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cis-Bis(dicyanamido)bis(4,4′-dimethyl-2,2′-bipyridyl)zinc(II) ethanol hemisolvate

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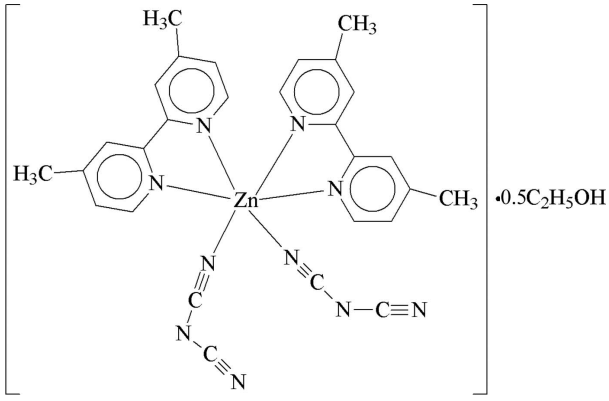
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.057; wR factor = 0.206; data-to-parameter ratio = 15.1.

In the title compound, $[Zn(C_2N_3)_2(C_{12}H_{12}N_2)_2]\cdot0.5C_2H_6O$, the Zn atom is in a distorted octahedral environment formed by six N atoms from two 4,4′-dimethyl-2,2′-bipyridine (dmbpy) ligands and two dicyanamide ligands that are *cis* to one another. There are weak π–π interactions between the dmbpy ligands in adjacent molecules [with centroid–centroid distances of 4.175 (3) and 3.838 (3) Å]. One dicyanamide ligand is disordered over two positions with occupancies 0.64 (2):0.36 (2). The ethanol molecule has a half-occupancy.

Related literature

For related literature, see: Jones & Rao (2001); Yiting *et al.* (2001).



Experimental

Crystal data

$[Zn(C_2N_3)_2(C_{12}H_{12}N_2)_2]\cdot0.5C_2H_6O$
M_r = 589.00
Monoclinic, $P2_1/c$
a = 15.694 (2) Å
b = 14.713 (2) Å
c = 13.8868 (19) Å
β = 112.674 (2)°
V = 2958.7 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.772, T_{max} = 0.870
16800 measured reflections
6059 independent reflections
4171 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.206
S = 1.08
6059 reflections
402 parameters
64 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker 2003); 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: PK2021).

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supplementary materials

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cis-Bis(dicyanamido)bis(4,4'-dimethyl-2,2'-bipyridyl)zinc(II) ethanol hemisolvate

X.-Z. Li, L.-N. Zhu, H. Qu, D.-D. Xu and D.-M. Kong

Comment

Polypyridine complexes of transition metals have received much attention in recent years on account of their photophysical properties (Yiting *et al.*, 2001). Hydrogen bonds and π···π stacking interactions have also proven to play important roles in the control of molecular arrangement in the crystalline state and the properties of matter (Jones & Rao, 2001).

The crystal structure of (I) contains half an ethanol molecule for each zinc(II) complex. The Zn atom is coordinated by six N atoms from two chelating dmbpy ligands and two dca ligands that are *cis* to one another (Fig.1). The Zn—N bond distances range from 2.101 (4) to 2.226 (3) Å and the *cis* N—Zn—N angles range from 74.87 (13) to 96.25 (13) °, indicating a distorted octahedral coordinated geometry around Zn atom. The dmbpy ligands are planar (maximum deviation from the least-squares planes are 0.0499 (44) Å (for the ligand containing N1 and 0.0436 (50) Å for the ligand containing N3.

The dihedral angle between the two dmbpy ligands is 79.31 (7) °. in the two dca ligands, all the C—N triple bond distances less than 1.13 Å. As depicted in Fig. 2, the complexes are linked *via* weak π···π stacking interactions between parallel dmbpy ligands to generate a one-dimensional chain along the [100] direction. The center-to-center distance between the pyridyl ring containing atom N1 and that containing $N2^{i}$ atom (i = 1 − *x*, 1 − *y*, 1 − *z*) is 4.175 (3) Å and that between the rings containing atom N3 and atom $N4^{ii}$ (ii = − *x*, 1 − *y*, −*z*) is 3.838 (3) Å. The one-dimensional chains are parallel in the crystal structure of (I) and the ethanol resides in a vacancy between the main complexes.

