Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis(dimethylformamide-κO)cadmium(II)]-di-μ_2-dicyanamido-$\kappa^4N^1:N^5$]

Jinfang Zhang

Molecular Materials Research Center, Scientific Research Academy, School of Chemistry and Chemical Engineering, Jiangsu University, Zhenjiang 212013, People's Republic of China
Correspondence e-mail: zjf260@ujs.edu.cn

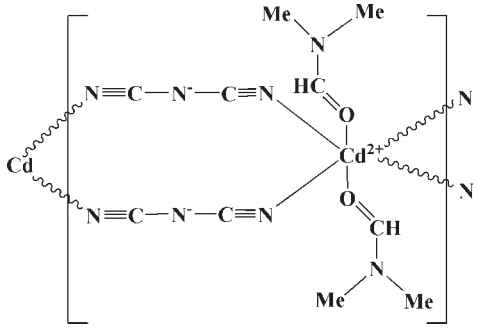
Received 22 October 2009; accepted 4 November 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(N–C) = 0.004 Å; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 14.5.

In the title compound, $[Cd(C_2N_3)_2(C_3H_7NO)_2]$, the Cd^{2+} ion lies on an inversion center and adopts an octahedral coordination geometry, in which four N atoms from four different dicyanamide ligands lie in the equatorial plane and two dimethylformamide O atoms occupy the axial positions. The Cd atoms are connected by two dicyanamide ligands, resulting in a neutral chain propagating parallel to [010].

Related literature

For architectures and topologies of metal-organic compounds, see: Eddaoudi *et al.* (2001); Zhang *et al.* (2008). For their potential applications, see: Banerjee *et al.* (2008); Zhang *et al.* (2007). For metal-organic compounds including dicyanamide ligands, see: Jensen *et al.* (1999); Zhang (2009).



Experimental

Crystal data

$[Cd(C_2N_3)_2(C_3H_7NO)_2]$
M_r = 390.70
Triclinic, $P\overline{1}$
a = 6.5325 (13) Å
b = 7.6003 (15) Å
c = 8.6051 (17) Å
α = 104.28 (3)°
β = 106.90 (3)°
γ = 97.05 (3)°
V = 387.35 (17) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.43 mm^{-1}
T = 293 K
0.20 × 0.16 × 0.12 mm

Data collection

Rigaku Saturn724+ diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.239, T_{max} = 0.480
3505 measured reflections
1410 independent reflections
1408 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.058
S = 1.10
1410 reflections
97 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXT07* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Foundation of Jiangsu University (08JDG036).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2226).

References

Banerjee, R., Phan, A., Wang, B., Knobler, C., Furukawa, H., O'Keeffe, M. & Yaghi O. M. (2008). *Science*, **319**, 939–943.
Eddaoudi, M., Moler, D. B., Li, H. L., Chen, B. L., Reineke, T. M., O'Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.
Jensen, P., Batten, S. R., Fallon, G. D., Moubaraki, B., Murray, K. S. & Price, D. J. (1999). *Chem. Commun.* pp. 177–178.
Rigaku (2008). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, J. (2009). *Acta Cryst.* E**65**, m1044.
Zhang, C., Song, Y. L. & Wang, X. (2007). *Coord. Chem. Rev.* **251**, 111–141.
Zhang, J. F., Song, Y. L., Yang, J. Y., Humphrey, M. G. & Zhang, C. (2008). *Cryst. Growth Des.* **8**, 387–390.

supplementary materials

Acta Cryst. (2009). E**65**, m1550 [**doi:10.1107/S1600536809046364**]

catena-Poly[[bis(dimethylformamide-κ*O*)cadmium(II)]-di-μ_2-dicyanamido-$\kappa^4N^1:N^5$]

J. Zhang

Comment

The designed syntheses of metal-organic compounds have attracted great attention in recent years because of not only their intriguing variety of architectures and topologies (Eddaoudi *et al.*, 2001; Zhang *et al.*, 2008) but also their potential applications (Banerjee *et al.*, 2008; Zhang *et al.*, 2007). Dicyanamide acting as flexible bridging ligands can construct metal-organic compounds with various structures (Jensen *et al.*, 1999; Zhang, 2009). The one-dimensional neutral compounds $\{Cd[N(CN)_2]_2(dmf)_2\}_n$ are constructed by this bridging ligands through diffusion reactions. In this paper, the crystal structure of the title compound, (I), is presented.

As illustrated in Fig. 1, Cd^{2+} which lies on an inversion center, adopts an octahedral coordination geometry, where four N atoms from four different dicyanamide ligands lies in equatorial plane and two O atoms from dmf occupy the axial positions. Every two neighboring Cd atoms connected by two dicyanamide ligands, gives rise to a one-dimensional neutral chain.

