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Diaquabis[*N*-(2-pyridylmethyl)-benzamide-κ^2O,N]zinc(II) dinitrate

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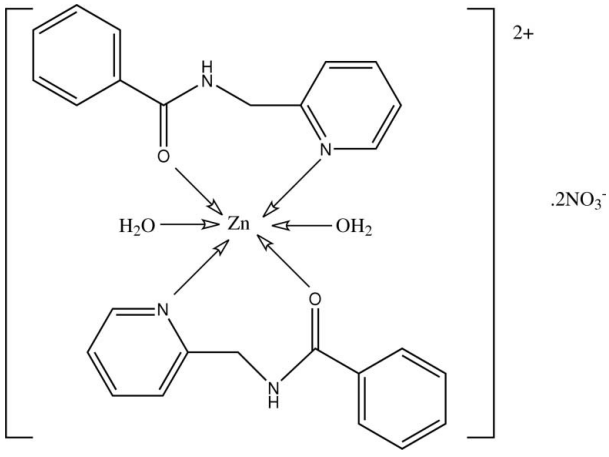
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.101; data-to-parameter ratio = 14.5.

In the title compound, $[Zn(C_{13}H_{12}N_2O)_2(H_2O)_2](NO_3)_2$, the Zn^{II} ion is located on an inversion center. Each Zn center is six-coordinated by two O atoms and two N atoms from two benzamide ligands, and two O atoms from two water molecules, in a distorted octahedral geometry with normal values of Zn—N [2.1977 (19) Å] and Zn—O [2.0853 (17) and 2.1081 (18) Å] coordinating bonds. Intermolecular N—H···O and O—H···O hydrogen bonds link cations and anions into layers parallel to the *bc* plane.

Related literature

For details of pharmacological properties of aminopyridine derivatives, see: Arora *et al.* (2005); Nielsen *et al.* (2004). For general background, see: Fekner *et al.* (2004).



Experimental

Crystal data

$[Zn(C_{13}H_{12}N_2O)_2(H_2O)_2](NO_3)_2$
M_r = 649.93
Monoclinic, $P2_1/c$
a = 11.054 (2) Å
b = 8.9058 (18) Å
c = 15.306 (3) Å
β = 105.037 (3)°
V = 1455.1 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.91 mm^{-1}
T = 293 (2) K
0.30 × 0.19 × 0.08 mm

Data collection

Simens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.772, T_{max} = 0.931
7832 measured reflections
2849 independent reflections
2313 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.03
2849 reflections
196 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2^{i}	0.82	2.24	2.934 (4)	142
N2—H2A···O3	0.86	2.17	2.919 (4)	146
C1—H1A···O1^{ii}	0.93	2.34	2.901 (3)	118

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2353).

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supplementary materials

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Diaquabis[*N*-(2-pyridylmethyl)benzamide-$\kappa^2 O,N$]zinc(II) dinitrate

X.-R. Zhang, B.-P. Qi, F. Li and S. Bi

Comment

Some benzamide molecules with the aminopyridine structure exhibit anti-ulcerogenic, sedative or anti-inflammatory properties (Arora *et al.*, 2005; Nielsen *et al.*, 2004). In order to search for aminopyridine derivatives with higher pharmacological properties, the title complex, (I), was synthesized and its structure is presented here.

The Zn^{II} atoms, which are located on inversion centers, is six-coordinated by two O atoms and two N atoms from two benzamide ligands, and two O atoms from two water molecules (Fig. 1). The geometry around the Zn atom is distorted octahedral with the normal values of Zn—N [2.1977 (19) Å] and Zn—O [2.0853 (17), 2.1081 (18) Å] coordinating bonds. Two nitrate anions lie outside the coordination sphere, balancing the charge. The character due to donation of the non-bonding electron pair on the nitrogen (Fekner *et al.*, 2004). The benzamide chelate is not planar and the two aromatic rings make a dihedral angle of 60.06 (1)°. There is an intramolecular C1—H1A···O1 hydrogen bond, which forms a six-number ring.