Experimental

An ethanol solution (20 ml) of dmbpy (36.8 mg, 0.2 mmol) was added to a mixed aqueous solution (10 ml) of the hexahydrate of zinc(II) perchlorate (37.2 mg, 0.1 mmol) and sodium dicyanamide (17.8 mg, 0.2 mmol) under continuous stirring. After 30 min, the reaction mixture was filtered. Colorless crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of the filtrate at room temperature. Yield 67%. Spectroscopic analysis: IR (KBr, νcm^{-1}): 3433, 2295, 2231, 2200,2170, 1616, 1562, 1485, 1354, 1120, 1016, 921, 837. (IR spectra were recorded on a BIO-RAD FTS 3000 infrared spectrophotometer). Analysis, required for $C_{58}H_{54}N_{20}OZn_2$: C 59.14, H 4.62, N 23.78%; found: C 59.32, H 4.39, N 23.85%.

Refinement

The dca ligand containing atom N8 is disordered over two positions with refined site-occupancy factors of 0.64 (2) and 0.36 (2). All H atoms were located in a difference Fourier map and were refined using a riding model, with distances between 0.93–0.97 Å (CH) and an OH distance of 0.82 Å. U_{iso}(H) values were set to either 1.2Ueq or 1.5Ueq (CH_3, OH) of the attached atom.

Figures

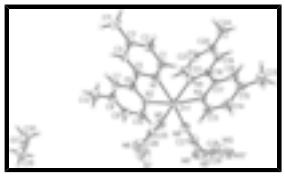


Fig. 1. View of the assymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

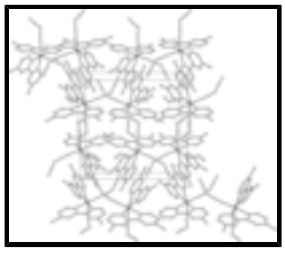


Fig. 2. The molecular packing, viewed along *c* axis.

cis-Bis(4,4'-dimethyl-2,2'-bipyridyl)bis(dicyanamide)zinc(II) ethanol hemisolvate

Crystal data

$[Zn(C_2N_3)_2(C_{12}H_{12}N_2)_2]\cdot 0.5C_2H_6O$	F_{000} = 1220
M_r = 589.00	D_x = 1.322 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5956 reflections
a = 15.694 (2) Å	θ = 2.8–25.4º
b = 14.713 (2) Å	μ = 0.87 mm^{-1}
c = 13.8868 (19) Å	T = 294 (2) K
β = 112.674 (2)º	Block, colourless
V = 2958.7 (7) Å^3	0.24 × 0.20 × 0.16 mm
Z = 4	

Data collection

Bruker APEX II CCD area-detector diffractometer	6059 independent reflections
Radiation source: fine-focus sealed tube	4171 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −19→9
T_{min} = 0.772, T_{max} = 0.870	k = −18→17
16800 measured reflections	l = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.206$	$w = 1/[\sigma^2(F_o^2) + (0.1227P)^2 + 1.4831P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.003$
6059 reflections	$\Delta\rho_{max} = 0.95$ e Å^{-3}
402 parameters	$\Delta\rho_{min} = -0.45$ e Å^{-3}
64 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.26488 (3)	0.45836 (3)	0.21113 (3)	0.0488 (2)	
N1	0.3197 (2)	0.5743 (2)	0.3162 (3)	0.0502 (8)	
N2	0.3189 (2)	0.3995 (2)	0.3645 (3)	0.0510 (8)	
N3	0.1999 (2)	0.5370 (2)	0.0733 (3)	0.0481 (8)	
N4	0.1283 (2)	0.4973 (3)	0.2124 (3)	0.0524 (8)	
N5	0.3916 (3)	0.4500 (3)	0.1909 (3)	0.0656 (10)	
N6	0.5474 (4)	0.4465 (4)	0.1965 (5)	0.0952 (15)	
N7	0.6198 (5)	0.5372 (4)	0.1048 (5)	0.1123 (19)	
N8	0.2159 (3)	0.3333 (3)	0.1376 (3)	0.0706 (10)	
C1	0.3184 (3)	0.6601 (3)	0.2883 (4)	0.0604 (11)	
H1	0.2911	0.6742	0.2176	0.073*	
C2	0.3553 (3)	0.7299 (3)	0.3580 (4)	0.0632 (11)	
H2	0.3533	0.7894	0.3344	0.076*	
C3	0.3950 (3)	0.7109 (3)	0.4623 (4)	0.0613 (11)	
C4	0.3968 (3)	0.6203 (3)	0.4924 (3)	0.0599 (11)	
H4	0.4233	0.6047	0.5627	0.072*	
C5	0.3590 (3)	0.5535 (3)	0.4176 (3)	0.0478 (9)	
C6	0.3579 (3)	0.4568 (3)	0.4447 (3)	0.0493 (9)	
C7	0.3940 (3)	0.4249 (3)	0.5452 (3)	0.0582 (10)	
H7	0.4213	0.4654	0.5998	0.070*	
C8	0.3906 (3)	0.3331 (3)	0.5671 (4)	0.0639 (11)	

