Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Poly[[μ_2-1,2-bis(4-pyridyl)ethene](μ_3-1,3-phenylenediacetato)cadmium]

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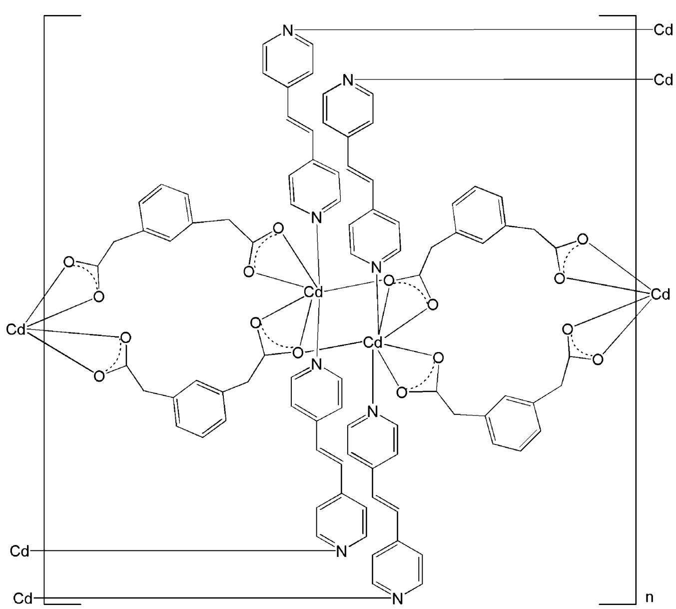
Received 19 October 2011; accepted 19 October 2011

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.005 Å; R factor = 0.033; wR factor = 0.083; data-to-parameter ratio = 16.2.

In the title coordination polymer, $[Cd(C_{10}H_8O_4)(C_{12}H_{10}N_2)]_n$, two centrosymmetrically related Cd^{II} atoms are bridged by two 1,3-phenylenediacetate ligands forming a chain along the [100] direction. The distorted pentagonal–bipyramidal coordination about each metal atom is completed by the N atoms of bridging 1,2-bis(4-pyridyl)ethene ligands, which link these one-dimensional chains into a two-dimensional net extending along the (101) plane.

Related literature

For two-dimensional nets constructed by Cd^{II}, dipyridyl ligands and dicarboxylate ligands, see: Tao *et al.* (2003); Tian *et al.* (2006); Wang *et al.* (2009).



Experimental

Crystal data

$[Cd(C_{10}H_8O_4)(C_{12}H_{10}N_2)]$
M_r = 486.79
Triclinic, $P\overline{1}$
a = 9.4626 (19) Å
b = 10.113 (2) Å
c = 11.351 (2) Å
α = 98.95 (3)°
β = 92.19 (3)°
γ = 116.88 (3)°
V = 949.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 223 K
0.40 × 0.30 × 0.25 mm

Data collection

Rigaku MercuryCCD area-detector diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998) T_{min} = 0.649, T_{max} = 0.757
8582 measured reflections
4256 independent reflections
3630 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.083
S = 1.09
4256 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

This work was supported by the Research Start-Up Fund for New Staff of Huaibei Normal University (grant No. 600581).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2313).

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supplementary materials

Acta Cryst. (2011). E**67**, m1599 [**doi:10.1107/S1600536811043467**]

Poly[[μ_2-1,2-bis(4-pyridyl)ethene](μ_3-1,3-phenylenediacetato)cadmium]

D. Liu

Comment

In recent years, particular attention has been devoted to coordination polymers because of their undisputed beauty and potential applications as materials for adsorption, separation, and catalysis (Tao *et al.*, 2003; Tian *et al.*, 2006; Wang *et al.*, 2009). Conformationally flexible dicarboxylate ligands, showing varied geometries, are often featured in these new classes of compounds (Wang *et al.*, 2009).

In this work, the reaction between $Cd(NO_3)_2$, 1,3-phenylenediacetic acid (1,3-H_2pda) and 1,2-bis(4-pyridyl)ethene (bpe) afforded the title coordination polymer, $[Cd(C_{12}H_{10}N_2)(C_{10}H_8O_4)]_n$ (I). In (I), each Cd^{II} atom is located in a pentagonal bipyramidally environment, coordinated by five O atoms from three different 1,3-pda ligands at the basal positions and two N atom from two different bpe ligands at the apical position (Fig. 1). Two centrosymmetrically related Cd^{II} atoms are linked by two 1,3-pda ligands to form a one-dimensional chain along the *a* axis (Fig. 2). Such a chain is connected to its adjacent ones *via* pairs of bpe ligands to form a two-dimensional net extending along the *ac* plane (Fig. 3).

