

(Ethylenediamine- κ^2N,N')bis[3-(2-pyridyl)-5-(4-pyridyl)-1,2,4-triazolato- κ^2N^2,N^3]zinc(II) methanol solvate dihydrate

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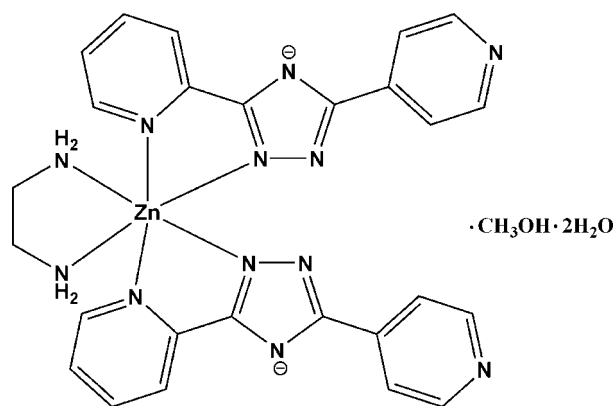
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.006$ Å; R factor = 0.055; wR factor = 0.130; data-to-parameter ratio = 14.5.

The asymmetric unit of the title compound, $[Zn(C_{12}H_8N_5)_2(C_2H_8N_2)] \cdot CH_3OH \cdot 2H_2O$, contains a Zn^{II} cation, octahedrally coordinated by two 3-(2-pyridyl)-5-(4-pyridyl)-1,2,4-triazolate anions, a chelating ethane-1,2-diamine molecule, a methanol solvent molecule, and two crystal water molecules. In the crystal packing, complex molecules are linked by hydrogen bonds into a two-dimensional layer.

Related literature

For related structures, see: Wang *et al.* (2005). For general background, see: Kesanli & Lin (2003).



Experimental

Crystal data

$[Zn(C_{12}H_8N_5)_2(C_2H_8N_2)] \cdot CH_3OH \cdot 2H_2O$

$M_r = 638.02$
Triclinic, $P\bar{1}$

$a = 8.3323$ (8) Å
 $b = 13.0268$ (12) Å
 $c = 14.9444$ (14) Å
 $\alpha = 66.404$ (2)°
 $\beta = 79.751$ (2)°
 $\gamma = 81.437$ (2)°

$V = 1457.3$ (2) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.90$ mm⁻¹
 $T = 293$ (2) K
 $0.25 \times 0.22 \times 0.16$ mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2000)
 $T_{\min} = 0.807$, $T_{\max} = 0.870$

11395 measured reflections
5643 independent reflections
4532 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.130$
 $S = 1.04$
5643 reflections

388 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.61$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.56$ e Å⁻³

Table 1

Selected bond lengths (Å).

Zn1—N7	2.096 (3)	Zn1—N12	2.148 (3)
Zn1—N2	2.103 (2)	Zn1—N1	2.269 (3)
Zn1—N11	2.133 (3)	Zn1—N6	2.293 (3)

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>
N11—H11B...O1W ⁱ	0.90	2.27	3.166 (4)	172
N11—H11C...O2W ⁱⁱ	0.90	2.17	3.034 (4)	161
N12—H12B...N5 ⁱⁱⁱ	0.90	2.54	3.321 (4)	146
N12—H12C...O1W	0.90	2.45	3.331 (4)	165
O1—H1B...N4 ^{iv}	0.90	2.02	2.897 (4)	163
O1W—H1WA...N3 ^v	0.85	2.04	2.887 (4)	171
O1W—H1WB...N8	0.85	2.09	2.859 (4)	150
O2W—H2WA...O1	0.85	1.94	2.778 (4)	169
O2W—H2WB...O1W	0.85	2.00	2.787 (4)	153

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2199).