In the crystal strucure, intermolecular N—H···O and O—H···O hydrogen bonds (Table 1) link cations and anions into the layers parallell to *bc* plane (Fig. 2). The packing is further stabilized by C—H···π (C6—H6A···*Cg*1^{iii}) interactions with the distance of H6A···*Cg*1^{iii} 2.85 Å, where *Cg*1 denotes the centroid of N1/C1—C5 pyridine ring [symmetry code: (iii) $-x + 1, y + 1/2, -z + 1/2$].

Experimental

To a cold solution of 2-(2-aminomethyl)pyridine (2 ml, 19 mmol) and triethylamine (2.63 ml, 19 mmol) in dry CH_2Cl_2 (25 ml) was added dropwise a solution of benzyl chloride (2 ml, 17.2 mmol) in dry CH_2Cl_2 (15 ml). Stirring was continued at room temperature for 1 h, then at 333 K for 5 h. After filtering, the filtrate was washed with water, dried over anhydrous Na_2SO_4, and then evaporated to give *N*-(pyridin-2-ylmethyl)benzamide as a yellow oil. To a solution of ligand (0.34 g, 1.6 mmol) in ethyl acetate (15 ml) was added slowly a solution of $Zn(NO_3)_2{\cdot}6H_2O$ (0.24 g, 0.80 mmol) in ethyl acetate (10 ml). The mixture was stirred for 2 h until a white solid appeared. Light yellow crystals suitable for an X-ray diffraction study were obtained by slow evaporation of an ethyl acetate solution.

Refinement

All H atoms were located in difference Fourier map, placed in idealized positions [O—H 0.82 Å, C—H 0.93–0.97 Å] and refined as riding, with $U_{iso}(H) = 1.2\ U_{eq}$ of the parent atom.

Figures

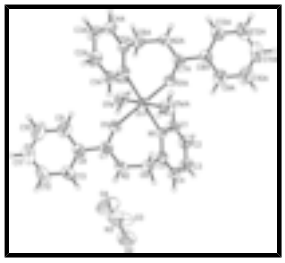

Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme [symmetry codes: (A) $-x+1, -y+1, -z$].

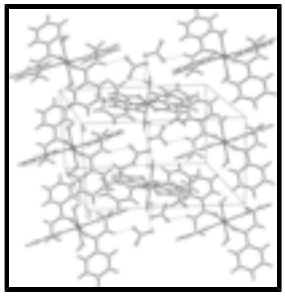

Fig. 2. A portion of the crystal packing of (I). Hydrogen bonds are indicated by dashed lines.

Diaquabis[*N*-(2-pyridylmethyl)benzamide-$\kappa^2 O,N$]zinc(II) dinitrate

Crystal data

$[Zn(C_{13}H_{12}N_2O)_2(H_2O)_2](NO_3)_2$	$F_{000} = 672$
$M_r = 649.93$	$D_x = 1.483$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.054$ (2) Å	Cell parameters from 3058 reflections
$b = 8.9058$ (18) Å	$\theta = 2.7$–25.6°
$c = 15.306$ (3) Å	$\mu = 0.91$ mm^{-1}
$\beta = 105.037$ (3)°	$T = 293$ (2) K
$V = 1455.1$ (5) Å^3	Prism, colourless
$Z = 2$	0.30 × 0.19 × 0.08 mm