Experimental

To a 25 ml Teflon-lined stainless steel autoclave was loaded $Cd(NO_3)_2.4H_2O$ (154 mg, 0.5 mmol), 1,3-phenylenediacetic acid (97 mg, 0.5 mmol), 1,2-bis(4-pyridyl)ethene (91 mg, 0.5 mmol), NaOH (40 mg, 1 mmol) and H_2O (15 ml). The autoclave was sealed and heated in an oven to 433 K for three days, and then cooled to ambient temperature at the rate of 5 K/h to form yellow crystals. Yield: 180 mg (74% yield based on Cd). Anal. calcd. for $C_{22}H_{18}CdN_2O_4$: C, 54.28; H, 3.73; N, 5.75. Found: C, 53.96; H, 3.77; N, 6.03.

Refinement

The C-bound H atoms were positioned geometrically, with C–H = 0.97 Å (methylene) or 0.94 Å (phenyl, pyridyl and vinyl), and refined as riding, with U_{iso}(H) = 1.5U_{eq}(C) for methylene groups or 1.2U_{eq}(C) otherwise.

Figures

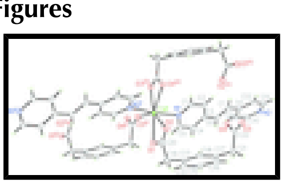


Fig. 1. Coordination environment of Cd^{II} atom in the compound with nonhydrogen atoms represented by thermal ellipsoids draw at 30% probability level. [Symmetry codes: i: *x*, *y* + 1, *z* + 1; ii: *x* – 1, *y*, *z*; iii: – *x* + 1, – *y* + 1, – *z*.]

Fig. 2. View of the one-dimensional chain in the title compound.

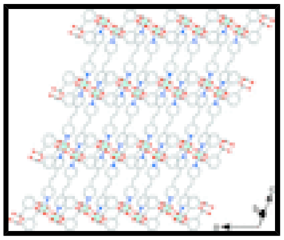


Fig. 3. View of the two-dimensional net of the title compound.

Poly[[μ_2-1,2-bis(4-pyridyl)ethene](μ_3-1,3-phenylenediacetato)cadmium]

Crystal data

$[Cd(C_{10}H_8O_4)(C_{12}H_{10}N_2)]$	$Z = 2$
$M_r = 486.79$	$F(000) = 488$
Triclinic, $P\overline{1}$	$D_x = 1.702$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.4626$ (19) Å	Cell parameters from 4814 reflections
$b = 10.113$ (2) Å	$\theta = 3.2–27.5°$
$c = 11.351$ (2) Å	$\mu = 1.18$ mm^{-1}
$\alpha = 98.95$ (3)°	$T = 223$ K
$\beta = 92.19$ (3)°	Block, yellow
$\gamma = 116.88$ (3)°	0.40 × 0.30 × 0.25 mm
$V = 949.8$ (3) Å^3	

Data collection

Rigaku MercuryCCD area-detector diffractometer	4256 independent reflections
Radiation source: fine-focus sealed tube	3630 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.029$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
Absorption correction: multi-scan (REQAB; Jacobson, 1998)	$h = -12 \rightarrow 11$
$T_{min} = 0.649$, $T_{max} = 0.757$	$k = -12 \rightarrow 12$
8582 measured reflections	$l = -11 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
4256 reflections	$\Delta\rho_{max} = 1.16$ e Å^{-3}
263 parameters	$\Delta\rho_{min} = -0.85$ e Å^{-3}

