

(Dicyanamido)[tris(2-pyridylmethyl)-amine]zinc(II) perchlorateHong Li,^{a*} Hong Yan Zhao^b and Shi Guo Zhang^a^aDepartment of Chemistry and Chemical Engineering, Institute of Materials Chemistry, Binzhou University, Binzhou 256603, People's Republic of China, and^bDepartment of Chemistry, Shandong Normal University, Jinan 250014, People's Republic of China

Correspondence e-mail: honglizhang1968@yahoo.cn

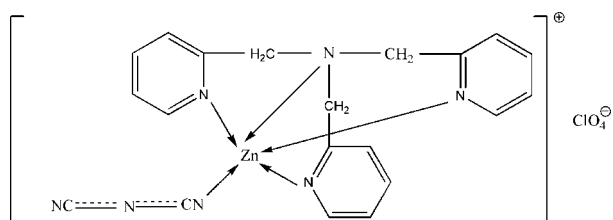
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; disorder in main residue; R factor = 0.043; wR factor = 0.107; data-to-parameter ratio = 15.6.

In the title complex, $[\text{Zn}(\text{C}_2\text{N}_3)(\text{C}_{18}\text{H}_{18}\text{N}_4)]\text{ClO}_4$, the Zn^{II} ion has a slightly distorted trigonal-bipyramidal ZnN_5 coordination geometry. The crystal structure is stabilized by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds. In addition, there are relatively close contacts between the O atoms of the perchlorate anion and symmetry-related pyridine rings [$\text{O}\cdots\text{Cg} = 3.179$ (3) and 3.236 (3) Å, where Cg is the centroid of a pyridine ring], and between the terminal N atom of the dicyanamide ligand and pyridine rings [$\text{N}\cdots\text{Cg} = 3.381$ (4)– 3.761 (3) Å]. The central N atom of the dicyanamide ligand is disordered over two sites in an approximately 0.6:0.4 ratio.

Related literature

For related literature, see: Makowska-Grzyska *et al.* (2003); Sun *et al.* (2003); Martin *et al.* (2001).

**Experimental***Crystal data* $[\text{Zn}(\text{C}_2\text{N}_3)(\text{C}_{18}\text{H}_{18}\text{N}_4)]\text{ClO}_4$ $M_r = 521.23$ Monoclinic, $P2_1/c$ $a = 13.931$ (2) Å $b = 10.8578$ (18) Å $c = 14.653$ (2) Å $\beta = 91.590$ (3)° $V = 2215.5$ (6) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 1.27$ mm⁻¹ $T = 298$ (2) K $0.30 \times 0.20 \times 0.18$ mm*Data collection*

Bruker SMART APEX CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\text{min}} = 0.702$, $T_{\text{max}} = 0.803$

12346 measured reflections

4800 independent reflections

3352 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.035$ *Refinement* $R[F^2 > 2\sigma(F^2)] = 0.043$ $wR(F^2) = 0.106$ $S = 0.99$

4800 reflections

308 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.36$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³**Table 1**

Selected geometric parameters (Å, °).

N1–Zn1	2.053 (2)	N4–Zn1	2.215 (2)
N2–Zn1	2.048 (2)	N5–Zn1	2.021 (3)
N3–Zn1	2.059 (2)		
N5–Zn1–N2	101.94 (10)	N1–Zn1–N3	112.99 (9)
N5–Zn1–N1	100.96 (11)	N5–Zn1–N4	179.41 (10)
N2–Zn1–N1	118.19 (9)	N2–Zn1–N4	78.60 (9)
N5–Zn1–N3	100.98 (10)	N1–Zn1–N4	78.95 (9)
N2–Zn1–N3	117.58 (9)	N3–Zn1–N4	78.55 (9)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C3–H3 \cdots O4 ⁱ	0.93	2.53	3.272 (4)	138
C7–H7B \cdots O2 ⁱⁱ	0.97	2.59	3.455 (4)	148
C10–H10 \cdots O1 ⁱⁱⁱ	0.93	2.58	3.511 (5)	179
C13–H13A \cdots N6 ^{iv}	0.97	2.61	3.457 (5)	146
C16–H16 \cdots N7 ^v	0.93	2.48	3.412 (18)	178

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2594).