C9	0.3523 (3)	0.2761 (3)	0.4843 (4)	0.0664 (12)	
H9	0.3504	0.2139	0.4952	0.080*	
C10	0.3168 (3)	0.3102 (3)	0.3857 (4)	0.0601 (11)	
H10	0.2900	0.2702	0.3304	0.072*	
C11	0.4351 (4)	0.7839 (4)	0.5419 (5)	0.0880 (17)	
H11A	0.4643	0.8288	0.5149	0.132*	
H11B	0.4800	0.7578	0.6043	0.132*	
H11C	0.3868	0.8118	0.5578	0.132*	
C12	0.4267 (4)	0.3001 (4)	0.6780 (4)	0.0894 (17)	
H12A	0.3817	0.3117	0.7077	0.134*	
H12B	0.4830	0.3316	0.7177	0.134*	
H12C	0.4386	0.2360	0.6796	0.134*	
C13	0.2371 (3)	0.5524 (3)	0.0024 (3)	0.0574 (11)	
H13	0.2918	0.5230	0.0103	0.069*	
C14	0.1983 (4)	0.6092 (3)	−0.0804 (4)	0.0670 (12)	
H14	0.2261	0.6174	−0.1280	0.080*	
C15	0.1173 (4)	0.6545 (3)	−0.0936 (4)	0.0666 (12)	
C16	0.0785 (3)	0.6362 (3)	−0.0229 (4)	0.0620 (11)	
H16	0.0228	0.6635	−0.0306	0.074*	
C17	0.1205 (3)	0.5779 (3)	0.0597 (3)	0.0470 (9)	
C18	0.0799 (3)	0.5560 (3)	0.1380 (3)	0.0476 (9)	
C19	−0.0018 (3)	0.5927 (3)	0.1341 (4)	0.0567 (10)	
H19	−0.0341	0.6329	0.0807	0.068*	
C20	−0.0367 (3)	0.5707 (3)	0.2085 (4)	0.0625 (11)	
C21	0.0135 (4)	0.5108 (4)	0.2844 (4)	0.0731 (13)	
H21	−0.0071	0.4938	0.3363	0.088*	
C22	0.0943 (4)	0.4759 (4)	0.2837 (4)	0.0676 (12)	
H22	0.1271	0.4350	0.3359	0.081*	
C23	0.0748 (5)	0.7225 (4)	−0.1791 (5)	0.102 (2)	
H23A	0.0182	0.6984	−0.2292	0.153*	
H23B	0.1167	0.7350	−0.2127	0.153*	
H23C	0.0621	0.7776	−0.1501	0.153*	
C24	−0.1243 (4)	0.6141 (4)	0.2073 (5)	0.0829 (16)	
H24A	−0.1688	0.5672	0.2003	0.124*	
H24B	−0.1481	0.6550	0.1491	0.124*	
H24C	−0.1121	0.6470	0.2709	0.124*	
C25	0.4622 (3)	0.4524 (3)	0.1893 (3)	0.0533 (10)	
C26	0.5817 (4)	0.4974 (4)	0.1456 (5)	0.0753 (14)	
C27	0.1844 (4)	0.2722 (3)	0.0877 (4)	0.0698 (13)	
N9	0.1507 (7)	0.2111 (7)	0.0119 (11)	0.088 (3)	0.64 (2)
C28	0.0769 (4)	0.1747 (4)	−0.0020 (5)	0.0834 (16)	0.64 (2)
N10	0.0048 (6)	0.1397 (7)	−0.0195 (11)	0.105 (4)	0.64 (2)
N9'	0.1659 (9)	0.1872 (10)	0.0591 (15)	0.070 (5)	0.36 (2)
C28'	0.0769 (4)	0.1747 (4)	−0.0020 (5)	0.0834 (16)	0.36 (2)
N10'	0.0058 (8)	0.1591 (13)	−0.0634 (15)	0.094 (6)	0.36 (2)
C29	0.7949 (9)	0.0355 (7)	0.9106 (12)	0.096 (4)	0.50
H29A	0.8388	0.0226	0.8797	0.144*	0.50
H29B	0.7404	−0.0005	0.8772	0.144*	0.50
H29C	0.8216	0.0212	0.9837	0.144*	0.50

