Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[tetra-μ-cyanido-dipyridine-cadmium(II)zinc(II)]

Sheng Li,* Kun Tang and Fu-Li Zhang

College of Medicine, Henan University, Kaifeng 475003, People's Republic of China
Correspondence e-mail: lisheng0821@sina.com

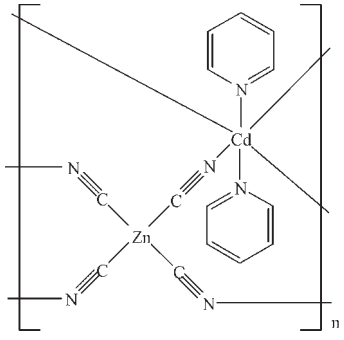
Received 26 October 2009; accepted 18 December 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.010 Å; R factor = 0.050; wR factor = 0.136; data-to-parameter ratio = 14.5.

In the title coordination polymer, $[CdZn(CN)_4(C_5H_5N)_2]_n$, the Zn^{II} atom (site symmetry 222) adopts a distorted ZnC_4 tetrahedral geometry, being coordinated by four crystallographically equivalent cyanide ions. The cyanide ion bridges to a Cd^{II} centre *via* its N atom. The Cd atom (site symmetry 2/*m*) coordination is a distorted CdN_6 octahedron, arising from four cyanide N atoms and two pyridine N atoms. The complete pyridine molecule is generated by *m* symmetry, with the N atom and one C atom lying on the reflecting plane. In the crystal, the bridging cyanide ions result in a three-dimensional network.

Related literature

For background to cyanide-containing coordination networks, see: Vasylyev & Neumann (2006).



Experimental

Crystal data

$[CdZn(CN)_4(C_5H_5N)_2]$
M_r = 440.05
Orthorhombic, *Cccm*
a = 9.514 (4) Å
b = 13.935 (6) Å
c = 13.965 (6) Å
V = 1851.5 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.45 mm^{-1}
T = 296 K
0.44 × 0.28 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.412, T_{max} = 0.615
4068 measured reflections
827 independent reflections
711 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.136
S = 1.00
827 reflections
57 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 2.77 e Å^{-3}
$\Delta\rho_{min}$ = −1.34 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd—N3	2.345 (4)	Zn1—C4	2.037 (4)
Cd—N1	2.354 (5)		

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful for financial support from Henan University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5184).

References

Bruker (2001). *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison,Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Vasylyev, M. & Neumann, R. (2006). *Chem. Mater.* **18**, 2781–2783.

supplementary materials

Acta Cryst. (2010). E**66**, m108 [**doi:10.1107/S1600536809054579**]

Poly[tetra-μ-cyanido-dipyridinecadmium(II)zinc(II)]

S. Li, K. Tang and F.-L. Zhang

Comment

It has always been the interest of many chemists to design and synthesize novel metal cyano compounds which possess broad applications in host–guest chemistry, catalysis, photochemistry and electrical conductivity *etc* (Vasylyev & Neumann, 2006). Herein, we report a new crystal structure.

In the asymmetric unit of complex **I**, there exhibit one cyano ios, half pyridine, one Cd(II), and one Zn^{II}, figure 1. The Zn^{II} ion surrounded by four $cyano^{-1}$ ligands is tetra-coordinated by four C atoms, with tetrahedral coordination sphere. The bond distances of Zn—C is 2.037 (4) /%A in the normal range compared to the reported complexes containing the Zn—C—N—Cd atoms (Vasylyev & Neumann, 2006). The cadmium(II) is hexacoordianted by six N atoms from four cyano ions and two pyridine, located in the center of the coordinated octahedral geometry. It is worthy noting that the complex exhibits three-dimensional structure *via* the bridge of cyano ions, figure 2.

Experimental

The starting materials of sodium cyanide (0.049 g, 1 mmol) and $ZnSO_4.7H_2O$ (0.07 g, 0.25 mmol), and $CdSO_4$ (0.05 g, 0.25 mmol) were refluxed in the mixture solution (CH_3OH: pyridine = 10:1) until all solid was dissolved. The solution was cooled to room temperature and filtered. Colourless blocks of (I) were obtained by allowing slow evaporation.

Refinement

All hydrogen atoms bound to carbon were refined using a riding model with distance C—H = 0.93 Å, $U_{iso} = 1.2U_{eq}$ (C) for aromatic atoms.