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supplementary materials

Acta Cryst. (2008). E64, m495 [doi:10.1107/S1600536808004741]

(Dicyanamido)[tris(2-pyridylmethyl)amine]zinc(II) perchlorate

H. Li, H. Y. Zhao and S. G. Zhang

Comment

Tris[(2-pyridyl)methylene]amine is a very common terminal ligand and many complexes containing this ligand have been reported, including some Zn(II) complexes with perchlorate anions (*e.g.* Makowska-Grzyska *et al.*, 2003) such as in the title compound. The dicyanamide anion can play a role as bridging ligand to form multi-nuclear complexes (*e.g.* Sun *et al.*, 2003; Martin *et al.*, 2001). As part of our work we wanted to prepare a coordination polymer with dicyanamide group acting as a bridging ligand and tris[(2-pyridyl)methylene]amine as terminal ligand, but instead we obtained the title mononuclear five-coordinated Zn(II) complex (I) and its crystal structure is reported herein. At this time there appears to be no other published examples of crystal structures of complexes of the two above mentioned ligands both coordinated to a transition metal.

The title complex is shown in Fig. 1. The Zn^{II} ion is in a slightly distorted trigonal-bipyramidal coordination geometry. In the crystal structure, there are weak hydrogen bonds formed between complex cations and perchlorate anions, and between symmetry related complex cations (Fig. 2). In addition there also exists interactions between Cl—O bonds and π -rings systems and between C—N bonds and π -ring systems, and the relevant distances (Å) are as follows: Cl1—O2...Cg1ⁱ = 3.236 (3), Cl1—O2...Cg1ⁱ_{perp} = 3.120; Cl1—O4...Cg2ⁱ = 3.179 (3), Cl1—O4...Cg2ⁱ_{perp} = 3.111; C20—N6...Cg2ⁱⁱ = 3.381 (4), C20—N6...Cg2ⁱⁱ_{perp} = 3.360; C20—N6...Cg1ⁱⁱⁱ = 3.453 (4), C20—N6...Cg1ⁱⁱⁱ_{perp} = 3.156; C20—N6...Cg3ⁱⁱⁱ = 3.761 (3), C20—N6...Cg3ⁱⁱⁱ_{perp} = 3.365; (Cg1, Cg2 and Cg3 are the centroids of N2/C1—C5 ring, N1/C8—C12 ring and N3/C14—C18 ring, respectively; A—B...Cg_j_{perp} is the perpendicular distance from B atom to ring j; symmetry codes: (i) $x, -1 + y, z$; (ii) $1 - x, 2 - y, -z$; (iii) $1 - x, 1/2 + y, 1/2 - z$).

Experimental

A 10 ml methanol solution of tris[(2-pyridyl)methylene]amine (0.2103 g, 0.72 mmol) was added into 20 ml H₂O solution containing Zn(ClO₄)₆H₂O (0.2621 g, 0.70 mmol) and sodium dicyanamide (0.0645 g, 0.72 mmol), and the mixture was stirred for a few minutes. Colorless single crystals were obtained after the filtrate had been allowed to stand at room temperature for 10 d.

Refinement

The central N atom of the dicyanamide ligand is disordered over two sites in a 0.40 (7): 60 (7) ratio (sum constrained to unity). H atoms were placed in calculated positions (C—H = 0.97 Å for methylene group and C—H = 0.93 Å for other H atoms) and refined as riding with $U_{\text{iso}} = 1.2 U_{\text{eq}}(\text{C})$.

Figures

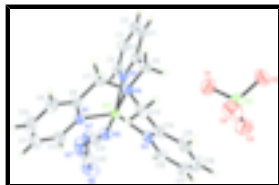


Fig. 1. View of complex (I), showing the the atom numbering scheme with thermal ellipsoids drawn at the 30% probability level.

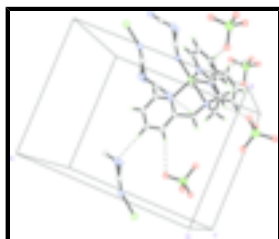


Fig. 2. Part of the crystal structure showing weak hydrogen bonds as dashed lines.