References

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supplementary materials

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Comment

Recently, there has been significant interest in the rational design and synthesis of chiral coordination polymers due to their potential functions, such as enantioselective separations and catalysis, which could be obtained by using chiral and achiral ligands (Kesanli *et al.* 2003; Wang *et al.* 2005). The use of achiral ligands is more attractive since usually such ligands are easier to be generated. Asymmetric ligands, as achiral ligands, have been widely used to construct those non-centrosymmetrical polymers. Unfortunately, here, we synthesised a centrosymmetrical complex $Zn(C_{12}H_8N_5)_2(C_2H_8N_2).CH_3OH.2H_2O$, with an asymmetric 3-(2-pyridyl)-5-(4-pyridyl)-4_H-1,2,4-triazole ligand.

The asymmetric unit of the title compound, contains one Zn^{II} cation, two 3-(2-pyridyl)-5-(4-pyridyl)-1,2,4-triazolato anions, one chelating ethane-1,2-diamine, methanol solvate and two crystal water molecules. The complex is mononuclear with Zn^{II} in a distorted octahedral geometry of two chelating triazolato anions, and one chelating ethane-1,2-diamine ligand. Each triazolato group acts as a bidentate chelating ligand whereas the N atom of 4-pyridyl group does not take part in coordination (Table 1 and Fig. 1). In the crystal, the complex molecules are linked by N—H \cdots O, O—H \cdots N and O—H \cdots O hydrogen bonds into a two-dimensional layer (Table 2 and Fig. 2).

Experimental

A mixture of 3-(2-pyridyl)-5-(4-pyridyl)-4_H-1,2,4-triazole (0.0446 g, 0.2 mmol), $ZnSO_4 \cdot 7 H_2O$ (0.0288 g, 0.1 mmol), ethane-1,2-diamine (0.1 ml), methanol (2 ml) and water (2 ml) was stirred for 0.5 h at room temperature, and then filtered. The filtrate was allowed to evaporate slowly at room temperature. After 2 weeks, colourless needle crystals were obtained in 34% yield (0.0217 g) based on Zn^{II} .

Refinement

H atoms bonded to N and O atoms were located in a difference map with the distances of N—H = 0.90 and O—H = 0.85–0.90 Å. Other H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97 Å and with $U_{iso}(H) = 1.2$.

Figures

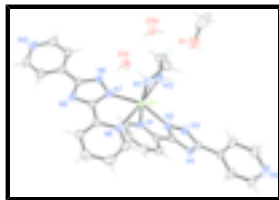


Fig. 1. Coordination environment of Zn^{II} with the 30% displacement ellipsoids.

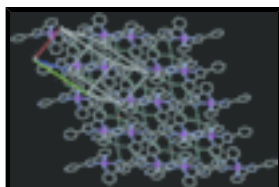


Fig. 2. The two-dimensional hydrogen bond network of the title compound.

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Crystal data

[Zn(C₁₂H₈N₅)₂(C₂H₈N₂)]·CH₃O·2H₂O

$M_r = 638.02$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.3323$ (8) Å

$b = 13.0268$ (12) Å

$c = 14.9444$ (14) Å

$\alpha = 66.404$ (2)°

$\beta = 79.751$ (2)°

$\gamma = 81.437$ (2)°

$V = 1457.3$ (2) Å³

$Z = 2$

$F_{000} = 664$

$D_x = 1.454$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 783 reflections

$\theta = 2.5$ – 28.0 °

$\mu = 0.90$ mm⁻¹

$T = 293$ (2) K

Needle, colourless

$0.25 \times 0.22 \times 0.16$ mm

Data collection

Bruker APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2000)

