

Bis(4-amino-3,5-di-2-pyridyl-1,2,4-triazole- κ^2N^1,N^5)diaquazinc(II) dinitrate

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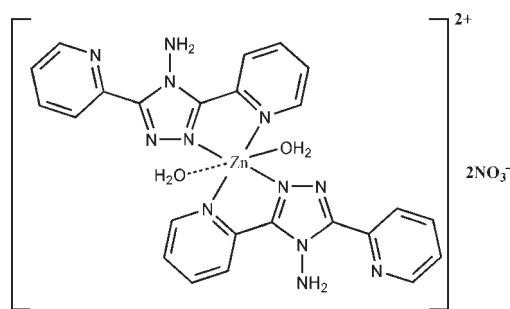
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.045; wR factor = 0.101; data-to-parameter ratio = 14.1.

The asymmetric unit of the title compound, $[Zn(C_{12}H_{10}N_6)_2(H_2O)_2](NO_3)_2$, contains one-half of the complex molecule and one NO_3^- anion. The Zn^{II} ion displays a distorted tetragonal-pyramidal geometry with four N atoms from two chelating 4-amino-3,5-di-2-pyridyl-1,2,4-triazole (2-bpt) ligands in the basal plane and one water molecule occupying the apical site. Another water molecule at the opposite of the apical site has a weak interaction with the Zn^{II} ion [$Zn-O = 2.852$ (5) Å]. The Zn^{II} ion and the two water molecules lie on a twofold rotation axis. An extensive system of hydrogen bonds involving the NH_2 groups of the 2-bpt ligands, water molecules and nitrate anions links all residues into a three-dimensional network.

Related literature

For transition metal complexes of 4-amino-3,5-di-2-pyridyl-1,2,4-triazole (2-bpt), see: Shao & Geng (2009); Hartmann & Vahrenkamp (1995); Keij *et al.* (1984); Kitchen *et al.* (2008); Koningsbruggen *et al.* (1998); Tong *et al.* (2007). For rare earth metal complexes of 2-bpt, see: Garcia *et al.* (1986); Rheingold *et al.* (1993). For hydrogen-bonding interactions involving 2-bpt in organic compounds, see: Mernari *et al.* (1998).



Experimental

Crystal data

$[Zn(C_{12}H_{10}N_6)_2(H_2O)_2](NO_3)_2$
 $M_r = 701.94$
Monoclinic, $C2/c$
 $a = 14.856$ (3) Å
 $b = 9.4185$ (19) Å
 $c = 20.230$ (4) Å
 $\beta = 91.99$ (3)°

$V = 2829$ (1) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.95$ mm⁻¹
 $T = 298$ K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{min} = 0.797$, $T_{max} = 0.828$

13550 measured reflections
3210 independent reflections
2424 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.067$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.101$
 $S = 1.03$
3210 reflections
228 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.32$ e Å⁻³
 $\Delta\rho_{min} = -0.64$ e Å⁻³

Table 1

Selected bond lengths (Å).

Zn1—O1W	2.008 (3)	Zn1—N1	2.078 (2)
Zn1—O2W	2.852 (5)	Zn1—N5	2.141 (2)

Table 2

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>
N4—H4A...O2 ⁱ	0.94 (4)	2.25 (4)	3.100 (3)	149 (3)
N4—H4A...O2	0.94 (4)	2.55 (4)	3.192 (4)	126 (3)
N4—H4B...N6	0.89 (4)	2.13 (4)	2.875 (3)	141 (3)
N4—H4B...O3	0.89 (4)	2.43 (4)	3.005 (3)	122 (3)
O1W—H1W...O3 ⁱⁱ	0.79 (3)	1.93 (3)	2.714 (3)	170 (3)
O2W—H2W...O1 ⁱⁱⁱ	0.92 (5)	2.02 (5)	2.900 (4)	161 (5)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999) and *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2215).

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supplementary materials

Acta Cryst. (2009). E65, m1106-m1107 [doi:10.1107/S1600536809032103]

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Comment

Recently, 4-amino-3,5-di-2-pyridyl-1,2,4-triazole (2-bpt) has been used as ligand because it has potential ability of multi-coordination modes, generating hydrogen-bonding and/or aromatic stacking interactions. The zinc(II) complex of 2-bpt has been reported previously. Hartmann & Vahrenkamp (1995) prepared the complexes based on 2-bpt with $Zn(ClO_4)_2$, $ZnCl_2$, $Zn(NO_3)_2$ and $Zn(BF_4)_2$. But they just obtained the single-crystal structure of $Zn(ClO_4)_2$ complex, in which Zn^{II} atom adopts octahedral geometry. Herein, we reported the crystal structure of the title compound obtained by reacting 2-bpt with $Zn(NO_3)_2$, in which 2-bpt acts as a chelating ligand and hydrogen-bonding interactions play an important role in stabilizing the solid-state structure.