(Dicyanamido)[tris(2-pyridylmethyl)amine]zinc(II) perchlorate

Crystal data

$[\text{Zn}(\text{C}_2\text{N}_3)(\text{C}_{18}\text{H}_{18}\text{N}_4)]\text{ClO}_4$

$M_r = 521.23$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 13.931\ (2)\ \text{\AA}$

$b = 10.8578\ (18)\ \text{\AA}$

$c = 14.653\ (2)\ \text{\AA}$

$\beta = 91.590\ (3)^\circ$

$V = 2215.5\ (6)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1064$

$D_x = 1.563\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2616 reflections

$\theta = 2.3\text{--}22.0^\circ$

$\mu = 1.27\ \text{mm}^{-1}$

$T = 298\ (2)\ \text{K}$

Block, colorless

$0.30 \times 0.20 \times 0.18\ \text{mm}$

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298\ (2)\ \text{K}$

φ and ω scans

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

$T_{\min} = 0.702$, $T_{\max} = 0.803$

12346 measured reflections

4800 independent reflections

3352 reflections with $I > 2\sigma(I)$

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

$\theta_{\max} = 27.0^\circ$

$\theta_{\min} = 2.3^\circ$

$h = -15 \rightarrow 17$

$k = -13 \rightarrow 12$

$l = -18 \rightarrow 16$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.043$$

$$wR(F^2) = 0.106$$

$$S = 0.99$$

4800 reflections

308 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.053P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.36 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$$

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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.0860 (2)	0.9139 (3)	0.2853 (2)	0.0612 (9)	
H1	0.0337	0.8627	0.2947	0.073*	
C2	0.1044 (3)	1.0115 (4)	0.3423 (2)	0.0697 (10)	
H2	0.0648	1.0272	0.3910	0.084*	
C3	0.1813 (3)	1.0854 (3)	0.3270 (2)	0.0674 (9)	
H3	0.1952	1.1517	0.3654	0.081*	
C4	0.2375 (2)	1.0607 (3)	0.2547 (2)	0.0545 (8)	
H4	0.2894	1.1122	0.2439	0.065*	
C5	0.14649 (19)	0.8927 (3)	0.21361 (19)	0.0461 (7)	
C6	0.1355 (2)	0.7823 (3)	0.1528 (2)	0.0562 (8)	
H6A	0.1669	0.7122	0.1816	0.067*	
H6B	0.0678	0.7629	0.1445	0.067*	
C7	0.1151 (2)	0.8761 (3)	0.0017 (2)	0.0629 (9)	
H7A	0.0784	0.9345	0.0367	0.076*	
H7B	0.0702	0.8217	-0.0301	0.076*	
C8	0.1729 (2)	0.9441 (3)	-0.0664 (2)	0.0519 (7)	
C9	0.1372 (3)	0.9713 (3)	-0.1530 (2)	0.0691 (9)	
H9	0.0769	0.9431	-0.1722	0.083*	
C10	0.1913 (4)	1.0397 (4)	-0.2098 (2)	0.0812 (11)	
H10	0.1684	1.0590	-0.2683	0.097*	
C11	0.2798 (3)	1.0797 (3)	-0.1801 (2)	0.0786 (11)	