Data collection

Simens SMART 1000 CCD area-detector diffractometer	2849 independent reflections
Radiation source: fine-focus sealed tube	2313 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.019$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.1^\circ$
$T = 293(2)$ K	$\theta_{min} = 1.9^\circ$
ω scans	$h = -13 \rightarrow 13$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -7 \rightarrow 10$
$T_{min} = 0.772$, $T_{max} = 0.931$	$l = -18 \rightarrow 18$
7832 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2 + 0.6788P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2849 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
196 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.5000	0.0000	0.03717 (14)
N1	0.59165 (18)	0.5211 (2)	0.14516 (12)	0.0389 (4)
O1	0.31996 (16)	0.50820 (19)	0.01892 (11)	0.0513 (4)
O1W	0.49296 (15)	0.2660 (2)	0.01872 (12)	0.0559 (5)
H1WA	0.5626	0.2298	0.0235	0.067*
H1WB	0.4714	0.2486	0.0651	0.067*
C5	0.5456 (2)	0.5925 (3)	0.20741 (15)	0.0424 (5)
C4	0.6129 (3)	0.6010 (3)	0.29739 (16)	0.0570 (7)
H4A	0.5787	0.6497	0.3392	0.068*
N2	0.31605 (19)	0.5545 (3)	0.16206 (14)	0.0507 (5)
H2A	0.2841	0.5330	0.2061	0.061*
C1	0.7055 (2)	0.4593 (3)	0.17359 (16)	0.0485 (6)
H1A	0.7380	0.4090	0.1315	0.058*
C6	0.4180 (2)	0.6636 (3)	0.17684 (17)	0.0507 (6)
H6A	0.4082	0.7355	0.2221	0.061*
H6B	0.4123	0.7180	0.1210	0.061*
C8	0.1587 (2)	0.3897 (3)	0.06956 (17)	0.0477 (6)
C7	0.2714 (2)	0.4878 (3)	0.08311 (16)	0.0432 (5)

N3	0.3019 (2)	0.4922 (2)	0.38825 (16)	0.0549 (6)
C2	0.7769 (3)	0.4663 (3)	0.26170 (18)	0.0601 (7)
H2B	0.8562	0.4231	0.2781	0.072*
C12	−0.0099 (3)	0.2758 (4)	0.1182 (3)	0.0782 (9)
H12A	−0.0520	0.2610	0.1628	0.094*
C13	0.0940 (2)	0.3680 (3)	0.1351 (2)	0.0650 (8)
H13A	0.1208	0.4159	0.1907	0.078*
O3	0.2683 (3)	0.5981 (3)	0.33914 (19)	0.1082 (10)
C3	0.7297 (3)	0.5377 (4)	0.32484 (18)	0.0633 (8)
H3A	0.7758	0.5433	0.3849	0.076*
C9	0.1180 (3)	0.3175 (4)	−0.0121 (2)	0.0702 (8)
H9A	0.1605	0.3305	−0.0567	0.084*
O2	0.3366 (3)	0.5101 (3)	0.47054 (17)	0.1026 (10)
C11	−0.0506 (3)	0.2070 (4)	0.0371 (3)	0.0862 (11)
H11A	−0.1220	0.1473	0.0253	0.103*
O4	0.3071 (4)	0.3698 (3)	0.3566 (2)	0.1251 (11)
C10	0.0136 (3)	0.2255 (5)	−0.0280 (3)	0.0949 (12)
H10A	−0.0133	0.1758	−0.0831	0.114*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0382 (2)	0.0444 (2)	0.0298 (2)	−0.00112 (15)	0.01025 (14)	0.00098 (15)
N1	0.0431 (10)	0.0437 (11)	0.0311 (9)	−0.0027 (8)	0.0119 (8)	−0.0016 (8)
O1	0.0410 (9)	0.0788 (13)	0.0366 (9)	−0.0026 (8)	0.0147 (7)	−0.0025 (8)
O1W	0.0628 (11)	0.0495 (10)	0.0563 (11)	−0.0011 (8)	0.0172 (9)	0.0093 (8)
C5	0.0519 (13)	0.0405 (12)	0.0381 (12)	−0.0098 (10)	0.0175 (10)	−0.0053 (10)
C4	0.0722 (18)	0.0623 (17)	0.0391 (13)	−0.0146 (14)	0.0191 (12)	−0.0146 (12)
N2	0.0493 (12)	0.0671 (13)	0.0426 (11)	−0.0068 (10)	0.0241 (9)	−0.0072 (10)
C1	0.0485 (14)	0.0596 (15)	0.0368 (12)	0.0062 (11)	0.0102 (10)	0.0017 (11)
C6	0.0545 (14)	0.0513 (14)	0.0504 (14)	−0.0026 (12)	0.0212 (11)	−0.0135 (11)
C8	0.0370 (11)	0.0530 (14)	0.0527 (14)	0.0046 (10)	0.0110 (10)	0.0048 (11)
C7	0.0374 (11)	0.0533 (14)	0.0408 (12)	0.0074 (10)	0.0136 (10)	0.0016 (10)
N3	0.0655 (14)	0.0513 (13)	0.0534 (14)	0.0030 (10)	0.0253 (11)	0.0008 (11)
C2	0.0557 (16)	0.0741 (19)	0.0432 (14)	0.0062 (13)	−0.0004 (12)	0.0042 (13)
C12	0.0532 (16)	0.082 (2)	0.109 (3)	−0.0063 (16)	0.0385 (18)	0.001 (2)
C13	0.0516 (15)	0.0738 (19)	0.0772 (19)	−0.0072 (14)	0.0306 (14)	−0.0094 (15)
O3	0.185 (3)	0.0732 (16)	0.0937 (18)	0.0554 (18)	0.0855 (19)	0.0338 (14)
C3	0.0707 (19)	0.0769 (19)	0.0346 (13)	−0.0110 (15)	−0.0003 (13)	−0.0049 (13)
C9	0.0664 (18)	0.084 (2)	0.0568 (17)	−0.0173 (16)	0.0100 (14)	−0.0020 (15)
O2	0.0866 (18)	0.167 (3)	0.0527 (14)	0.0014 (15)	0.0158 (13)	−0.0032 (14)
C11	0.0543 (18)	0.082 (2)	0.117 (3)	−0.0193 (17)	0.0126 (19)	0.009 (2)
O4	0.203 (3)	0.0602 (16)	0.118 (2)	0.0137 (18)	0.052 (2)	−0.0138 (15)
C10	0.089 (2)	0.107 (3)	0.075 (2)	−0.039 (2)	−0.0028 (19)	−0.010 (2)