$T_{\min} = 0.807$, $T_{\max} = 0.870$

11395 measured reflections

5643 independent reflections

4532 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\text{max}} = 26.0$ °

$\theta_{\text{min}} = 1.8$ °

$h = -10 \rightarrow 10$

$k = -16 \rightarrow 16$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.853P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
5643 reflections	$(\Delta/\sigma)_{\max} < 0.001$
388 parameters	$\Delta\rho_{\max} = 0.61 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.56 \text{ e } \text{\AA}^{-3}$
	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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.71857 (5)	0.78434 (3)	0.29062 (3)	0.03871 (14)
C1	0.4382 (5)	0.9641 (3)	0.1713 (3)	0.0551 (10)
H1A	0.4027	0.9023	0.1664	0.066*
C2	0.3536 (5)	1.0670 (4)	0.1313 (3)	0.0636 (11)
H2A	0.2637	1.0748	0.0993	0.076*
C3	0.4042 (5)	1.1584 (3)	0.1393 (3)	0.0609 (11)
H3A	0.3492	1.2293	0.1127	0.073*
C4	0.5377 (4)	1.1433 (3)	0.1875 (3)	0.0477 (9)
H4A	0.5729	1.2036	0.1949	0.057*
C5	0.6183 (4)	1.0380 (3)	0.2245 (2)	0.0357 (7)
C6	0.7672 (4)	1.0124 (3)	0.2716 (2)	0.0350 (7)
C7	0.9746 (4)	1.0178 (3)	0.3288 (2)	0.0364 (7)
C8	1.0995 (4)	1.0544 (3)	0.3656 (2)	0.0378 (7)
C9	1.1963 (4)	0.9778 (3)	0.4322 (3)	0.0456 (8)
H9A	1.1866	0.9012	0.4534	0.055*
C10	1.3081 (4)	1.0159 (3)	0.4672 (3)	0.0549 (10)
H10A	1.3723	0.9627	0.5123	0.066*
C11	1.2366 (5)	1.1968 (3)	0.3747 (3)	0.0597 (11)

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H11A	1.2510	1.2728	0.3531	0.072*
C12	1.1207 (5)	1.1674 (3)	0.3365 (3)	0.0512 (9)
H12A	1.0575	1.2223	0.2918	0.061*
C13	1.0318 (4)	0.8471 (3)	0.1141 (3)	0.0522 (9)
H13A	1.0659	0.8844	0.1482	0.063*
C14	1.1280 (5)	0.8449 (3)	0.0311 (3)	0.0601 (11)
H14A	1.2243	0.8807	0.0088	0.072*