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H11	0.3177	1.1267	-0.2180	0.094*	
C12	0.3118 (3)	1.0497 (3)	-0.0937 (2)	0.0617 (8)	
H12	0.3719	1.0774	-0.0736	0.074*	
C13	0.2121 (2)	0.6901 (3)	0.0215 (2)	0.0628 (9)	
H13A	0.2159	0.7016	-0.0439	0.075*	
H13B	0.1676	0.6233	0.0324	0.075*	
C14	0.3093 (2)	0.6574 (3)	0.0606 (2)	0.0554 (8)	
C15	0.3413 (4)	0.5360 (3)	0.0654 (3)	0.0844 (12)	
H15	0.3010	0.4718	0.0469	0.101*	
C16	0.4314 (4)	0.5126 (4)	0.0972 (3)	0.1041 (15)	
H16	0.4535	0.4318	0.1008	0.125*	
C17	0.4900 (3)	0.6072 (4)	0.1240 (3)	0.0947 (14)	
H17	0.5526	0.5922	0.1448	0.114*	
C18	0.4545 (2)	0.7252 (3)	0.1195 (2)	0.0681 (9)	
H18	0.4936	0.7899	0.1392	0.082*	
C19	0.4657 (2)	1.1134 (3)	0.1232 (2)	0.0594 (8)	
C20	0.5964 (3)	1.2341 (3)	0.1587 (2)	0.0670 (9)	
C11	0.13251 (5)	0.26686 (7)	0.06625 (5)	0.0551 (2)	
N1	0.25963 (17)	0.9822 (2)	-0.03743 (15)	0.0474 (6)	
N2	0.22133 (15)	0.9657 (2)	0.19860 (14)	0.0425 (5)	
N3	0.36571 (17)	0.7501 (2)	0.08790 (16)	0.0500 (6)	
N4	0.17686 (15)	0.8038 (2)	0.06381 (15)	0.0461 (6)	
N5	0.42095 (18)	1.0295 (3)	0.11270 (19)	0.0626 (7)	
N6	0.6718 (3)	1.2592 (3)	0.1805 (2)	0.1036 (12)	
N7	0.5015 (14)	1.214 (2)	0.157 (3)	0.066 (7)	0.40 (7)
N7'	0.5148 (16)	1.2179 (15)	0.116 (3)	0.100 (5)	0.60 (7)
O1	0.1054 (2)	0.3925 (2)	0.06831 (17)	0.0854 (8)	
O2	0.08216 (17)	0.2017 (2)	0.13439 (16)	0.0821 (7)	
O3	0.23268 (17)	0.2569 (3)	0.0827 (2)	0.0980 (8)	
O4	0.1080 (2)	0.2177 (2)	-0.02084 (16)	0.0905 (8)	
Zn1	0.30405 (2)	0.92245 (3)	0.08979 (2)	0.04138 (12)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0467 (17)	0.086 (3)	0.0509 (19)	0.0100 (16)	0.0088 (14)	0.0197 (18)
C2	0.081 (3)	0.086 (3)	0.0423 (19)	0.024 (2)	0.0134 (17)	0.0048 (18)
C3	0.089 (3)	0.067 (2)	0.0456 (19)	0.0119 (19)	0.0039 (18)	-0.0042 (16)
C4	0.0615 (19)	0.056 (2)	0.0459 (18)	0.0023 (14)	-0.0017 (15)	0.0004 (14)
C5	0.0401 (15)	0.0575 (18)	0.0404 (16)	0.0022 (13)	-0.0029 (12)	0.0081 (13)
C6	0.0447 (17)	0.068 (2)	0.0564 (19)	-0.0167 (15)	0.0066 (14)	0.0053 (15)
C7	0.0424 (17)	0.090 (2)	0.056 (2)	-0.0105 (16)	-0.0095 (15)	0.0053 (18)
C8	0.0528 (18)	0.0588 (19)	0.0437 (17)	0.0085 (14)	-0.0041 (14)	0.0003 (14)
C9	0.083 (2)	0.076 (2)	0.048 (2)	0.0142 (19)	-0.0125 (18)	-0.0030 (18)
C10	0.123 (4)	0.075 (3)	0.045 (2)	0.025 (2)	-0.006 (2)	0.0083 (18)
C11	0.120 (3)	0.062 (2)	0.055 (2)	0.005 (2)	0.020 (2)	0.0158 (17)
C12	0.074 (2)	0.0515 (19)	0.061 (2)	-0.0001 (16)	0.0158 (17)	0.0026 (15)
C13	0.074 (2)	0.056 (2)	0.059 (2)	-0.0263 (17)	0.0047 (17)	-0.0095 (15)