Geometric parameters (Å, °)

Zn1—O1^{i}	2.0853 (17)	C6—H6A	0.9700

Zn1—O1	2.0853 (17)	C6—H6B	0.9700
Zn1—O1W	2.1081 (18)	C8—C9	1.373 (4)
Zn1—O1W^{i}	2.1081 (18)	C8—C13	1.388 (4)
Zn1—N1^{i}	2.1977 (19)	C8—C7	1.492 (3)
Zn1—N1	2.1977 (19)	N3—O4	1.201 (3)
N1—C1	1.338 (3)	N3—O3	1.203 (3)
N1—C5	1.350 (3)	N3—O2	1.228 (3)
O1—C7	1.249 (3)	C2—C3	1.368 (4)
O1W—H1WA	0.8200	C2—H2B	0.9300
O1W—H1WB	0.8201	C12—C11	1.353 (5)
C5—C4	1.387 (3)	C12—C13	1.380 (4)
C5—C6	1.505 (3)	C12—H12A	0.9300
C4—C3	1.371 (4)	C13—H13A	0.9300
C4—H4A	0.9300	C3—H3A	0.9300
N2—C7	1.322 (3)	C9—C10	1.385 (4)
N2—C6	1.460 (3)	C9—H9A	0.9300
N2—H2A	0.8600	C11—C10	1.374 (5)
C1—C2	1.376 (4)	C11—H11A	0.9300
C1—H1A	0.9300	C10—H10A	0.9300
O1^{i}—Zn1—O1	180.00 (13)	N2—C6—H6A	109.0
O1^{i}—Zn1—O1W	93.12 (7)	C5—C6—H6A	109.0
O1—Zn1—O1W	86.88 (7)	N2—C6—H6B	109.0
O1^{i}—Zn1—O1W^{i}	86.88 (7)	C5—C6—H6B	109.0
O1—Zn1—O1W^{i}	93.12 (7)	H6A—C6—H6B	107.8
O1W—Zn1—O1W^{i}	180.000 (15)	C9—C8—C13	119.0 (2)
O1^{i}—Zn1—N1^{i}	93.60 (7)	C9—C8—C7	117.7 (2)
O1—Zn1—N1^{i}	86.40 (7)	C13—C8—C7	123.3 (2)
O1W—Zn1—N1^{i}	91.67 (7)	O1—C7—N2	121.3 (2)
O1W^{i}—Zn1—N1^{i}	88.33 (7)	O1—C7—C8	119.3 (2)
O1^{i}—Zn1—N1	86.40 (7)	N2—C7—C8	119.4 (2)
O1—Zn1—N1	93.60 (7)	O4—N3—O3	119.9 (3)
O1W—Zn1—N1	88.33 (7)	O4—N3—O2	119.8 (3)
O1W^{i}—Zn1—N1	91.67 (7)	O3—N3—O2	120.2 (3)
N1^{i}—Zn1—N1	180.00 (4)	C3—C2—C1	119.1 (3)
C1—N1—C5	117.3 (2)	C3—C2—H2B	120.5
C1—N1—Zn1	116.20 (15)	C1—C2—H2B	120.5
C5—N1—Zn1	126.46 (16)	C11—C12—C13	120.2 (3)
C7—O1—Zn1	136.42 (16)	C11—C12—H12A	119.9
Zn1—O1W—H1WA	109.5	C13—C12—H12A	119.9
Zn1—O1W—H1WB	109.5	C12—C13—C8	120.5 (3)
H1WA—O1W—H1WB	109.0	C12—C13—H13A	119.8
N1—C5—C4	121.5 (2)	C8—C13—H13A	119.8
N1—C5—C6	118.2 (2)	C2—C3—C4	118.4 (2)
C4—C5—C6	120.2 (2)	C2—C3—H3A	120.8
C3—C4—C5	120.1 (2)	C4—C3—H3A	120.8
C3—C4—H4A	119.9	C8—C9—C10	119.8 (3)

