7A	0.9700
O2—C8	1.236 (2)	C7—H7B	0.9700

O1W—Zn1—O1W^{i}	180.0	N5—C5—C4	122.90 (15)
O1W—Zn1—N5	90.67 (5)	N5—C5—C6	113.44 (14)
O1W^{i}—Zn1—N5	89.33 (5)	C4—C5—C6	123.65 (15)
O1W—Zn1—N5^{i}	89.33 (5)	N4—C6—N1	111.77 (14)
O1W^{i}—Zn1—N5^{i}	90.67 (5)	N4—C6—C5	127.65 (15)
N5—Zn1—N5^{i}	180.000 (1)	N1—C6—C5	120.58 (14)
O1W—Zn1—N1^{i}	88.14 (5)	C6—N4—N3	101.29 (13)
O1W^{i}—Zn1—N1^{i}	91.86 (5)	N5—C1—C2	122.66 (16)
N5—Zn1—N1^{i}	102.84 (5)	N5—C1—H1	118.7
N5^{i}—Zn1—N1^{i}	77.16 (5)	C2—C1—H1	118.7
O1W—Zn1—N1	91.86 (5)	C5—C4—C3	118.07 (17)
O1W^{i}—Zn1—N1	88.14 (5)	C5—C4—H4	121.0
N5—Zn1—N1	77.16 (5)	C3—C4—H4	121.0
N5^{i}—Zn1—N1	102.84 (5)	C3—C2—C1	118.66 (17)
N1^{i}—Zn1—N1	180.0	C3—C2—H2	120.7
N2—N1—C6	107.04 (13)	C1—C2—H2	120.7
N2—N1—Zn1	140.18 (11)	C2—C3—C4	119.59 (17)
C6—N1—Zn1	111.18 (10)	C2—C3—H3	120.2
Zn1—O1W—H1WA	108.1	C4—C3—H3	120.2
Zn1—O1W—H1WB	112.8	N3—C7—C8	113.54 (14)
H1WA—O1W—H1WB	111.8	N3—C7—H7A	108.9
C1—N5—C5	118.12 (14)	C8—C7—H7A	108.9
C1—N5—Zn1	125.41 (11)	N3—C7—H7B	108.9
C5—N5—Zn1	116.46 (11)	C8—C7—H7B	108.9
N3—N2—N1	105.00 (13)	H7A—C7—H7B	107.7
N2—N3—N4	114.90 (13)	O1—C8—O2	129.21 (17)
N2—N3—C7	121.74 (15)	O1—C8—C7	113.30 (16)
N4—N3—C7	123.35 (14)	O2—C8—C7	117.48 (15)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WB*···O1^{ii}	0.85	1.85	2.6891 (19)	172
O1*W*—H1*WA*···O2^{iii}	0.85	1.80	2.6365 (17)	169

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