C14	0.075 (2)	0.0442 (17)	0.0481 (17)	-0.0047 (15)	0.0153 (15)	-0.0035 (14)
C15	0.119 (4)	0.046 (2)	0.089 (3)	0.001 (2)	0.030 (3)	0.0011 (19)
C16	0.138 (4)	0.067 (3)	0.108 (4)	0.043 (3)	0.033 (3)	0.018 (3)
C17	0.090 (3)	0.100 (4)	0.095 (3)	0.048 (3)	0.007 (2)	0.012 (3)
C18	0.061 (2)	0.073 (2)	0.070 (2)	0.0125 (17)	0.0050 (18)	0.0036 (18)
C19	0.0489 (18)	0.0545 (18)	0.074 (2)	-0.0062 (12)	-0.0102 (16)	0.0012 (17)
C20	0.071 (2)	0.058 (2)	0.072 (2)	-0.0248 (18)	-0.0010 (19)	-0.0053 (17)
C11	0.0535 (4)	0.0568 (5)	0.0552 (5)	-0.0035 (3)	0.0042 (4)	0.0010 (4)
N1	0.0524 (14)	0.0476 (14)	0.0424 (13)	0.0022 (11)	0.0063 (11)	0.0037 (11)
N2	0.0419 (13)	0.0463 (13)	0.0391 (13)	0.0032 (10)	-0.0033 (10)	0.0028 (10)
N3	0.0524 (15)	0.0494 (14)	0.0484 (15)	0.0025 (11)	0.0044 (11)	0.0023 (11)
N4	0.0411 (13)	0.0553 (15)	0.0421 (13)	-0.0109 (11)	0.0025 (10)	0.0002 (11)
N5	0.0485 (15)	0.0609 (16)	0.0784 (19)	-0.0141 (11)	0.0000 (13)	-0.0056 (14)
N6	0.090 (2)	0.118 (3)	0.103 (3)	-0.050 (2)	0.010 (2)	-0.037 (2)
N7	0.060 (6)	0.040 (8)	0.096 (15)	-0.005 (5)	-0.014 (8)	0.007 (6)
N7'	0.089 (7)	0.082 (6)	0.128 (15)	-0.040 (5)	-0.042 (8)	0.052 (7)
O1	0.107 (2)	0.0644 (16)	0.0849 (19)	0.0212 (14)	0.0130 (15)	0.0035 (13)
O2	0.0737 (16)	0.1009 (19)	0.0720 (16)	-0.0049 (13)	0.0058 (13)	0.0369 (14)
O3	0.0550 (15)	0.0947 (19)	0.144 (2)	-0.0051 (13)	0.0035 (15)	0.0138 (17)
O4	0.110 (2)	0.098 (2)	0.0639 (16)	-0.0235 (16)	0.0170 (14)	-0.0221 (14)
Zn1	0.03599 (18)	0.0427 (2)	0.0454 (2)	-0.00542 (13)	0.00088 (13)	-0.00063 (14)

Geometric parameters (Å, °)

C1—C2	1.368 (5)	C13—C14	1.498 (4)
C1—C5	1.384 (4)	C13—H13A	0.9700
C1—H1	0.9300	C13—H13B	0.9700
C2—C3	1.362 (5)	C14—N3	1.332 (4)
C2—H2	0.9300	C14—C15	1.392 (5)
C3—C4	1.362 (4)	C15—C16	1.352 (6)
C3—H3	0.9300	C15—H15	0.9300
C4—N2	1.334 (3)	C16—C17	1.363 (6)
C4—H4	0.9300	C16—H16	0.9300
C5—N2	1.333 (3)	C17—C18	1.374 (5)
C5—C6	1.499 (4)	C17—H17	0.9300
C6—N4	1.458 (3)	C18—N3	1.336 (4)
C6—H6A	0.9700	C18—H18	0.9300
C6—H6B	0.9700	C19—N5	1.112 (4)
C7—N4	1.463 (4)	C19—N7	1.294 (17)
C7—C8	1.495 (4)	C19—N7'	1.331 (14)
C7—H7A	0.9700	C20—N6	1.122 (4)
C7—H7B	0.9700	C20—N7'	1.298 (16)
C8—N1	1.335 (4)	C20—N7	1.34 (2)
C8—C9	1.382 (4)	C11—O3	1.414 (2)
C9—C10	1.359 (5)	C11—O4	1.416 (2)
C9—H9	0.9300	C11—O1	1.416 (2)
C10—C11	1.367 (6)	C11—O2	1.424 (2)
C10—H10	0.9300	N1—Zn1	2.053 (2)
C11—C12	1.369 (5)	N2—Zn1	2.048 (2)