C5—C4—H4A	119.9	C8—C9—H9A	120.1
C7—N2—C6	122.0 (2)	C10—C9—H9A	120.1
C7—N2—H2A	119.0	C12—C11—C10	120.0 (3)
C6—N2—H2A	119.0	C12—C11—H11A	120.0
N1—C1—C2	123.5 (2)	C10—C11—H11A	120.0
N1—C1—H1A	118.2	C11—C10—C9	120.5 (3)
C2—C1—H1A	118.2	C11—C10—H10A	119.8
N2—C6—C5	113.0 (2)	C9—C10—H10A	119.8
O1^{i}—Zn1—N1—C1	−27.82 (17)	C7—N2—C6—C5	−88.9 (3)
O1—Zn1—N1—C1	152.18 (17)	N1—C5—C6—N2	76.4 (3)
O1W—Zn1—N1—C1	65.42 (17)	C4—C5—C6—N2	−103.6 (3)
O1W^{i}—Zn1—N1—C1	−114.58 (17)	Zn1—O1—C7—N2	50.2 (3)
N1^{i}—Zn1—N1—C1	150.85 (16)	Zn1—O1—C7—C8	−131.5 (2)
O1^{i}—Zn1—N1—C5	150.74 (18)	C6—N2—C7—O1	4.6 (4)
O1—Zn1—N1—C5	−29.26 (18)	C6—N2—C7—C8	−173.7 (2)
O1W—Zn1—N1—C5	−116.02 (18)	C9—C8—C7—O1	4.3 (3)
O1W^{i}—Zn1—N1—C5	63.98 (18)	C13—C8—C7—O1	−175.9 (2)
N1^{i}—Zn1—N1—C5	−30.6 (3)	C9—C8—C7—N2	−177.4 (3)
O1^{i}—Zn1—O1—C7	121 (100)	C13—C8—C7—N2	2.4 (4)
O1W—Zn1—O1—C7	68.7 (2)	N1—C1—C2—C3	1.1 (5)
O1W^{i}—Zn1—O1—C7	−111.3 (2)	C11—C12—C13—C8	−0.8 (5)
N1^{i}—Zn1—O1—C7	160.6 (2)	C9—C8—C13—C12	−0.3 (4)
N1—Zn1—O1—C7	−19.4 (2)	C7—C8—C13—C12	179.9 (3)
C1—N1—C5—C4	−0.3 (3)	C1—C2—C3—C4	−0.6 (5)
Zn1—N1—C5—C4	−178.86 (18)	C5—C4—C3—C2	−0.3 (4)
C1—N1—C5—C6	179.7 (2)	C13—C8—C9—C10	0.3 (5)
Zn1—N1—C5—C6	1.1 (3)	C7—C8—C9—C10	−179.9 (3)
N1—C5—C4—C3	0.8 (4)	C13—C12—C11—C10	1.8 (6)
C6—C5—C4—C3	−179.2 (2)	C12—C11—C10—C9	−1.8 (6)
C5—N1—C1—C2	−0.6 (4)	C8—C9—C10—C11	0.7 (6)
Zn1—N1—C1—C2	178.1 (2)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O2^{ii}	0.82	2.24	2.934 (4)	142
N2—H2A···O3	0.86	2.17	2.919 (4)	146
C1—H1A···O1^{i}	0.93	2.34	2.901 (3)	118