The structure analysis reveals that the asymmetric unit of the title compound contains half a Zn^{II} atom, one 2-bpt molecule, two half water molecules and one NO_3^- anion. As depicted in Fig. 1, the distorted tetragonal pyramidal Zn^{II} atom is located on an inversion center. The basal plane is defined by four N atoms from two 2-bpt ligands with a chelating mode, and the apical site is occupied by one water molecule (O1W) with a Zn—O distance of 2.008 (3) Å (Table 1). Another water molecule (O2W) has a weak interaction with the Zn atom [Zn1—O2W = 2.852 (5) Å], which makes the crystal structure differ from the recently reported nickel complex (Shao & Geng, 2009) because of Jahn-Teller effect. The 2-bpt molecule exhibits *trans*-conformation. The two 2-bpt molecules are not coplanar, with a dihedral angle of 48.54 (5)°. N—H \cdots O, N—H \cdots N and O—H \cdots O hydrogen bonds are observed in the crystal structure (Table 2; Fig. 2).

Experimental

To an ethanol solution (20 ml) of 2-bpt (0.012 g, 0.05 mmol) was added an aqueous solution (5 ml) of $Zn(NO_3)_2 \cdot 6H_2O$ (0.018 g, 0.05 mmol) with stirring. After vigorous stirring for *ca* 40 min, the resultant solution was filtered and left to stand at room temperature. Colorless block crystals suitable for X-ray analysis were produced by slow evaporation of the solvent for two weeks.

Refinement

C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms attached to N atom were found in a difference Fourier map. Their coordinates were refined and U_{iso} factors were fixed. H atoms of water molecules were found in a difference Fourier map and refined isotropically.

Figures

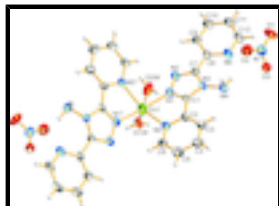


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $-x, y, 3/2 - z$.]

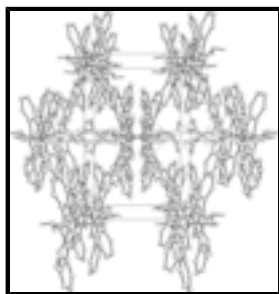


Fig. 2. The crystal packing of the title compound. Dashed lines denote hydrogen bonds.

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Crystal data

$[\text{Zn}(\text{C}_{12}\text{H}_{10}\text{N}_6)_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$

$M_r = 701.94$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 14.856\ (3)\ \text{\AA}$

$b = 9.4185\ (19)\ \text{\AA}$

$c = 20.230\ (4)\ \text{\AA}$

$\beta = 91.99\ (3)^\circ$

$V = 2829\ (1)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1440$

$D_x = 1.648\ \text{Mg m}^{-3}$

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

Cell parameters from 3210 reflections

$\theta = 3.2\text{--}27.4^\circ$

$\mu = 0.95\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Block, colorless

$0.25 \times 0.20 \times 0.20\ \text{mm}$

Data collection

Bruker SMART 1000 CCD diffractometer

Radiation source: sealed tube

Monochromator: graphite

$T = 298\ \text{K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.797$, $T_{\max} = 0.828$

