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

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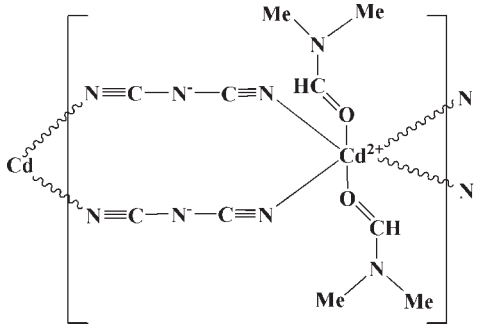
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(N–C) = 0.004 Å; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 14.5.

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*.

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

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supporting information

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

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S1. 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.

S2. 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.

S3. 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.

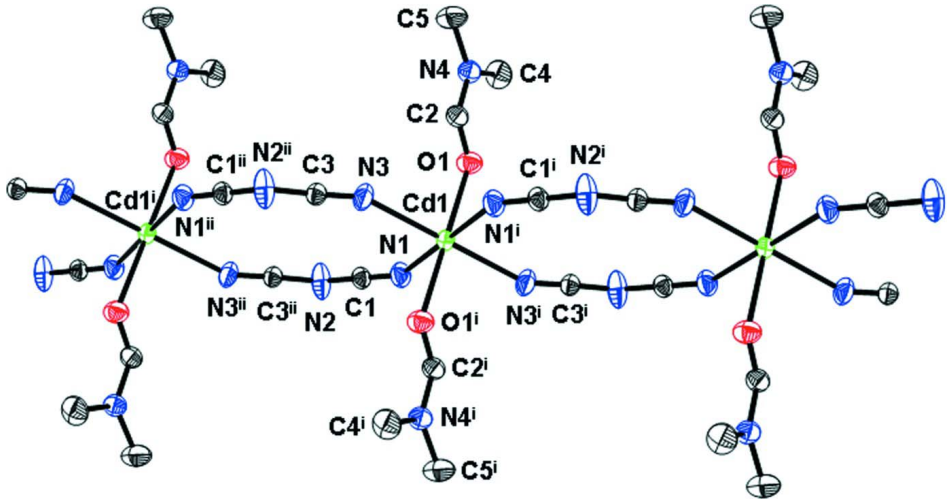

Figure 1

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*).

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
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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
F(000) = 194
D_x = 1.675 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 1884 reflections
θ = 3.3–28.4°
μ = 1.43 mm^{-1}
T = 293 K
Block, colorless
0.2 × 0.16 × 0.12 mm

Data collection

Rigaku Saturn724+ diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
dtprofit.ref scans
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
θ_{max} = 25.5°, θ_{min} = 3.3°
h = −7→7
k = −7→9
l = −9→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.058
S = 1.10
1410 reflections
97 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.0503P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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}
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, º)

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*.