Experimental

$Cd(NO_3)_2.4\ H_2O$ (123.2 mg, 0.4 mmol) was added into 2 ml dmf with thorough stirring for 5 minutes. After filtration, the filtrate was carefully laid on the surface with the solution of $NaN(CN)_2$ (89.1 mg, 1 mmol) in 1 ml dmf and 6 ml CH_3CN. colorless block crystals were obtained after eight days. Yield: 199.3 mg in pure form, 51.0% based on Cd.

Refinement

H atoms were positioned geometrically and refined with riding model, with U_{iso} = 1.5 and 1.2 U_{eq} for methyl and formyl H atoms, respectively. The C—H bonds are 0.96 Å in methyl and 0.93 Å in formyl.

Figures

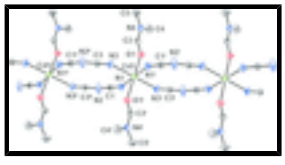


Fig. 1. The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids, all H atoms have been omitted (i -*x* + 1,-*y* + 1,-*z*; ii -*x* + 1,-*y*,-*z*).

catena-Poly[[bis(dimethylformamide-κ*O*)cadmium(II)]- di-μ_2-dicyanamido-$\kappa^4N^1:N^5$]

Crystal data

$[Cd(C_2N_3)_2(C_3H_7NO)_2]$	Z = 1
M_r = 390.70	F_{000} = 194

Triclinic, $P\overline{1}$	D_x = 1.675 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 6.5325 (13) Å	Cell parameters from 1884 reflections
b = 7.6003 (15) Å	θ = 3.3–28.4º
c = 8.6051 (17) Å	μ = 1.43 mm^{-1}
α = 104.28 (3)º	T = 293 K
β = 106.90 (3)º	Block, colorless
γ = 97.05 (3)º	0.2 × 0.16 × 0.12 mm
V = 387.35 (17) Å^3	

Data collection

Rigaku Saturn724+ diffractometer	1410 independent reflections
Radiation source: fine-focus sealed tube	1408 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 293 K	θ_{max} = 25.5º
dtprofit.ref scans	θ_{min} = 3.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7\rightarrow7$
T_{min} = 0.239, T_{max} = 0.480	$k = -7\rightarrow9$
3505 measured reflections	$l = -9\rightarrow10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.022	H-atom parameters constrained
$wR(F^2)$ = 0.058	$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.0503P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max} < 0.001$
1410 reflections	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
97 parameters	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.5000	0.0000	0.04117 (11)
O1	0.7512 (3)	0.6362 (3)	0.2708 (2)	0.0572 (5)
N1	0.2979 (4)	0.3110 (3)	0.0987 (3)	0.0570 (6)
N2	0.2301 (6)	0.0218 (4)	0.1653 (4)	0.0781 (9)
N4	1.1012 (4)	0.7109 (3)	0.4447 (3)	0.0500 (5)
N3	0.6991 (4)	0.2758 (3)	−0.0440 (3)	0.0598 (6)
C1	0.2690 (4)	0.1705 (3)	0.1214 (3)	0.0449 (5)
C5	1.3277 (5)	0.6980 (6)	0.4658 (4)	0.0755 (9)
H5A	1.3381	0.6327	0.3586	0.113*
H5B	1.3766	0.6322	0.5470	0.113*
H5C	1.4177	0.8205	0.5059	0.113*
C4	1.0524 (7)	0.8062 (5)	0.5930 (4)	0.0728 (9)
H4A	0.8984	0.8039	0.5624	0.109*
H4B	1.1323	0.9326	0.6357	0.109*
H4C	1.0943	0.7454	0.6792	0.109*
C2	0.9476 (4)	0.6352 (4)	0.2975 (3)	0.0468 (6)
H2A	0.9885	0.5765	0.2063	0.056*
C3	0.7261 (4)	0.1317 (3)	−0.0954 (3)	0.0427 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04194 (16)	0.03209 (15)	0.04955 (17)	0.01065 (10)	0.01353 (11)	0.01291 (10)
O1	0.0480 (11)	0.0673 (13)	0.0488 (9)	0.0118 (9)	0.0137 (8)	0.0076 (9)
N1	0.0607 (14)	0.0420 (12)	0.0744 (15)	0.0081 (10)	0.0296 (12)	0.0209 (11)
N2	0.136 (3)	0.0421 (13)	0.0862 (18)	0.0263 (15)	0.077 (2)	0.0210 (13)
N4	0.0533 (12)	0.0530 (12)	0.0389 (10)	0.0105 (10)	0.0105 (9)	0.0115 (9)
N3	0.0660 (15)	0.0466 (13)	0.0771 (15)	0.0271 (11)	0.0296 (12)	0.0221 (11)
C1	0.0469 (13)	0.0378 (13)	0.0505 (13)	0.0082 (10)	0.0217 (10)	0.0080 (10)
C5	0.0518 (17)	0.100 (3)	0.0616 (18)	0.0162 (17)	0.0065 (14)	0.0165 (17)
C4	0.093 (2)	0.076 (2)	0.0426 (14)	0.0225 (18)	0.0204 (15)	0.0069 (14)
C2	0.0495 (14)	0.0473 (14)	0.0397 (12)	0.0070 (11)	0.0134 (10)	0.0096 (10)
C3	0.0457 (13)	0.0391 (13)	0.0461 (12)	0.0110 (10)	0.0167 (10)	0.0150 (10)