C30	0.7712 (7)	0.1294 (7)	0.8976 (9)	0.077 (3)	0.50
H30A	0.7052	0.1346	0.8578	0.092*	0.50
H30B	0.7842	0.1559	0.9658	0.092*	0.50
O1	0.8149 (5)	0.1774 (6)	0.8501 (7)	0.098 (2)	0.50
H1A	0.8307	0.1439	0.8128	0.147*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0478 (3)	0.0516 (3)	0.0448 (3)	−0.0035 (2)	0.0155 (2)	−0.00216 (19)
N1	0.055 (2)	0.0476 (18)	0.0453 (18)	−0.0068 (15)	0.0164 (15)	−0.0053 (15)
N2	0.0515 (19)	0.0518 (19)	0.0479 (18)	−0.0030 (15)	0.0170 (15)	−0.0007 (15)
N3	0.0490 (19)	0.0537 (19)	0.0415 (17)	−0.0028 (15)	0.0173 (15)	−0.0023 (14)
N4	0.0475 (19)	0.062 (2)	0.050 (2)	−0.0020 (16)	0.0210 (16)	0.0010 (17)
N5	0.057 (2)	0.078 (3)	0.065 (2)	0.0031 (19)	0.0269 (19)	0.0028 (19)
N6	0.0927 (17)	0.0955 (18)	0.0974 (18)	0.0011 (10)	0.0367 (11)	0.0035 (10)
N7	0.111 (2)	0.114 (2)	0.114 (2)	0.0007 (10)	0.0455 (12)	0.0008 (10)
N8	0.0700 (13)	0.0688 (13)	0.0706 (13)	−0.0009 (9)	0.0245 (9)	−0.0025 (9)
C1	0.072 (3)	0.053 (2)	0.056 (2)	−0.006 (2)	0.023 (2)	−0.002 (2)
C2	0.068 (3)	0.051 (2)	0.066 (3)	−0.007 (2)	0.022 (2)	−0.004 (2)
C3	0.054 (3)	0.056 (2)	0.068 (3)	−0.007 (2)	0.017 (2)	−0.014 (2)
C4	0.054 (2)	0.066 (3)	0.049 (2)	0.000 (2)	0.0090 (19)	−0.007 (2)
C5	0.043 (2)	0.053 (2)	0.045 (2)	−0.0018 (17)	0.0147 (17)	−0.0053 (17)
C6	0.044 (2)	0.055 (2)	0.049 (2)	0.0001 (17)	0.0187 (18)	0.0022 (18)
C7	0.058 (3)	0.066 (3)	0.045 (2)	−0.002 (2)	0.0135 (19)	0.002 (2)
C8	0.058 (3)	0.073 (3)	0.059 (3)	0.002 (2)	0.020 (2)	0.013 (2)
C9	0.073 (3)	0.053 (2)	0.075 (3)	0.004 (2)	0.030 (3)	0.012 (2)
C10	0.068 (3)	0.050 (2)	0.062 (3)	−0.006 (2)	0.025 (2)	−0.001 (2)
C11	0.092 (4)	0.071 (3)	0.078 (4)	−0.006 (3)	0.007 (3)	−0.028 (3)
C12	0.096 (4)	0.095 (4)	0.068 (3)	0.006 (3)	0.022 (3)	0.030 (3)
C13	0.057 (3)	0.070 (3)	0.049 (2)	0.001 (2)	0.024 (2)	−0.001 (2)
C14	0.084 (3)	0.069 (3)	0.057 (3)	0.000 (3)	0.037 (3)	0.004 (2)
C15	0.081 (3)	0.062 (3)	0.054 (3)	0.000 (2)	0.024 (2)	0.004 (2)
C16	0.066 (3)	0.057 (3)	0.063 (3)	0.009 (2)	0.026 (2)	0.002 (2)
C17	0.050 (2)	0.045 (2)	0.047 (2)	−0.0037 (17)	0.0192 (17)	−0.0072 (17)
C18	0.045 (2)	0.048 (2)	0.047 (2)	−0.0049 (17)	0.0153 (17)	−0.0085 (17)
C19	0.054 (2)	0.057 (2)	0.060 (3)	0.0001 (19)	0.023 (2)	−0.008 (2)
C20	0.053 (3)	0.066 (3)	0.074 (3)	−0.007 (2)	0.031 (2)	−0.014 (2)
C21	0.065 (3)	0.091 (4)	0.077 (3)	−0.005 (3)	0.042 (3)	0.008 (3)
C22	0.064 (3)	0.082 (3)	0.064 (3)	−0.003 (2)	0.032 (2)	0.011 (2)
C23	0.125 (5)	0.097 (4)	0.084 (4)	0.032 (4)	0.040 (4)	0.037 (3)
C24	0.063 (3)	0.096 (4)	0.102 (4)	0.002 (3)	0.045 (3)	−0.011 (3)
C25	0.045 (2)	0.056 (2)	0.054 (2)	0.0052 (18)	0.0142 (19)	0.0010 (18)
C26	0.061 (3)	0.084 (4)	0.092 (4)	0.006 (3)	0.041 (3)	0.006 (3)
C27	0.067 (3)	0.057 (3)	0.079 (3)	−0.010 (2)	0.021 (3)	−0.016 (2)
N9	0.089 (3)	0.088 (3)	0.088 (3)	−0.0007 (10)	0.0342 (16)	−0.0016 (10)
C28	0.078 (4)	0.084 (4)	0.091 (4)	−0.009 (3)	0.035 (3)	−0.024 (3)
N10	0.105 (4)	0.105 (4)	0.105 (4)	−0.0011 (10)	0.0398 (17)	−0.0005 (10)