C15	1.0810 (5)	0.7890 (3)	-0.0194 (3)	0.0552 (10)
H15A	1.1451	0.7859	-0.0761	0.066*
C16	0.9368 (4)	0.7374 (3)	0.0155 (3)	0.0447 (8)
H16A	0.9026	0.6980	-0.0166	0.054*
C17	0.8445 (4)	0.7457 (3)	0.0990 (2)	0.0372 (7)
C18	0.6844 (4)	0.6996 (3)	0.1399 (2)	0.0360 (7)
C19	0.4638 (4)	0.6307 (3)	0.1630 (2)	0.0370 (7)
C20	0.3338 (4)	0.5731 (3)	0.1523 (3)	0.0389 (8)
C21	0.2038 (4)	0.5364 (3)	0.2252 (3)	0.0484 (9)
H21A	0.1938	0.5495	0.2828	0.058*
C22	0.0886 (5)	0.4799 (3)	0.2112 (3)	0.0583 (10)
H22A	0.0012	0.4566	0.2608	0.070*
C23	0.2181 (5)	0.4939 (4)	0.0620 (3)	0.0633 (11)
H23A	0.2245	0.4800	0.0051	0.076*
C24	0.3379 (5)	0.5521 (3)	0.0684 (3)	0.0527 (10)
H24A	0.4212	0.5771	0.0164	0.063*
C25	0.8006 (5)	0.6203 (3)	0.4815 (3)	0.0540 (10)
H25A	0.8431	0.6727	0.5008	0.065*
H25B	0.8377	0.5446	0.5230	0.065*
C26	0.6162 (5)	0.6348 (3)	0.4945 (3)	0.0562 (10)
H26A	0.5734	0.5796	0.4789	0.067*
H26B	0.5750	0.6239	0.5623	0.067*
N1	0.5690 (3)	0.9484 (2)	0.2168 (2)	0.0425 (7)
N2	0.8401 (3)	0.9090 (2)	0.3005 (2)	0.0379 (6)
N3	0.9767 (3)	0.9114 (2)	0.3379 (2)	0.0391 (6)
N4	0.8461 (3)	1.0852 (2)	0.2877 (2)	0.0384 (6)
N5	1.3297 (4)	1.1242 (3)	0.4403 (3)	0.0584 (9)
N6	0.8917 (3)	0.7990 (2)	0.1493 (2)	0.0425 (7)
N7	0.6034 (3)	0.7089 (2)	0.2217 (2)	0.0392 (6)
N8	0.4580 (3)	0.6639 (2)	0.2376 (2)	0.0405 (6)
N9	0.6030 (3)	0.6513 (2)	0.0994 (2)	0.0411 (7)
N10	0.0943 (4)	0.4566 (3)	0.1321 (3)	0.0618 (9)
N11	0.8616 (3)	0.6409 (2)	0.3777 (2)	0.0418 (7)
H11B	0.9644	0.6557	0.3761	0.050*
H11C	0.8363	0.5759	0.3779	0.050*
N12	0.5630 (3)	0.7487 (2)	0.4287 (2)	0.0466 (7)
H12B	0.5435	0.7894	0.4666	0.056*
H12C	0.4597	0.7511	0.4173	0.056*
C27	0.3055 (11)	0.6293 (5)	0.7695 (7)	0.204 (5)
H27A	0.2189	0.6451	0.8151	0.245*
H27B	0.4091	0.6254	0.7908	0.245*
H27C	0.2926	0.5587	0.7666	0.245*

