Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(dicyanamido-κN)(di-2-pyridylamine-$\kappa^2 N,N'$)-zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.044
wR factor = 0.108
Data-to-parameter ratio = 16.9

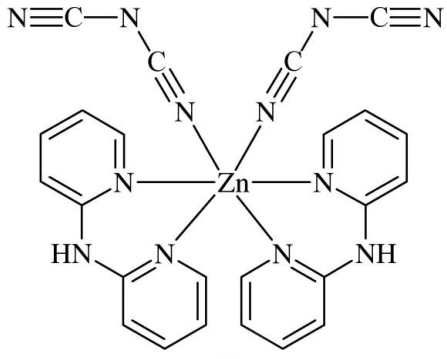
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 30 November 2006
Accepted 21 December 2006

The title mononuclear Zn^{II} complex, $[Zn(C_2N_3)_2(C_{10}H_9N_3)_2]$, is isostructural with its Mn^{II}, Co^{II} and Ni^{II} analogues. The Zn^{II} atom lies on a crystallographic twofold rotation axis and is coordinated by two bidentate di-2-pyridylamine ligands and by two dicyanamide ligands in a *cis* orientation.

Comment

The title Zn^{II} complex, (I), is isostructural with its Mn^{II}, Co^{II} and Ni^{II} analogues (Xu *et al.*, 2003; Huang *et al.*, 2006). The Zn^{II} atom lies on a crystallographic twofold rotation axis and is coordinated in a distorted octahedral geometry by two bidentate di-2-pyridylamine (dpaH) ligands and by two dicyanamide ligands (Fig. 1 and Table 1). The dihedral angle between the pyridine rings of the dpaH ligands lying *trans* to each other [coordinated through N3 and N3^{i}; symmetry code: (i) $-x$, y, $\frac{1}{2}-z$] is 25.5 (3)°. The two dicyanamide ligands adopt a *cis* orientation, and each possesses approximate local C_{2v} symmetry, the N4—C11 and N5—C11 bond distances being comparable to N5—C12 and N6—C12, and with a C11—N5—C12 angle of 123.9 (3)°.



(I)

The complexes lie in layers parallel to (001) (Fig. 2), forming hydrogen bonds between the alkylamino NH groups of the dpaH ligand and the non-coordinated terminal N atoms of the dicyanamide ligands (Table 2).

Experimental

A methanol solution (5 ml) of sodium dicyanamide (0.32 g) and di-2-pyridylamine (0.16 g) was added to 10 ml of water. $Zn(NO_3)_2{\cdot}6H_2O$ (0.25 g) dissolved in methanol (10 ml) was layered on the top and colourless block-shaped crystals were obtained after standing at room temperature for several days.

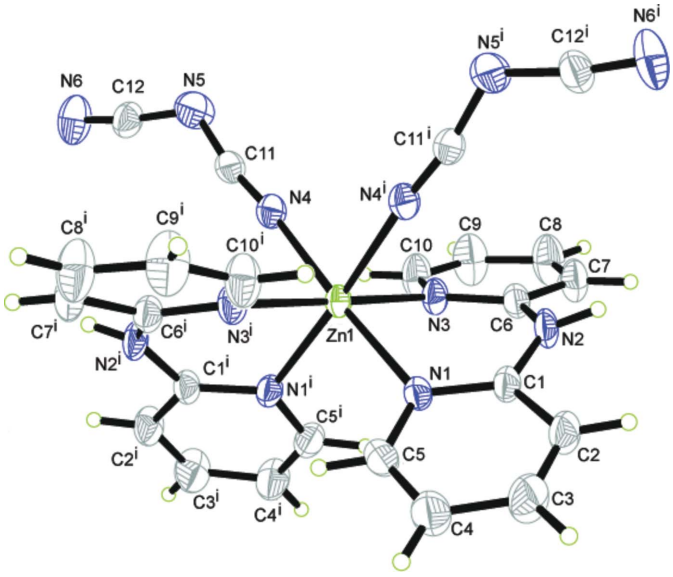


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms. [Symmetry code: (i) $-x, y, -z+\frac{1}{2}$.]

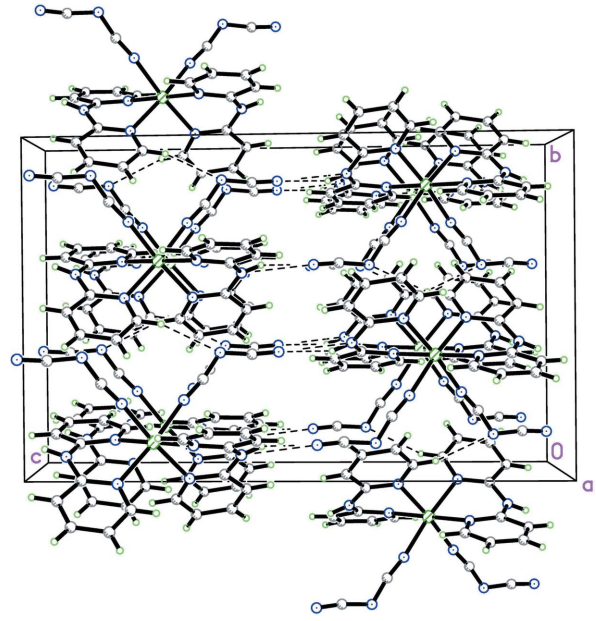


Figure 2
Packing diagram of (I). Dashed lines indicate hydrogen bonds.

Crystal data

$[Zn(C_2N_3)_2(C_{10}H_9N_3)_2]$
M_r = 539.89
Monoclinic, $C2/c$
a = 8.6474 (11) Å
b = 13.5964 (18) Å
c = 21.632 (3) Å
β = 94.549 (2)°
V = 2535.3 (6) Å^3
Z = 4
D_x = 1.414 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.30 × 0.10 mm

Data collection

Bruker APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.752, T_{max} = 0.906
7391 measured reflections
2836 independent reflections
1840 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 1.00
2836 reflections
168 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.141 (2)	Zn1—N3	2.178 (2)
Zn1—N4	2.157 (3)		
N1^i—Zn1—N1	95.27 (12)	N1—Zn1—N3	83.07 (9)
N1—Zn1—N4^i	87.30 (9)	N4^i—Zn1—N3	89.72 (9)
N1—Zn1—N4	173.16 (9)	N4—Zn1—N3	90.33 (9)
N4^i—Zn1—N4	90.88 (13)	N3—Zn1—N3^i	179.93 (13)
N1^i—Zn1—N3	96.89 (9)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N6^{ii}	0.86	2.09	2.904 (4)	157

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

H atoms were placed in calculated positions and allowed to ride during subsequent refinement, with C—H = 0.93Å or N—H = 0.86Å, and with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Education Office Foundation of Liaoning Province (project No. 605 L207).

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