N9'	0.070 (5)	0.069 (5)	0.071 (5)	0.0000 (10)	0.026 (2)	0.0000 (10)
C28'	0.078 (4)	0.084 (4)	0.091 (4)	−0.009 (3)	0.035 (3)	−0.024 (3)
N10'	0.094 (6)	0.094 (6)	0.094 (6)	−0.0005 (10)	0.036 (2)	−0.0002 (10)
C29	0.069 (6)	0.106 (7)	0.119 (8)	−0.011 (5)	0.041 (6)	0.008 (6)
C30	0.055 (5)	0.095 (6)	0.080 (6)	−0.001 (5)	0.026 (4)	0.003 (5)
O1	0.071 (4)	0.098 (5)	0.107 (5)	0.004 (4)	0.014 (4)	0.040 (4)

Geometric parameters (Å, °)

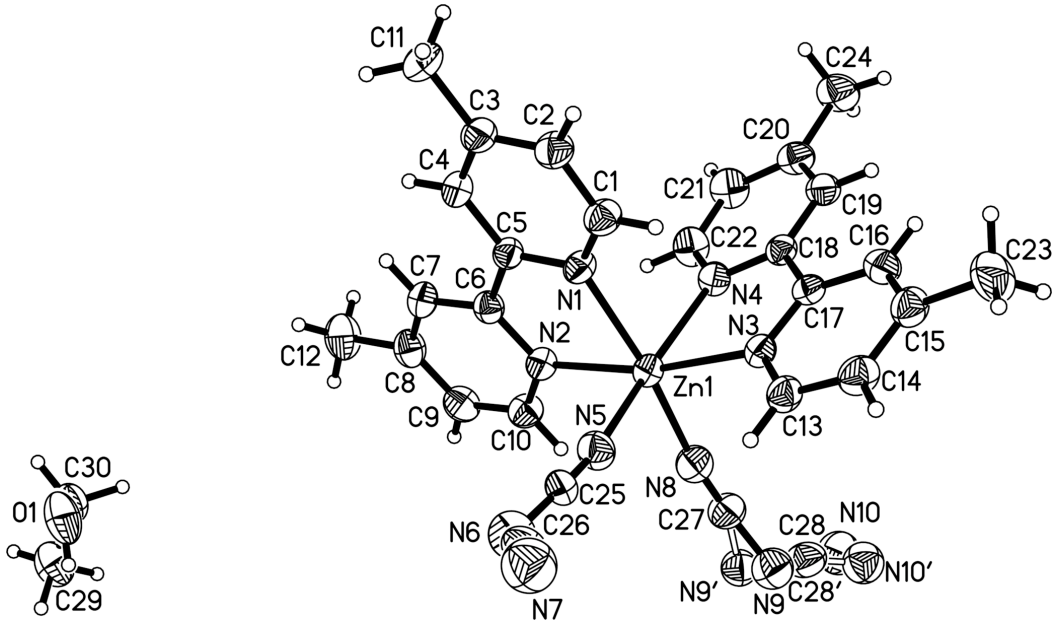
Zn1—N8	2.101 (4)	C12—H12A	0.9600
Zn1—N5	2.117 (4)	C12—H12B	0.9600
Zn1—N3	2.130 (3)	C12—H12C	0.9600
Zn1—N2	2.148 (3)	C13—C14	1.360 (6)
Zn1—N1	2.194 (3)	C13—H13	0.9300
Zn1—N4	2.226 (3)	C14—C15	1.384 (7)
N1—C1	1.319 (5)	C14—H14	0.9300
N1—C5	1.336 (5)	C15—C16	1.367 (6)
N2—C6	1.342 (5)	C15—C23	1.498 (7)
N2—C10	1.349 (5)	C16—C17	1.380 (6)
N3—C17	1.330 (5)	C16—H16	0.9300
N3—C13	1.342 (5)	C17—C18	1.492 (5)
N4—C22	1.331 (6)	C18—C19	1.373 (6)
N4—C18	1.336 (5)	C19—C20	1.382 (6)
N5—C25	1.118 (6)	C19—H19	0.9300
N6—C26	1.281 (7)	C20—C21	1.366 (7)
N6—C25	1.305 (7)	C20—C24	1.510 (6)
N7—C26	1.132 (7)	C21—C22	1.372 (7)
N8—C27	1.127 (6)	C21—H21	0.9300
C1—C2	1.377 (6)	C22—H22	0.9300
C1—H1	0.9300	C23—H23A	0.9600
C2—C3	1.367 (7)	C23—H23B	0.9600
C2—H2	0.9300	C23—H23C	0.9600
C3—C4	1.393 (6)	C24—H24A	0.9600
C3—C11	1.495 (6)	C24—H24B	0.9600
C4—C5	1.386 (6)	C24—H24C	0.9600
C4—H4	0.9300	C27—N9'	1.311 (14)
C5—C6	1.475 (5)	C27—N9	1.329 (10)
C6—C7	1.371 (6)	N9—C28	1.222 (10)
C7—C8	1.390 (6)	C28—N10	1.181 (8)
C7—H7	0.9300	C29—C30	1.425 (9)
C8—C9	1.361 (7)	C29—H29A	0.9600
C8—C12	1.503 (7)	C29—H29B	0.9600
C9—C10	1.360 (6)	C29—H29C	0.9600
C9—H9	0.9300	C30—O1	1.324 (8)
C10—H10	0.9300	C30—H30A	0.9700
C11—H11A	0.9600	C30—H30B	0.9700
C11—H11B	0.9600	O1—H1A	0.8200
C11—H11C	0.9600		
N8—Zn1—N5	94.05 (16)	C8—C12—H12B	109.5