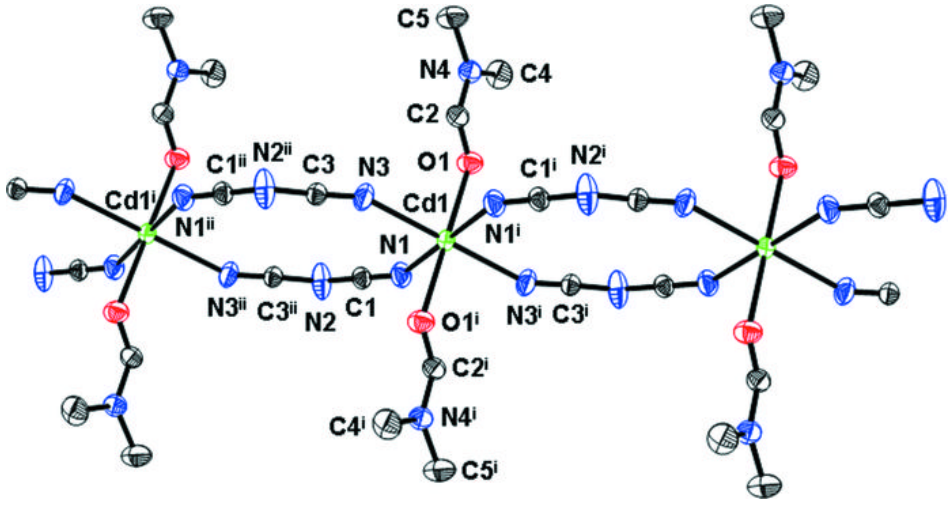
Geometric parameters (Å, °)

Cd1—N3^{i}	2.291 (2)	N4—C4	1.446 (4)
Cd1—N3	2.291 (2)	N4—C5	1.456 (4)
Cd1—N1	2.306 (2)	N3—C3	1.132 (3)
Cd1—N1^{i}	2.306 (2)	C5—H5A	0.9600
Cd1—O1	2.316 (2)	C5—H5B	0.9600
Cd1—O1^{i}	2.316 (2)	C5—H5C	0.9600

O1—C2	1.237 (3)	C4—H4A	0.9600
N1—C1	1.136 (3)	C4—H4B	0.9600
N2—C3^{ii}	1.281 (4)	C4—H4C	0.9600
N2—C1	1.296 (4)	C2—H2A	0.9300
N4—C2	1.305 (3)	C3—N2^{ii}	1.281 (4)
N3^{i}—Cd1—N3	180.0	C4—N4—C5	117.7 (3)
N3^{i}—Cd1—N1	91.27 (9)	C3—N3—Cd1	156.3 (2)
N3—Cd1—N1	88.73 (9)	N1—C1—N2	172.2 (3)
N3^{i}—Cd1—N1^{i}	88.73 (9)	N4—C5—H5A	109.5
N3—Cd1—N1^{i}	91.27 (9)	N4—C5—H5B	109.5
N1—Cd1—N1^{i}	180.00 (11)	H5A—C5—H5B	109.5
N3^{i}—Cd1—O1	90.45 (9)	N4—C5—H5C	109.5
N3—Cd1—O1	89.55 (9)	H5A—C5—H5C	109.5
N1—Cd1—O1	91.26 (9)	H5B—C5—H5C	109.5
N1^{i}—Cd1—O1	88.74 (9)	N4—C4—H4A	109.5
N3^{i}—Cd1—O1^{i}	89.55 (9)	N4—C4—H4B	109.5
N3—Cd1—O1^{i}	90.45 (9)	H4A—C4—H4B	109.5
N1—Cd1—O1^{i}	88.74 (9)	N4—C4—H4C	109.5
N1^{i}—Cd1—O1^{i}	91.26 (9)	H4A—C4—H4C	109.5
O1—Cd1—O1^{i}	180.00 (11)	H4B—C4—H4C	109.5
C2—O1—Cd1	120.12 (16)	O1—C2—N4	124.5 (2)
C1—N1—Cd1	145.5 (2)	O1—C2—H2A	117.7
C3^{ii}—N2—C1	122.3 (2)	N4—C2—H2A	117.7
C2—N4—C4	121.4 (3)	N3—C3—N2^{ii}	172.2 (3)
C2—N4—C5	120.8 (2)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+1, −*y*, −*z*.

Fig. 1


C5
N4
C4
C2
O1
C1ii
N2ii
C3
N3
Cd1i
N1ii
Cd1
N1
C1i
N2i
N1i
N3ii
C3ii
N2
C1
O1i
N3i
C3i
C2i
C4i
N4i
C5i