13550 measured reflections

3210 independent reflections

2424 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.067$

$\theta_{\max} = 27.4^\circ$

$\theta_{\min} = 3.2^\circ$

$h = -19 \rightarrow 19$

$k = -12 \rightarrow 12$

$l = -22 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 4.1918P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
3210 reflections	$(\Delta/\sigma)_{\max} < 0.001$
228 parameters	$\Delta\rho_{\max} = 0.32 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.64 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.0000	0.04107 (5)	0.7500	0.03188 (15)
O1W	0.0000	-0.1721 (3)	0.7500	0.0441 (8)
O2W	0.0000	0.3439 (5)	0.7500	0.1050 (19)
O1	0.09893 (16)	0.4526 (3)	1.17312 (12)	0.0646 (7)
O2	0.03688 (16)	0.4946 (2)	1.07668 (12)	0.0586 (6)
O3	-0.01516 (15)	0.3294 (2)	1.13778 (10)	0.0511 (6)
N1	0.03975 (14)	0.0690 (2)	0.84865 (10)	0.0298 (5)
N2	0.11637 (14)	0.0466 (2)	0.88711 (10)	0.0304 (5)
N3	0.01446 (13)	0.1534 (2)	0.94627 (9)	0.0250 (4)
N4	-0.03229 (16)	0.2187 (3)	0.99862 (11)	0.0345 (5)
N5	-0.12105 (14)	0.1149 (2)	0.79303 (10)	0.0305 (5)
N6	0.13761 (15)	0.1407 (2)	1.06063 (10)	0.0335 (5)
N7	0.04037 (16)	0.4274 (2)	1.12933 (12)	0.0371 (5)
C1	-0.02138 (16)	0.1310 (3)	0.88464 (11)	0.0251 (5)
C2	-0.11171 (16)	0.1616 (3)	0.85638 (12)	0.0267 (5)
C3	-0.18075 (18)	0.2271 (3)	0.88886 (14)	0.0349 (6)
H3	-0.1720	0.2599	0.9320	0.080*
C4	-0.26341 (18)	0.2426 (3)	0.85559 (15)	0.0409 (7)
H4	-0.3112	0.2859	0.8762	0.080*
C5	-0.27402 (18)	0.1930 (3)	0.79131 (15)	0.0428 (7)
H5	-0.3291	0.2014	0.7684	0.080*
C6	-0.20152 (18)	0.1311 (3)	0.76189 (13)	0.0378 (7)
H6	-0.2087	0.0990	0.7185	0.080*
C7	0.10017 (17)	0.0992 (3)	0.94616 (12)	0.0268 (5)
C8	0.16653 (17)	0.0977 (3)	1.00174 (12)	0.0282 (5)
C9	0.25491 (18)	0.0556 (3)	0.99173 (13)	0.0331 (6)
H9	0.2726	0.0256	0.9503	0.080*
C10	0.31574 (18)	0.0597 (3)	1.04516 (15)	0.0393 (7)
H10	0.3750	0.0306	1.0404	0.080*

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C11	0.2877 (2)	0.1073 (3)	1.10541 (15)	0.0416 (7)
H11	0.3279	0.1131	1.1415	0.080*
C12	0.1988 (2)	0.1460 (3)	1.11125 (13)	0.0381 (6)
H12	0.1802	0.1774	1.1522	0.080*
H4A	-0.026 (3)	0.317 (4)	0.9919 (19)	0.080*
H4B	0.004 (3)	0.204 (4)	1.034 (2)	0.080*
H1W	0.001 (2)	-0.214 (3)	0.7165 (14)	0.046 (10)*
H2W	0.040 (3)	0.410 (5)	0.734 (3)	0.13 (2)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0277 (2)	0.0478 (3)	0.0200 (2)	0.000	-0.00160 (16)	0.000
O1W	0.066 (2)	0.0431 (18)	0.0229 (16)	0.000	-0.0029 (15)	0.000
O2W	0.151 (5)	0.057 (3)	0.111 (4)	0.000	0.071 (4)	0.000
O1	0.0634 (15)	0.0664 (16)	0.0616 (16)	-0.0025 (13)	-0.0322 (13)	-0.0026 (13)
O2	0.0622 (15)	0.0615 (15)	0.0514 (14)	-0.0047 (12)	-0.0083 (12)	0.0277 (12)
O3	0.0537 (13)	0.0614 (15)	0.0383 (12)	-0.0128 (12)	0.0016 (10)	0.0083 (10)
N1	0.0270 (11)	0.0368 (13)	0.0253 (11)	0.0028 (9)	-0.0030 (9)	-0.0018 (9)
N2	0.0271 (11)	0.0375 (12)	0.0261 (11)	0.0024 (10)	-0.0054 (9)	-0.0002 (10)
N3	0.0267 (10)	0.0266 (11)	0.0215 (10)	0.0003 (9)	-0.0009 (8)	-0.0023 (8)
N4	0.0344 (12)	0.0418 (13)	0.0273 (12)	0.0038 (11)	0.0018 (10)	-0.0097 (10)
N5	0.0278 (11)	0.0394 (13)	0.0242 (11)	0.0010 (10)	-0.0028 (9)	0.0017 (9)
N6	0.0422 (13)	0.0328 (12)	0.0250 (11)	0.0006 (10)	-0.0047 (10)	0.0003 (9)
N7	0.0366 (13)	0.0393 (14)	0.0350 (13)	0.0044 (11)	-0.0049 (10)	0.0015 (11)
C1	0.0262 (12)	0.0264 (12)	0.0225 (12)	-0.0008 (10)	-0.0026 (10)	0.0001 (10)
C2	0.0278 (12)	0.0245 (12)	0.0275 (13)	0.0000 (10)	-0.0022 (10)	0.0012 (10)
C3	0.0326 (14)	0.0338 (14)	0.0380 (15)	0.0030 (12)	-0.0006 (12)	-0.0029 (12)
C4	0.0293 (14)	0.0428 (16)	0.0505 (18)	0.0073 (12)	-0.0015 (13)	-0.0043 (14)
C5	0.0302 (14)	0.0546 (19)	0.0430 (17)	0.0058 (13)	-0.0079 (13)	0.0075 (14)
C6	0.0300 (14)	0.0540 (18)	0.0288 (14)	0.0012 (13)	-0.0068 (11)	0.0038 (13)
C7	0.0278 (12)	0.0265 (12)	0.0261 (13)	0.0003 (10)	-0.0014 (10)	0.0010 (10)
C8	0.0328 (13)	0.0265 (13)	0.0252 (12)	-0.0028 (11)	-0.0027 (11)	0.0017 (10)
C9	0.0317 (13)	0.0338 (14)	0.0334 (14)	-0.0006 (12)	-0.0040 (11)	-0.0006 (12)
C10	0.0320 (14)	0.0390 (16)	0.0463 (17)	-0.0017 (12)	-0.0092 (13)	0.0050 (13)
C11	0.0438 (17)	0.0413 (16)	0.0384 (16)	-0.0059 (13)	-0.0173 (13)	0.0066 (13)
C12	0.0479 (17)	0.0404 (16)	0.0251 (13)	-0.0030 (13)	-0.0097 (12)	0.0019 (12)