N8—Zn1—N3	94.59 (14)	H12A—C12—H12B	109.5
N5—Zn1—N3	93.49 (14)	C8—C12—H12C	109.5
N8—Zn1—N2	93.40 (14)	H12A—C12—H12C	109.5
N5—Zn1—N2	94.37 (14)	H12B—C12—H12C	109.5
N3—Zn1—N2	168.36 (13)	N3—C13—C14	123.0 (4)
N8—Zn1—N1	168.71 (14)	N3—C13—H13	118.5
N5—Zn1—N1	89.18 (14)	C14—C13—H13	118.5
N3—Zn1—N1	96.01 (13)	C13—C14—C15	119.8 (4)
N2—Zn1—N1	75.55 (12)	C13—C14—H14	120.1
N8—Zn1—N4	93.27 (15)	C15—C14—H14	120.1
N5—Zn1—N4	166.71 (14)	C16—C15—C14	116.8 (4)
N3—Zn1—N4	74.87 (13)	C16—C15—C23	121.0 (5)
N2—Zn1—N4	96.25 (13)	C14—C15—C23	122.2 (5)
N1—Zn1—N4	85.78 (13)	C15—C16—C17	121.1 (4)
C1—N1—C5	118.5 (4)	C15—C16—H16	119.5
C1—N1—Zn1	126.2 (3)	C17—C16—H16	119.5
C5—N1—Zn1	115.2 (3)	N3—C17—C16	121.4 (4)
C6—N2—C10	118.1 (4)	N3—C17—C18	116.1 (4)
C6—N2—Zn1	116.7 (3)	C16—C17—C18	122.5 (4)
C10—N2—Zn1	125.2 (3)	N4—C18—C19	121.9 (4)
C17—N3—C13	117.9 (4)	N4—C18—C17	115.4 (3)
C17—N3—Zn1	118.1 (3)	C19—C18—C17	122.8 (4)
C13—N3—Zn1	123.9 (3)	C18—C19—C20	120.7 (4)
C22—N4—C18	117.2 (4)	C18—C19—H19	119.6
C22—N4—Zn1	127.5 (3)	C20—C19—H19	119.6
C18—N4—Zn1	114.9 (3)	C21—C20—C19	116.9 (4)
C25—N5—Zn1	172.1 (4)	C21—C20—C24	122.2 (5)
C26—N6—C25	123.7 (5)	C19—C20—C24	120.9 (5)
C27—N8—Zn1	171.7 (4)	C20—C21—C22	119.7 (4)
N1—C1—C2	123.6 (4)	C20—C21—H21	120.2
N1—C1—H1	118.2	C22—C21—H21	120.2
C2—C1—H1	118.2	N4—C22—C21	123.6 (5)
C3—C2—C1	119.2 (4)	N4—C22—H22	118.2
C3—C2—H2	120.4	C21—C22—H22	118.2
C1—C2—H2	120.4	C15—C23—H23A	109.5
C2—C3—C4	117.5 (4)	C15—C23—H23B	109.5
C2—C3—C11	121.7 (5)	H23A—C23—H23B	109.5
C4—C3—C11	120.7 (5)	C15—C23—H23C	109.5
C5—C4—C3	120.0 (4)	H23A—C23—H23C	109.5
C5—C4—H4	120.0	H23B—C23—H23C	109.5
C3—C4—H4	120.0	C20—C24—H24A	108.7
N1—C5—C4	121.2 (4)	C20—C24—H24B	109.4
N1—C5—C6	116.3 (4)	H24A—C24—H24B	109.5
C4—C5—C6	122.5 (4)	C20—C24—H24C	110.2
N2—C6—C7	120.5 (4)	H24A—C24—H24C	109.5
N2—C6—C5	116.2 (4)	H24B—C24—H24C	109.5
C7—C6—C5	123.3 (4)	N5—C25—N6	172.4 (5)
C6—C7—C8	121.3 (4)	N7—C26—N6	173.0 (7)
C6—C7—H7	119.3	N8—C27—N9'	160.3 (10)