supplementary materials

C11—H11	0.9300	N3—Zn1	2.059 (2)
C12—N1	1.334 (4)	N4—Zn1	2.215 (2)
C12—H12	0.9300	N5—Zn1	2.021 (3)
C13—N4	1.472 (4)		
C2—C1—C5	119.0 (3)	C16—C15—C14	119.3 (4)
C2—C1—H1	120.5	C16—C15—H15	120.4
C5—C1—H1	120.5	C14—C15—H15	120.4
C3—C2—C1	119.4 (3)	C15—C16—C17	120.0 (4)
C3—C2—H2	120.3	C15—C16—H16	120.0
C1—C2—H2	120.3	C17—C16—H16	120.0
C2—C3—C4	118.9 (3)	C16—C17—C18	118.5 (4)
C2—C3—H3	120.5	C16—C17—H17	120.7
C4—C3—H3	120.5	C18—C17—H17	120.7
N2—C4—C3	122.7 (3)	N3—C18—C17	122.3 (4)
N2—C4—H4	118.6	N3—C18—H18	118.9
C3—C4—H4	118.6	C17—C18—H18	118.9
N2—C5—C1	121.4 (3)	N5—C19—N7	162.3 (19)
N2—C5—C6	116.4 (2)	N5—C19—N7'	166.9 (17)
C1—C5—C6	122.0 (3)	N6—C20—N7'	166.3 (18)
N4—C6—C5	111.5 (2)	N6—C20—N7	163.6 (17)
N4—C6—H6A	109.3	O3—C11—O4	109.71 (18)
C5—C6—H6A	109.3	O3—C11—O1	109.44 (17)
N4—C6—H6B	109.3	O4—C11—O1	108.92 (16)
C5—C6—H6B	109.3	O3—C11—O2	110.20 (16)
H6A—C6—H6B	108.0	O4—C11—O2	109.48 (16)
N4—C7—C8	111.2 (2)	O1—C11—O2	109.07 (16)
N4—C7—H7A	109.4	C12—N1—C8	118.5 (3)
C8—C7—H7A	109.4	C12—N1—Zn1	125.4 (2)
N4—C7—H7B	109.4	C8—N1—Zn1	115.97 (19)
C8—C7—H7B	109.4	C5—N2—C4	118.6 (3)
H7A—C7—H7B	108.0	C5—N2—Zn1	116.86 (19)
N1—C8—C9	121.7 (3)	C4—N2—Zn1	124.6 (2)
N1—C8—C7	116.1 (2)	C14—N3—C18	118.9 (3)
C9—C8—C7	122.1 (3)	C14—N3—Zn1	116.6 (2)
C10—C9—C8	119.2 (4)	C18—N3—Zn1	124.2 (2)
C10—C9—H9	120.4	C6—N4—C7	113.7 (2)
C8—C9—H9	120.4	C6—N4—C13	112.7 (2)
C9—C10—C11	119.3 (3)	C7—N4—C13	112.7 (2)
C9—C10—H10	120.4	C6—N4—Zn1	105.89 (16)
C11—C10—H10	120.4	C7—N4—Zn1	104.41 (17)
C10—C11—C12	119.1 (3)	C13—N4—Zn1	106.58 (17)
C10—C11—H11	120.4	C19—N5—Zn1	160.0 (3)
C12—C11—H11	120.4	C19—N7—C20	120.9 (14)
N1—C12—C11	122.2 (3)	C20—N7'—C19	121.4 (13)
N1—C12—H12	118.9	N5—Zn1—N2	101.94 (10)
C11—C12—H12	118.9	N5—Zn1—N1	100.96 (11)
N4—C13—C14	110.3 (2)	N2—Zn1—N1	118.19 (9)
N4—C13—H13A	109.6	N5—Zn1—N3	100.98 (10)
C14—C13—H13A	109.6	N2—Zn1—N3	117.58 (9)