O1	0.2993 (5)	0.7199 (3)	0.6702 (3)	0.1036 (12)
H1B	0.2698	0.7879	0.6733	0.124*
O1W	0.2078 (3)	0.7151 (2)	0.37517 (18)	0.0555 (7)
H1WA	0.1489	0.7772	0.3615	0.067*
H1WB	0.2587	0.7179	0.3197	0.067*
O2W	0.1847 (4)	0.6019 (2)	0.5789 (2)	0.0810 (10)
H2WA	0.2278	0.6300	0.6105	0.097*
H2WB	0.1918	0.6143	0.5181	0.097*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0371 (2)	0.0371 (2)	0.0476 (2)	-0.00668 (16)	-0.01032 (17)	-0.01898 (18)
C1	0.052 (2)	0.050 (2)	0.069 (3)	-0.0071 (18)	-0.028 (2)	-0.020 (2)
C2	0.054 (2)	0.061 (3)	0.076 (3)	-0.001 (2)	-0.039 (2)	-0.016 (2)
C3	0.053 (2)	0.050 (2)	0.074 (3)	0.0077 (19)	-0.027 (2)	-0.014 (2)
C4	0.046 (2)	0.039 (2)	0.059 (2)	-0.0010 (16)	-0.0134 (18)	-0.0178 (17)
C5	0.0318 (17)	0.0397 (18)	0.0380 (17)	-0.0050 (14)	-0.0062 (14)	-0.0158 (15)
C6	0.0333 (17)	0.0350 (18)	0.0391 (17)	-0.0033 (14)	-0.0081 (14)	-0.0149 (14)
C7	0.0344 (18)	0.0375 (18)	0.0420 (18)	-0.0040 (14)	-0.0065 (14)	-0.0192 (15)
C8	0.0310 (17)	0.0443 (19)	0.0476 (19)	-0.0059 (14)	-0.0057 (15)	-0.0262 (16)
C9	0.0368 (19)	0.047 (2)	0.061 (2)	-0.0030 (16)	-0.0128 (17)	-0.0254 (18)
C10	0.042 (2)	0.064 (3)	0.068 (3)	0.0016 (19)	-0.0218 (19)	-0.031 (2)
C11	0.060 (3)	0.051 (2)	0.083 (3)	-0.013 (2)	-0.019 (2)	-0.035 (2)
C12	0.053 (2)	0.043 (2)	0.067 (2)	-0.0042 (17)	-0.0212 (19)	-0.0254 (19)
C13	0.044 (2)	0.052 (2)	0.064 (2)	-0.0126 (18)	-0.0050 (19)	-0.024 (2)
C14	0.041 (2)	0.063 (3)	0.070 (3)	-0.0196 (19)	0.003 (2)	-0.019 (2)
C15	0.043 (2)	0.066 (3)	0.055 (2)	-0.0031 (19)	0.0010 (18)	-0.025 (2)
C16	0.0366 (19)	0.053 (2)	0.047 (2)	-0.0043 (16)	-0.0047 (15)	-0.0214 (17)
C17	0.0324 (17)	0.0382 (18)	0.0387 (17)	-0.0017 (14)	-0.0086 (14)	-0.0112 (15)
C18	0.0346 (17)	0.0354 (18)	0.0393 (17)	-0.0014 (14)	-0.0034 (14)	-0.0168 (15)
C19	0.0341 (18)	0.0350 (18)	0.0436 (18)	-0.0027 (14)	-0.0032 (15)	-0.0177 (15)
C20	0.0337 (18)	0.0342 (18)	0.052 (2)	0.0006 (14)	-0.0074 (15)	-0.0208 (16)
C21	0.045 (2)	0.053 (2)	0.052 (2)	-0.0113 (17)	-0.0020 (17)	-0.0247 (18)
C22	0.047 (2)	0.058 (2)	0.070 (3)	-0.0210 (19)	0.003 (2)	-0.023 (2)
C23	0.064 (3)	0.069 (3)	0.076 (3)	-0.016 (2)	-0.006 (2)	-0.046 (2)
C24	0.046 (2)	0.062 (2)	0.064 (2)	-0.0148 (19)	0.0027 (18)	-0.039 (2)
C25	0.055 (2)	0.054 (2)	0.050 (2)	0.0056 (19)	-0.0161 (18)	-0.0174 (19)
C26	0.054 (2)	0.059 (3)	0.053 (2)	-0.014 (2)	0.0035 (19)	-0.019 (2)
N1	0.0390 (16)	0.0405 (16)	0.0522 (17)	-0.0042 (13)	-0.0187 (13)	-0.0166 (14)
N2	0.0332 (15)	0.0340 (15)	0.0532 (17)	-0.0018 (12)	-0.0155 (13)	-0.0199 (13)
N3	0.0335 (15)	0.0385 (16)	0.0516 (17)	-0.0014 (12)	-0.0130 (13)	-0.0212 (13)
N4	0.0373 (15)	0.0340 (15)	0.0491 (16)	-0.0019 (12)	-0.0140 (13)	-0.0181 (13)
N5	0.0494 (19)	0.066 (2)	0.076 (2)	-0.0097 (17)	-0.0190 (17)	-0.0386 (19)
N6	0.0380 (16)	0.0419 (16)	0.0487 (17)	-0.0085 (13)	-0.0056 (13)	-0.0169 (14)
N7	0.0336 (15)	0.0425 (16)	0.0463 (16)	-0.0072 (12)	-0.0037 (12)	-0.0213 (13)
N8	0.0341 (15)	0.0464 (17)	0.0470 (16)	-0.0084 (13)	0.0008 (12)	-0.0252 (14)
N9	0.0357 (15)	0.0474 (17)	0.0475 (16)	-0.0072 (13)	-0.0029 (13)	-0.0254 (14)