Figures

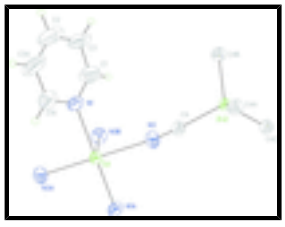


Fig. 1. A view of (I) with the unique atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

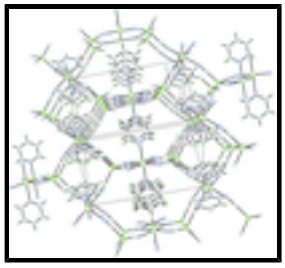


Fig. 2. A view of (I) supramolecular strcuture.

Poly[tetra-μ-cyanido-dipyridinecadmium(II)zinc(II)]

Crystal data

$[CdZn(CN)_4(C_5H_5N)_2]$	$F(000) = 856$
$M_r = 440.05$	$D_x = 1.579$ Mg m^{-3}
Orthorhombic, *Cccm*	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2 2c	Cell parameters from 2697 reflections
$a = 9.514$ (4) Å	$\theta = 2.6$–$27.9°$
$b = 13.935$ (6) Å	$\mu = 2.45$ mm^{-1}
$c = 13.965$ (6) Å	$T = 296$ K
$V = 1851.5$ (14) Å^3	Block, colourless
$Z = 4$	0.44 × 0.28 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer	827 independent reflections
Radiation source: fine-focus sealed tube	711 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.051$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.9°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$h = -11 \rightarrow 11$
$T_{min} = 0.412$, $T_{max} = 0.615$	$k = -16 \rightarrow 8$
4068 measured reflections	$l = -16 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.050$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.136$	H-atom parameters not refined
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.115P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
827 reflections	$(\Delta/\sigma)_{max} = 0.001$
57 parameters	$\Delta\rho_{max} = 2.77$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -1.34$ e Å^{-3}

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}
Cd	1.2500	0.2500	0.5000	0.04119 (16)
Zn1	1.0000	0.5000	0.2500	0.0357 (2)
C4	1.1171 (4)	0.4109 (3)	0.3337 (3)	0.0495 (9)
N3	1.1750 (4)	0.3577 (3)	0.3815 (3)	0.0643 (10)
N1	1.0252 (5)	0.1795 (4)	0.5000	0.0592 (13)
C1	0.9588 (8)	0.1595 (5)	0.4210 (4)	0.104 (2)
H1A	1.0043	0.1715	0.3633	0.125*
C2	0.7615 (11)	0.1001 (9)	0.5000	0.131 (4)
H2A	0.6741	0.0703	0.5000	0.157*
C3	0.8239 (8)	0.1213 (6)	0.4180 (6)	0.132 (3)
H3A	0.7787	0.1109	0.3598	0.158*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.0414 (3)	0.0350 (3)	0.0472 (3)	0.0062 (2)	0.000	0.000
Zn1	0.0399 (4)	0.0276 (4)	0.0396 (4)	0.000	0.000	0.000
C4	0.051 (2)	0.0422 (18)	0.0553 (18)	−0.0008 (18)	−0.0004 (16)	0.0053 (16)
N3	0.069 (3)	0.055 (2)	0.069 (2)	0.010 (2)	−0.0084 (17)	0.0112 (17)
N1	0.050 (3)	0.052 (3)	0.076 (3)	−0.010 (2)	0.000	0.000
C1	0.101 (4)	0.124 (5)	0.087 (4)	−0.045 (4)	−0.003 (3)	−0.020 (3)
C2	0.086 (6)	0.105 (7)	0.201 (12)	−0.048 (5)	0.000	0.000
C3	0.115 (5)	0.147 (7)	0.133 (6)	−0.083 (5)	−0.026 (4)	−0.003 (5)

Geometric parameters (Å, °)

Cd—N3^{i}	2.345 (4)	C4—N3	1.140 (5)
Cd—N3^{ii}	2.345 (4)	N1—C1	1.301 (6)
Cd—N3^{iii}	2.345 (4)	N1—C1^{iii}	1.301 (6)
Cd—N3	2.345 (4)	C1—C3	1.390 (10)
Cd—N1	2.354 (5)	C1—H1A	0.9300
Cd—N1^{ii}	2.354 (5)	C2—C3^{iii}	1.324 (9)