N4—C13—H13B	109.6	N1—Zn1—N3	112.99 (9)
C14—C13—H13B	109.6	N5—Zn1—N4	179.41 (10)
H13A—C13—H13B	108.1	N2—Zn1—N4	78.60 (9)
N3—C14—C15	121.0 (3)	N1—Zn1—N4	78.95 (9)
N3—C14—C13	117.1 (3)	N3—Zn1—N4	78.55 (9)
C15—C14—C13	121.9 (3)		
C5—C1—C2—C3	0.2 (5)	C14—C13—N4—Zn1	34.9 (3)
C1—C2—C3—C4	0.6 (5)	N7—C19—N5—Zn1	63 (5)
C2—C3—C4—N2	-1.0 (5)	N7'—C19—N5—Zn1	-71 (7)
C2—C1—C5—N2	-0.6 (4)	N5—C19—N7—C20	138.7 (19)
C2—C1—C5—C6	175.2 (3)	N7'—C19—N7—C20	-61 (3)
N2—C5—C6—N4	-27.9 (3)	N6—C20—N7—C19	-134 (2)
C1—C5—C6—N4	156.1 (3)	N7'—C20—N7—C19	65 (3)
N4—C7—C8—N1	-33.0 (4)	N6—C20—N7'—C19	141 (3)
N4—C7—C8—C9	150.0 (3)	N7—C20—N7'—C19	-62 (2)
N1—C8—C9—C10	-0.7 (5)	N5—C19—N7'—C20	-142 (3)
C7—C8—C9—C10	176.1 (3)	N7—C19—N7'—C20	66 (3)
C8—C9—C10—C11	0.1 (6)	C19—N5—Zn1—N2	-60.5 (8)
C9—C10—C11—C12	0.1 (6)	C19—N5—Zn1—N1	61.7 (8)
C10—C11—C12—N1	0.2 (5)	C19—N5—Zn1—N3	178.0 (8)
N4—C13—C14—N3	-30.8 (4)	C5—N2—Zn1—N5	-167.30 (19)
N4—C13—C14—C15	151.5 (3)	C4—N2—Zn1—N5	12.5 (2)
N3—C14—C15—C16	-0.8 (5)	C5—N2—Zn1—N1	83.2 (2)
C13—C14—C15—C16	176.8 (4)	C4—N2—Zn1—N1	-97.0 (2)
C14—C15—C16—C17	-0.1 (7)	C5—N2—Zn1—N3	-58.0 (2)
C15—C16—C17—C18	1.3 (7)	C4—N2—Zn1—N3	121.8 (2)
C16—C17—C18—N3	-1.6 (6)	C5—N2—Zn1—N4	12.47 (18)
C11—C12—N1—C8	-0.8 (5)	C4—N2—Zn1—N4	-167.7 (2)
C11—C12—N1—Zn1	175.7 (2)	C12—N1—Zn1—N5	14.7 (3)
C9—C8—N1—C12	1.0 (4)	C8—N1—Zn1—N5	-168.7 (2)
C7—C8—N1—C12	-176.0 (3)	C12—N1—Zn1—N2	124.8 (2)
C9—C8—N1—Zn1	-175.8 (2)	C8—N1—Zn1—N2	-58.7 (2)
C7—C8—N1—Zn1	7.2 (3)	C12—N1—Zn1—N3	-92.3 (2)
C1—C5—N2—C4	0.2 (4)	C8—N1—Zn1—N3	84.2 (2)
C6—C5—N2—C4	-175.8 (2)	C12—N1—Zn1—N4	-164.7 (3)
C1—C5—N2—Zn1	-180.0 (2)	C8—N1—Zn1—N4	11.9 (2)
C6—C5—N2—Zn1	4.0 (3)	C14—N3—Zn1—N5	-170.4 (2)
C3—C4—N2—C5	0.6 (4)	C18—N3—Zn1—N5	15.8 (3)
C3—C4—N2—Zn1	-179.2 (2)	C14—N3—Zn1—N2	79.8 (2)
C15—C14—N3—C18	0.6 (4)	C18—N3—Zn1—N2	-94.1 (3)
C13—C14—N3—C18	-177.2 (3)	C14—N3—Zn1—N1	-63.4 (2)
C15—C14—N3—Zn1	-173.6 (2)	C18—N3—Zn1—N1	122.8 (2)
C13—C14—N3—Zn1	8.6 (3)	C14—N3—Zn1—N4	9.3 (2)
C17—C18—N3—C14	0.7 (5)	C18—N3—Zn1—N4	-164.6 (3)
C17—C18—N3—Zn1	174.4 (3)	C6—N4—Zn1—N2	-25.66 (18)
C5—C6—N4—C7	-79.4 (3)	C7—N4—Zn1—N2	94.61 (19)
C5—C6—N4—C13	150.8 (2)	C13—N4—Zn1—N2	-145.91 (19)
C5—C6—N4—Zn1	34.7 (3)	C6—N4—Zn1—N1	-147.68 (19)
C8—C7—N4—C6	153.5 (3)	C7—N4—Zn1—N1	-27.42 (18)