supplementary materials

N10	0.054 (2)	0.061 (2)	0.084 (2)	-0.0211 (17)	-0.0054 (19)	-0.038 (2)
N11	0.0400 (16)	0.0351 (15)	0.0536 (17)	-0.0051 (12)	-0.0088 (13)	-0.0188 (13)
N12	0.0365 (16)	0.0554 (19)	0.0568 (18)	-0.0042 (14)	-0.0047 (14)	-0.0313 (16)
C27	0.250 (10)	0.067 (4)	0.335 (13)	0.000 (5)	-0.219 (10)	-0.048 (6)
O1	0.139 (3)	0.066 (2)	0.123 (3)	0.013 (2)	-0.044 (3)	-0.051 (2)
O1W	0.0514 (16)	0.0555 (16)	0.0523 (15)	0.0069 (12)	-0.0001 (12)	-0.0199 (13)
O2W	0.119 (3)	0.068 (2)	0.0630 (19)	-0.0367 (19)	-0.0044 (18)	-0.0249 (16)

Geometric parameters (Å, °)

Zn1—N7	2.096 (3)	C16—H16A	0.9300
Zn1—N2	2.103 (2)	C17—N6	1.343 (4)
Zn1—N11	2.133 (3)	C17—C18	1.473 (4)
Zn1—N12	2.148 (3)	C18—N7	1.329 (4)
Zn1—N1	2.269 (3)	C18—N9	1.341 (4)
Zn1—N6	2.293 (3)	C19—N8	1.340 (4)
C1—N1	1.334 (4)	C19—N9	1.347 (4)
C1—C2	1.370 (5)	C19—C20	1.470 (4)
C1—H1A	0.9300	C20—C24	1.379 (5)
C2—C3	1.376 (6)	C20—C21	1.381 (5)
C2—H2A	0.9300	C21—C22	1.382 (5)
C3—C4	1.379 (5)	C21—H21A	0.9300
C3—H3A	0.9300	C22—N10	1.324 (5)
C4—C5	1.374 (5)	C22—H22A	0.9300
C4—H4A	0.9300	C23—N10	1.325 (5)
C5—N1	1.347 (4)	C23—C24	1.377 (5)
C5—C6	1.465 (4)	C23—H23A	0.9300
C6—N2	1.324 (4)	C24—H24A	0.9300
C6—N4	1.347 (4)	C25—N11	1.470 (4)
C7—N3	1.335 (4)	C25—C26	1.507 (5)
C7—N4	1.348 (4)	C25—H25A	0.9700
C7—C8	1.475 (4)	C25—H25B	0.9700
C8—C9	1.374 (5)	C26—N12	1.468 (5)
C8—C12	1.387 (5)	C26—H26A	0.9700
C9—C10	1.380 (5)	C26—H26B	0.9700
C9—H9A	0.9300	N2—N3	1.364 (3)
C10—N5	1.335 (5)	N7—N8	1.366 (4)
C10—H10A	0.9300	N11—H11B	0.8999
C11—N5	1.330 (5)	N11—H11C	0.9001
C11—C12	1.374 (5)	N12—H12B	0.9006
C11—H11A	0.9300	N12—H12C	0.8999
C12—H12A	0.9300	C27—O1	1.485 (8)
C13—N6	1.330 (4)	C27—H27A	0.9600
C13—C14	1.361 (5)	C27—H27B	0.9600
C13—H13A	0.9300	C27—H27C	0.9600
C14—C15	1.372 (5)	O1—H1B	0.9002
C14—H14A	0.9300	O1W—H1WA	0.8500
C15—C16	1.379 (5)	O1W—H1WB	0.8506
C15—H15A	0.9300	O2W—H2WA	0.8501