C8—C7—H7	119.3	N8—C27—N9	166.7 (8)
C9—C8—C7	117.1 (4)	C28—N9—C27	119.0 (8)
C9—C8—C12	122.4 (5)	N10—C28—N9	177.5 (10)
C7—C8—C12	120.4 (5)	C30—C29—H29A	109.5
C10—C9—C8	119.9 (4)	C30—C29—H29B	109.5
C10—C9—H9	120.0	H29A—C29—H29B	109.5
C8—C9—H9	120.0	C30—C29—H29C	109.5
N2—C10—C9	123.0 (4)	H29A—C29—H29C	109.5
N2—C10—H10	118.5	H29B—C29—H29C	109.5
C9—C10—H10	118.5	O1—C30—C29	114.8 (9)
C3—C11—H11A	109.5	O1—C30—H30A	108.6
C3—C11—H11B	109.5	C29—C30—H30A	108.6
H11A—C11—H11B	109.5	O1—C30—H30B	108.6
C3—C11—H11C	109.5	C29—C30—H30B	108.6
H11A—C11—H11C	109.5	H30A—C30—H30B	107.5
H11B—C11—H11C	109.5	C30—O1—H1A	109.6
C8—C12—H12A	109.5		
N8—Zn1—N1—C1	−167.9 (7)	C3—C4—C5—N1	−0.7 (7)
N5—Zn1—N1—C1	85.3 (4)	C3—C4—C5—C6	−179.3 (4)
N3—Zn1—N1—C1	−8.1 (4)	C10—N2—C6—C7	−0.4 (6)
N2—Zn1—N1—C1	−180.0 (4)	Zn1—N2—C6—C7	179.9 (3)
N4—Zn1—N1—C1	−82.4 (4)	C10—N2—C6—C5	179.6 (4)
N8—Zn1—N1—C5	13.2 (9)	Zn1—N2—C6—C5	−0.1 (5)
N5—Zn1—N1—C5	−93.6 (3)	N1—C5—C6—N2	1.1 (5)
N3—Zn1—N1—C5	173.0 (3)	C4—C5—C6—N2	179.8 (4)
N2—Zn1—N1—C5	1.1 (3)	N1—C5—C6—C7	−178.9 (4)
N4—Zn1—N1—C5	98.7 (3)	C4—C5—C6—C7	−0.2 (7)
N8—Zn1—N2—C6	−178.2 (3)	N2—C6—C7—C8	−0.6 (7)
N5—Zn1—N2—C6	87.5 (3)	C5—C6—C7—C8	179.4 (4)
N3—Zn1—N2—C6	−44.8 (8)	C6—C7—C8—C9	1.8 (7)
N1—Zn1—N2—C6	−0.5 (3)	C6—C7—C8—C12	−177.2 (5)
N4—Zn1—N2—C6	−84.5 (3)	C7—C8—C9—C10	−2.1 (7)
N8—Zn1—N2—C10	2.1 (4)	C12—C8—C9—C10	177.0 (5)
N5—Zn1—N2—C10	−92.2 (4)	C6—N2—C10—C9	0.1 (7)
N3—Zn1—N2—C10	135.5 (6)	Zn1—N2—C10—C9	179.8 (3)
N1—Zn1—N2—C10	179.8 (4)	C8—C9—C10—N2	1.2 (7)
N4—Zn1—N2—C10	95.8 (4)	C17—N3—C13—C14	1.6 (6)