Geometric parameters (\AA , $^\circ$)

Zn1—O1W	2.008 (3)	N6—C12	1.346 (3)
Zn1—O2W	2.852 (5)	C1—C2	1.469 (3)
Zn1—N1	2.078 (2)	C2—C3	1.382 (4)
Zn1—N5	2.141 (2)	C3—C4	1.387 (4)
O1W—H1W	0.79 (3)	C3—H3	0.9300
O2W—H2W	0.92 (5)	C4—C5	1.386 (4)
O1—N7	1.243 (3)	C4—H4	0.9300
O2—N7	1.238 (3)	C5—C6	1.378 (4)
O3—N7	1.253 (3)	C5—H5	0.9300

N1—C1	1.319 (3)	C6—H6	0.9300
N1—N2	1.373 (3)	C7—C8	1.469 (3)
N2—C7	1.323 (3)	C8—C9	1.393 (4)
N3—C1	1.355 (3)	C9—C10	1.385 (4)
N3—C7	1.372 (3)	C9—H9	0.9300
N3—N4	1.426 (3)	C10—C11	1.377 (4)
N4—H4A	0.94 (4)	C10—H10	0.9300
N4—H4B	0.89 (4)	C11—C12	1.379 (4)
N5—C6	1.340 (3)	C11—H11	0.9300
N5—C2	1.358 (3)	C12—H12	0.9300
N6—C8	1.343 (3)		
O1W—Zn1—N1	97.28 (6)	N5—C2—C3	122.7 (2)
O1W—Zn1—N1 ⁱ	97.28 (6)	N5—C2—C1	111.5 (2)
N1—Zn1—N1 ⁱ	165.44 (12)	C3—C2—C1	125.9 (2)
O1W—Zn1—N5 ⁱ	108.96 (6)	C2—C3—C4	118.4 (3)
N1—Zn1—N5 ⁱ	97.73 (8)	C2—C3—H3	120.8
N1 ⁱ —Zn1—N5 ⁱ	77.47 (8)	C4—C3—H3	120.8
O1W—Zn1—N5	108.96 (6)	C5—C4—C3	119.3 (3)
N1—Zn1—N5	77.47 (8)	C5—C4—H4	120.3
N1 ⁱ —Zn1—N5	97.73 (8)	C3—C4—H4	120.3
N5 ⁱ —Zn1—N5	142.09 (12)	C6—C5—C4	118.9 (3)
O2W—Zn1—N1	82.73 (5)	C6—C5—H5	120.6
O2W—Zn1—N5	71.05 (5)	C4—C5—H5	120.6
Zn1—O1W—H1W	120 (2)	N5—C6—C5	122.9 (3)
C1—N1—N2	109.2 (2)	N5—C6—H6	118.6
C1—N1—Zn1	114.07 (16)	C5—C6—H6	118.6
N2—N1—Zn1	136.65 (16)	N2—C7—N3	109.8 (2)
C7—N2—N1	106.3 (2)	N2—C7—C8	123.3 (2)
C1—N3—C7	106.0 (2)	N3—C7—C8	126.9 (2)
C1—N3—N4	124.4 (2)	N6—C8—C9	123.1 (2)
C7—N3—N4	129.6 (2)	N6—C8—C7	116.7 (2)
N3—N4—H4A	105 (2)	C9—C8—C7	120.2 (2)
N3—N4—H4B	104 (2)	C10—C9—C8	118.1 (3)
H4A—N4—H4B	102 (3)	C10—C9—H9	120.9
C6—N5—C2	117.9 (2)	C8—C9—H9	120.9
C6—N5—Zn1	126.42 (18)	C11—C10—C9	119.4 (3)
C2—N5—Zn1	115.42 (16)	C11—C10—H10	120.3
C8—N6—C12	117.3 (2)	C9—C10—H10	120.3
O2—N7—O1	121.5 (3)	C10—C11—C12	118.8 (3)
O2—N7—O3	119.0 (2)	C10—C11—H11	120.6
O1—N7—O3	119.4 (2)	C12—C11—H11	120.6
N1—C1—N3	108.7 (2)	N6—C12—C11	123.2 (3)
N1—C1—C2	120.6 (2)	N6—C12—H12	118.4
N3—C1—C2	130.7 (2)	C11—C12—H12	118.4