C16—C17	1.379 (5)	O2W—H2WB	0.8506
N7—Zn1—N2	156.47 (11)	N8—C19—N9	114.0 (3)
N7—Zn1—N11	99.48 (10)	N8—C19—C20	123.6 (3)
N2—Zn1—N11	98.05 (10)	N9—C19—C20	122.4 (3)
N7—Zn1—N12	101.58 (10)	C24—C20—C21	116.9 (3)
N2—Zn1—N12	96.28 (11)	C24—C20—C19	121.0 (3)
N11—Zn1—N12	81.99 (11)	C21—C20—C19	122.2 (3)
N7—Zn1—N1	89.05 (10)	C20—C21—C22	119.0 (3)
N2—Zn1—N1	74.90 (10)	C20—C21—H21A	120.5
N11—Zn1—N1	170.61 (10)	C22—C21—H21A	120.5
N12—Zn1—N1	92.50 (11)	N10—C22—C21	124.5 (4)
N7—Zn1—N6	75.35 (10)	N10—C22—H22A	117.7
N2—Zn1—N6	88.45 (10)	C21—C22—H22A	117.7
N11—Zn1—N6	92.21 (10)	N10—C23—C24	124.0 (4)
N12—Zn1—N6	172.96 (10)	N10—C23—H23A	118.0
N1—Zn1—N6	93.77 (10)	C24—C23—H23A	118.0
N1—C1—C2	123.1 (3)	C23—C24—C20	119.8 (4)
N1—C1—H1A	118.5	C23—C24—H24A	120.1
C2—C1—H1A	118.5	C20—C24—H24A	120.1
C1—C2—C3	118.7 (3)	N11—C25—C26	109.3 (3)
C1—C2—H2A	120.6	N11—C25—H25A	109.8
C3—C2—H2A	120.6	C26—C25—H25A	109.8
C2—C3—C4	118.9 (4)	N11—C25—H25B	109.8
C2—C3—H3A	120.5	C26—C25—H25B	109.8
C4—C3—H3A	120.5	H25A—C25—H25B	108.3
C5—C4—C3	119.2 (3)	N12—C26—C25	108.8 (3)
C5—C4—H4A	120.4	N12—C26—H26A	109.9
C3—C4—H4A	120.4	C25—C26—H26A	109.9
N1—C5—C4	122.0 (3)	N12—C26—H26B	109.9
N1—C5—C6	113.5 (3)	C25—C26—H26B	109.9
C4—C5—C6	124.5 (3)	H26A—C26—H26B	108.3
N2—C6—N4	113.5 (3)	C1—N1—C5	118.1 (3)
N2—C6—C5	119.7 (3)	C1—N1—Zn1	127.8 (2)
N4—C6—C5	126.8 (3)	C5—N1—Zn1	114.1 (2)
N3—C7—N4	114.2 (3)	C6—N2—N3	106.6 (2)
N3—C7—C8	121.6 (3)	C6—N2—Zn1	117.1 (2)
N4—C7—C8	124.1 (3)	N3—N2—Zn1	136.0 (2)
C9—C8—C12	117.5 (3)	C7—N3—N2	104.7 (3)
C9—C8—C7	121.1 (3)	C6—N4—C7	101.1 (3)
C12—C8—C7	121.4 (3)	C11—N5—C10	115.7 (3)
C8—C9—C10	119.3 (3)	C13—N6—C17	117.3 (3)
C8—C9—H9A	120.4	C13—N6—Zn1	129.4 (2)
C10—C9—H9A	120.4	C17—N6—Zn1	113.2 (2)
N5—C10—C9	124.1 (4)	C18—N7—N8	106.3 (2)
N5—C10—H10A	117.9	C18—N7—Zn1	117.0 (2)
C9—C10—H10A	117.9	N8—N7—Zn1	136.7 (2)
N5—C11—C12	124.6 (4)	C19—N8—N7	104.7 (2)
N5—C11—H11A	117.7	C18—N9—C19	101.3 (3)
C12—C11—H11A	117.7	C22—N10—C23	115.9 (3)