supplementary materials

C8—C7—N4—C13	-76.7 (3)	C13—N4—Zn1—N1	92.06 (19)
C8—C7—N4—Zn1	38.6 (3)	C6—N4—Zn1—N3	95.86 (18)
C14—C13—N4—C6	-80.8 (3)	C7—N4—Zn1—N3	-143.9 (2)
C14—C13—N4—C7	148.9 (2)	C13—N4—Zn1—N3	-24.39 (18)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 \cdots O4 ⁱ	0.93	2.53	3.272 (4)	138
C7—H7B \cdots O2 ⁱⁱ	0.97	2.59	3.455 (4)	148
C10—H10 \cdots O1 ⁱⁱⁱ	0.93	2.58	3.511 (5)	179
C13—H13A \cdots N6 ^{iv}	0.97	2.61	3.457 (5)	146
C16—H16 \cdots N7 ^v	0.93	2.48	3.412 (18)	178

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

Fig. 1

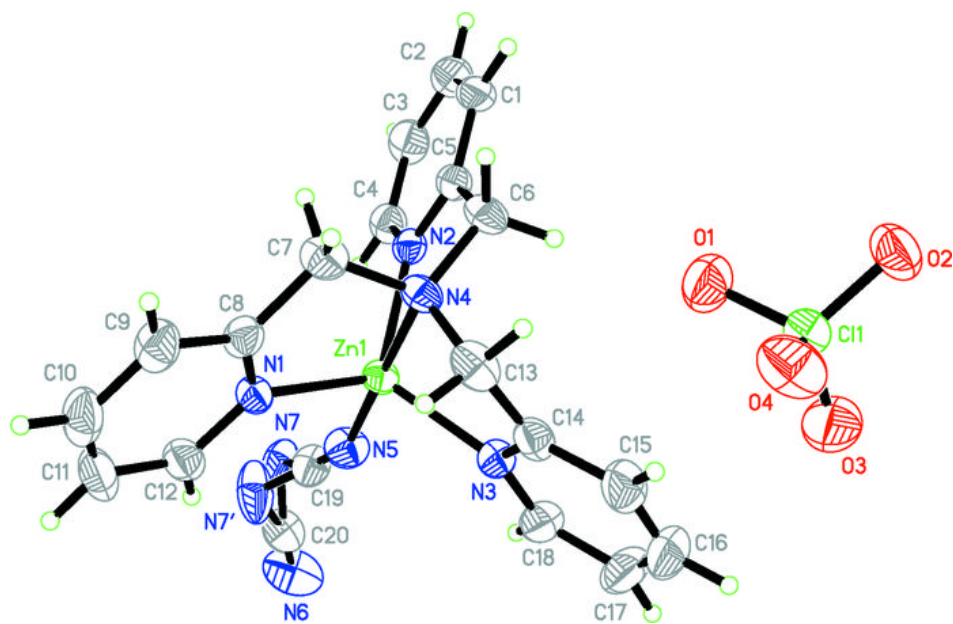


Fig. 2