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

supplementary materials

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N4—H4A \cdots O2 ⁱⁱ	0.94 (4)	2.25 (4)	3.100 (3)	149 (3)
N4—H4A \cdots O2	0.94 (4)	2.55 (4)	3.192 (4)	126 (3)
N4—H4B \cdots N6	0.89 (4)	2.13 (4)	2.875 (3)	141 (3)
N4—H4B \cdots O3	0.89 (4)	2.43 (4)	3.005 (3)	122 (3)
O1W—H1W \cdots O3 ⁱⁱⁱ	0.79 (3)	1.93 (3)	2.714 (3)	170 (3)
O2W—H2W \cdots O1 ^{iv}	0.92 (5)	2.02 (5)	2.900 (4)	161 (5)

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

Fig. 1

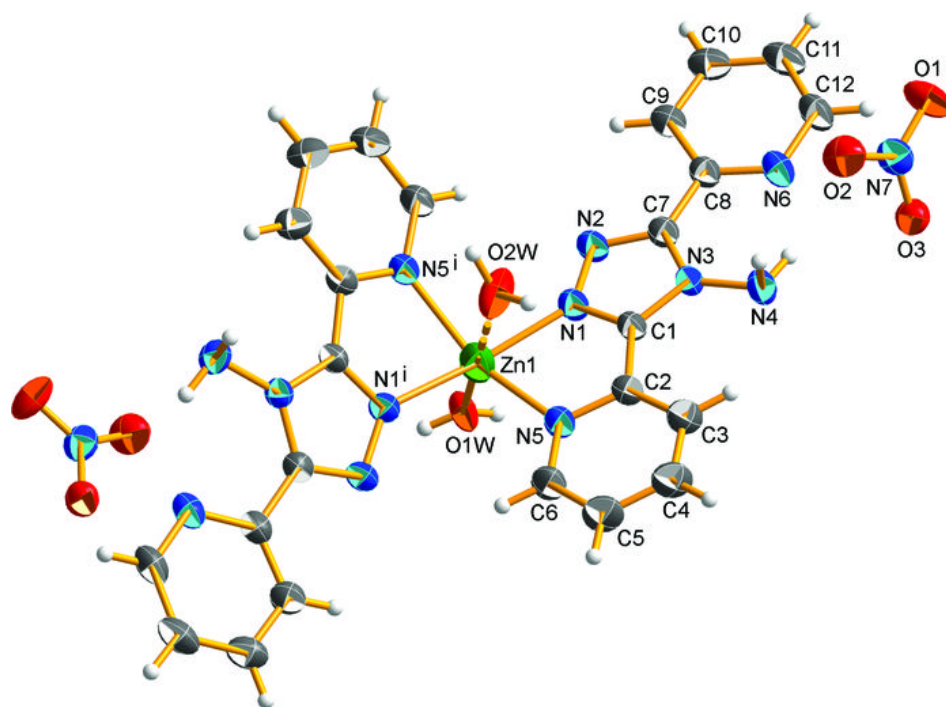


Fig. 2