Zn1—C4^{iv}	2.037 (4)	C2—C3	1.324 (9)
Zn1—C4	2.037 (4)	C2—H2A	0.9300
Zn1—C4^{v}	2.037 (4)	C3—H3A	0.9300
Zn1—C4^{vi}	2.037 (4)		
N3^{i}—Cd—N3^{ii}	89.74 (19)	C4^{iv}—Zn1—C4^{vi}	113.7 (2)
N3^{i}—Cd—N3^{iii}	180.0	C4—Zn1—C4^{vi}	109.9 (2)
N3^{ii}—Cd—N3^{iii}	90.26 (19)	C4^{v}—Zn1—C4^{vi}	104.9 (2)
N3^{i}—Cd—N3	90.26 (18)	N3—C4—Zn1	175.6 (4)
N3^{ii}—Cd—N3	180.0	C4—N3—Cd	167.6 (3)
N3^{iii}—Cd—N3	89.74 (19)	C1—N1—C1^{iii}	116.0 (7)
N3^{i}—Cd—N1	90.54 (14)	C1—N1—Cd	122.0 (3)
N3^{ii}—Cd—N1	90.54 (14)	C1^{iii}—N1—Cd	122.0 (3)
N3^{iii}—Cd—N1	89.46 (14)	N1—C1—C3	123.8 (6)
N3—Cd—N1	89.46 (14)	N1—C1—H1A	118.1
N3^{i}—Cd—N1^{ii}	89.46 (14)	C3—C1—H1A	118.1
N3^{ii}—Cd—N1^{ii}	89.46 (14)	C3^{iii}—C2—C3	119.9 (10)
N3^{iii}—Cd—N1^{ii}	90.54 (14)	C3^{iii}—C2—H2A	120.1
N3—Cd—N1^{ii}	90.54 (14)	C3—C2—H2A	120.1
N1—Cd—N1^{ii}	180.0	C2—C3—C1	118.2 (7)
C4^{iv}—Zn1—C4	104.9 (2)	C2—C3—H3A	120.9
C4^{iv}—Zn1—C4^{v}	109.9 (2)	C1—C3—H3A	120.9
C4—Zn1—C4^{v}	113.7 (2)		

Symmetry codes: (i) −*x*+5/2, −*y*+1/2, *z*; (ii) −*x*+5/2, −*y*+1/2, −*z*+1; (iii) *x*, *y*, −*z*+1; (iv) −*x*+2, *y*, −*z*+1/2; (v) *x*, −*y*+1, −*z*+1/2; (vi) −*x*+2, −*y*+1, *z*.

Fig. 1

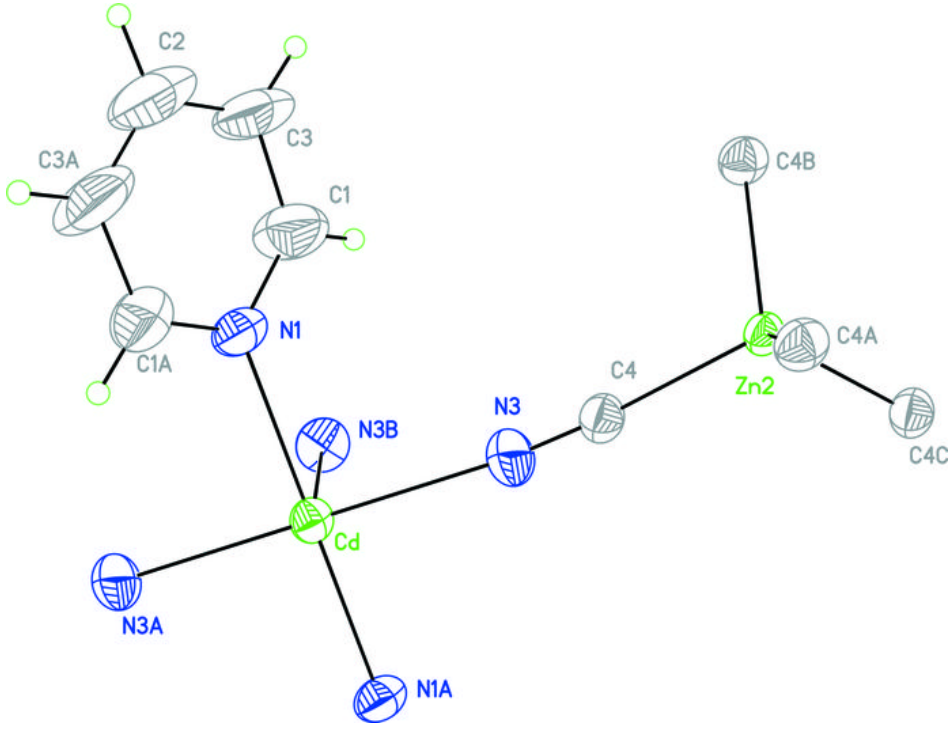


Fig. 2