N8—Zn1—N3—C17	99.3 (3)	Zn1—N3—C13—C14	−174.2 (3)
N5—Zn1—N3—C17	−166.3 (3)	N3—C13—C14—C15	0.6 (7)
N2—Zn1—N3—C17	−33.9 (8)	C13—C14—C15—C16	−2.5 (7)
N1—Zn1—N3—C17	−76.8 (3)	C13—C14—C15—C23	175.8 (5)
N4—Zn1—N3—C17	7.2 (3)	C14—C15—C16—C17	2.4 (7)
N8—Zn1—N3—C13	−85.0 (3)	C23—C15—C16—C17	−175.9 (5)
N5—Zn1—N3—C13	9.4 (3)	C13—N3—C17—C16	−1.7 (6)
N2—Zn1—N3—C13	141.8 (6)	Zn1—N3—C17—C16	174.3 (3)
N1—Zn1—N3—C13	98.9 (3)	C13—N3—C17—C18	177.7 (3)
N4—Zn1—N3—C13	−177.1 (3)	Zn1—N3—C17—C18	−6.3 (4)
N8—Zn1—N4—C22	85.9 (4)	C15—C16—C17—N3	−0.4 (7)
N5—Zn1—N4—C22	−150.8 (6)	C15—C16—C17—C18	−179.7 (4)

N3—Zn1—N4—C22	179.7 (4)	C22—N4—C18—C19	−0.3 (6)
N2—Zn1—N4—C22	−7.9 (4)	Zn1—N4—C18—C19	−174.1 (3)
N1—Zn1—N4—C22	−82.9 (4)	C22—N4—C18—C17	−179.9 (4)
N8—Zn1—N4—C18	−101.0 (3)	Zn1—N4—C18—C17	6.3 (4)
N5—Zn1—N4—C18	22.3 (8)	N3—C17—C18—N4	−0.3 (5)
N3—Zn1—N4—C18	−7.1 (3)	C16—C17—C18—N4	179.1 (4)
N2—Zn1—N4—C18	165.2 (3)	N3—C17—C18—C19	−179.8 (4)
N1—Zn1—N4—C18	90.3 (3)	C16—C17—C18—C19	−0.5 (6)
C5—N1—C1—C2	−0.1 (7)	N4—C18—C19—C20	0.7 (6)
Zn1—N1—C1—C2	−179.0 (3)	C17—C18—C19—C20	−179.8 (4)
N1—C1—C2—C3	−0.7 (8)	C18—C19—C20—C21	−0.5 (7)
C1—C2—C3—C4	0.8 (7)	C18—C19—C20—C24	177.3 (4)
C1—C2—C3—C11	−179.2 (5)	C19—C20—C21—C22	0.0 (8)
C2—C3—C4—C5	−0.1 (7)	C24—C20—C21—C22	−177.7 (5)
C11—C3—C4—C5	179.8 (5)	C18—N4—C22—C21	−0.2 (7)
C1—N1—C5—C4	0.8 (6)	Zn1—N4—C22—C21	172.8 (4)
Zn1—N1—C5—C4	179.8 (3)	C20—C21—C22—N4	0.4 (8)
C1—N1—C5—C6	179.5 (4)	N8—C27—N9—C28	−134 (3)
Zn1—N1—C5—C6	−1.5 (5)	N9'—C27—N9—C28	72.4 (17)

Fig. 1


C11
C24
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C29

Fig. 2