Symmetry codes: (ii) −*x*+1, *y*−1/2, −*z*+1/2; (i) −*x*+1, −*y*+1, −*z*.

Fig. 1

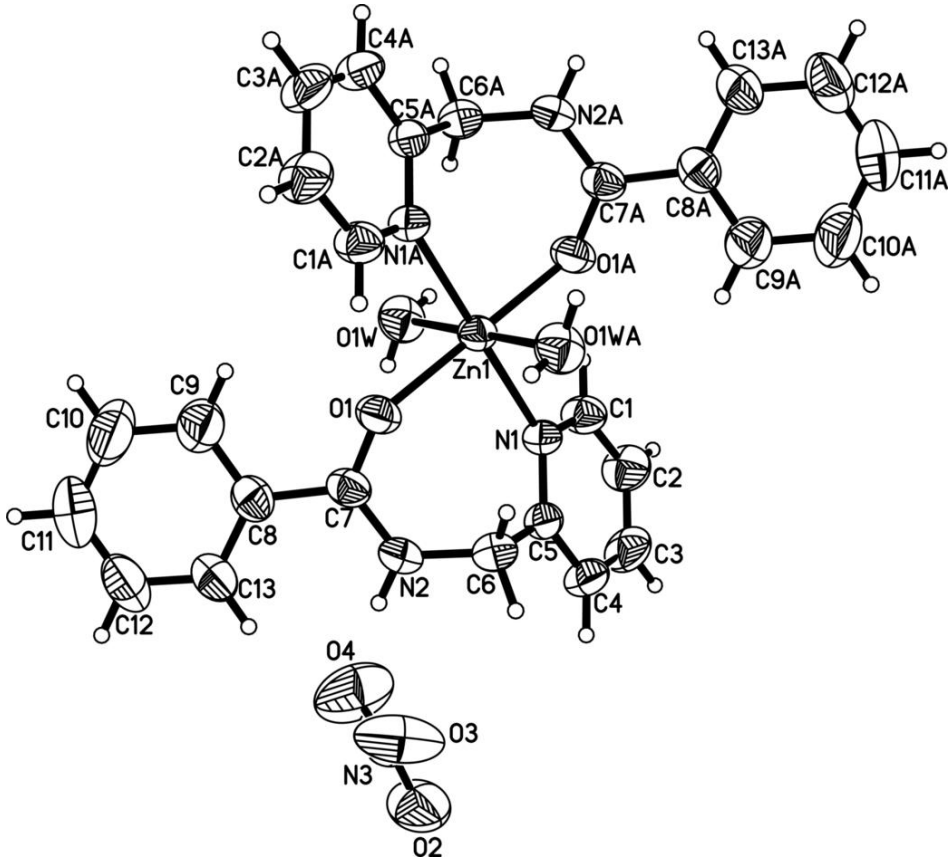
C4A
C3A
C6A
C5A
N2A
C13A
C12A
C2A
C7A
C8A
C11A
C1A
N1A
O1A
C10A
C9A
O1W
O1WA
Zn1
C9
O1
C1
C10
N1
C2
C7
C8
C11
C5
C3
C13
N2
C6
C4
C12
O4
O3
N3
O2

Fig. 2