supplementary materials

C11—C12—C8	118.9 (4)	C25—N11—Zn1	107.1 (2)
C11—C12—H12A	120.6	C25—N11—H11B	99.2
C8—C12—H12A	120.6	Zn1—N11—H11B	112.6
N6—C13—C14	123.6 (4)	C25—N11—H11C	97.5
N6—C13—H13A	118.2	Zn1—N11—H11C	113.1
C14—C13—H13A	118.2	H11B—N11—H11C	123.5
C13—C14—C15	119.1 (4)	C26—N12—Zn1	107.1 (2)
C13—C14—H14A	120.5	C26—N12—H12B	104.9
C15—C14—H14A	120.5	Zn1—N12—H12B	127.8
C14—C15—C16	118.8 (4)	C26—N12—H12C	110.1
C14—C15—H15A	120.6	Zn1—N12—H12C	107.7
C16—C15—H15A	120.6	H12B—N12—H12C	98.5
C17—C16—C15	118.5 (3)	O1—C27—H27A	109.5
C17—C16—H16A	120.7	O1—C27—H27B	109.5
C15—C16—H16A	120.7	H27A—C27—H27B	109.5
N6—C17—C16	122.7 (3)	O1—C27—H27C	109.5
N6—C17—C18	113.9 (3)	H27A—C27—H27C	109.5
C16—C17—C18	123.4 (3)	H27B—C27—H27C	109.5
N7—C18—N9	113.8 (3)	C27—O1—H1B	112.0
N7—C18—C17	120.1 (3)	H1WA—O1W—H1WB	104.0
N9—C18—C17	126.0 (3)	H2WA—O2W—H2WB	133.0

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N11—H11B \cdots O1W ⁱ	0.90	2.27	3.166 (4)	172
N11—H11C \cdots O2W ⁱⁱ	0.90	2.17	3.034 (4)	161
N12—H12B \cdots N5 ⁱⁱⁱ	0.90	2.54	3.321 (4)	146
N12—H12C \cdots O1W	0.90	2.45	3.331 (4)	165
O1—H1B \cdots N4 ^{iv}	0.90	2.02	2.897 (4)	163
O1W—H1WA \cdots N3 ^v	0.85	2.04	2.887 (4)	171
O1W—H1WB \cdots N8	0.85	2.09	2.859 (4)	150
O2W—H2WA \cdots O1	0.85	1.94	2.778 (4)	169
O2W—H2WB \cdots O1W	0.85	2.00	2.787 (4)	153

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

Fig. 1

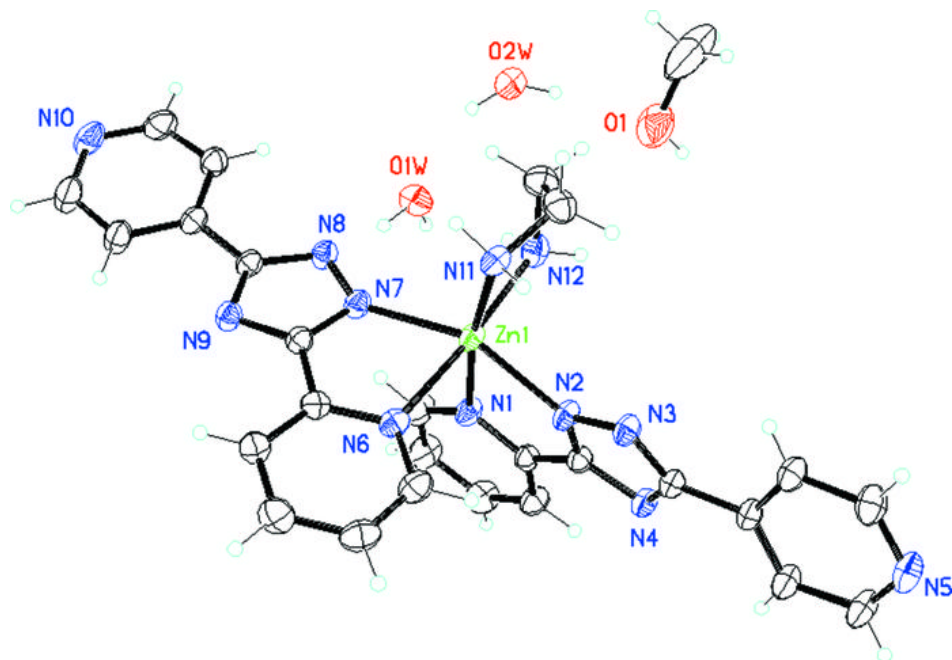


Fig. 2