0 restraints	Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.098 (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	0.16456 (3)	0.49799 (2)	0.10431 (2)	0.02493 (12)
N1	0.1884 (3)	0.3281 (3)	−0.0471 (3)	0.0287 (6)
N2	0.1751 (3)	−0.3077 (3)	−0.7491 (2)	0.0266 (6)
O1	0.1024 (3)	0.3142 (3)	0.2322 (2)	0.0353 (6)
O2	0.3550 (3)	0.4760 (2)	0.2348 (2)	0.0350 (6)
O3	0.8868 (3)	0.3906 (3)	0.0535 (2)	0.0362 (6)
O4	0.6363 (3)	0.2894 (3)	−0.0233 (2)	0.0336 (6)
C1	0.2978 (4)	0.3687 (4)	−0.1239 (3)	0.0338 (8)
H1	0.3788	0.4693	−0.1097	0.041*
C2	0.2974 (4)	0.2702 (4)	−0.2224 (3)	0.0325 (8)
H2	0.3759	0.3039	−0.2745	0.039*
C3	0.1791 (4)	0.1192 (3)	−0.2445 (3)	0.0288 (7)
C4	0.0700 (4)	0.0771 (4)	−0.1623 (3)	0.0355 (8)
H4	−0.0090	−0.0239	−0.1714	0.043*
C5	0.0775 (5)	0.1841 (4)	−0.0670 (3)	0.0365 (9)
H5	0.0006	0.1536	−0.0135	0.044*
C6	0.1591 (4)	0.0064 (4)	−0.3510 (3)	0.0337 (8)
H6	0.0776	−0.0924	−0.3543	0.040*
C7	0.2438 (4)	0.0293 (4)	−0.4427 (3)	0.0320 (8)
H7	0.3282	0.1267	−0.4391	0.038*
C8	0.2160 (4)	−0.0861 (3)	−0.5501 (3)	0.0291 (7)
C9	0.3390 (4)	−0.0707 (4)	−0.6182 (3)	0.0315 (8)
H9	0.4385	0.0162	−0.5989	0.038*
C10	0.3148 (4)	−0.1832 (4)	−0.7145 (3)	0.0315 (8)
H10	0.4008	−0.1718	−0.7580	0.038*
C11	0.0541 (4)	−0.3206 (4)	−0.6863 (3)	0.0299 (7)
H11	−0.0458	−0.4061	−0.7103	0.036*
C12	0.0698 (4)	−0.2139 (4)	−0.5878 (3)	0.0331 (8)
H12	−0.0183	−0.2276	−0.5462	0.040*

C13	0.4592 (4)	0.2971 (3)	0.3492 (3)	0.0284 (7)
C14	0.5692 (4)	0.3628 (4)	0.4528 (3)	0.0323 (8)
H14	0.5405	0.4004	0.5239	0.039*
C15	0.7199 (4)	0.3733 (4)	0.4519 (3)	0.0358 (8)
H15	0.7939	0.4199	0.5218	0.043*
C16	0.7619 (4)	0.3156 (4)	0.3491 (3)	0.0347 (8)
H16	0.8649	0.3239	0.3490	0.042*
C17	0.6528 (4)	0.2449 (4)	0.2447 (3)	0.0301 (8)
C18	0.5032 (4)	0.2396 (3)	0.2462 (3)	0.0305 (8)
H18	0.4304	0.1959	0.1757	0.037*
C19	0.2923 (4)	0.2811 (4)	0.3494 (3)	0.0320 (8)
H19A	0.2798	0.3177	0.4316	0.038*
H19B	0.2160	0.1733	0.3279	0.038*
C20	0.2475 (4)	0.3636 (3)	0.2656 (3)	0.0243 (7)
C21	0.6985 (4)	0.1814 (4)	0.1321 (3)	0.0334 (8)
H21A	0.6091	0.0842	0.0934	0.040*
H21B	0.7899	0.1645	0.1525	0.040*
C22	0.7419 (4)	0.2925 (3)	0.0462 (3)	0.0265 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03223 (17)	0.02483 (16)	0.01910 (16)	0.01568 (11)	0.00324 (10)	0.00013 (9)
N1	0.0356 (15)	0.0267 (14)	0.0227 (16)	0.0157 (12)	0.0049 (13)	−0.0021 (11)
N2	0.0348 (15)	0.0267 (13)	0.0190 (15)	0.0167 (12)	0.0024 (12)	−0.0013 (11)
O1	0.0246 (12)	0.0387 (13)	0.0438 (17)	0.0143 (10)	0.0011 (11)	0.0135 (11)
O2	0.0269 (12)	0.0334 (12)	0.0422 (16)	0.0094 (10)	0.0020 (11)	0.0162 (11)
O3	0.0282 (13)	0.0411 (14)	0.0372 (16)	0.0120 (11)	0.0061 (11)	0.0143 (12)
O4	0.0324 (13)	0.0397 (13)	0.0278 (15)	0.0161 (11)	0.0016 (11)	0.0067 (11)
C1	0.0317 (18)	0.0310 (17)	0.033 (2)	0.0129 (15)	0.0063 (16)	−0.0055 (15)
C2	0.0274 (17)	0.0378 (18)	0.028 (2)	0.0147 (15)	0.0067 (15)	−0.0035 (15)
C3	0.0362 (18)	0.0281 (16)	0.026 (2)	0.0199 (15)	0.0030 (15)	−0.0008 (14)
C4	0.047 (2)	0.0230 (16)	0.030 (2)	0.0120 (15)	0.0084 (17)	0.0004 (14)
C5	0.049 (2)	0.0311 (18)	0.027 (2)	0.0164 (16)	0.0148 (17)	0.0029 (15)
C6	0.039 (2)	0.0275 (17)	0.032 (2)	0.0159 (15)	0.0034 (16)	−0.0022 (14)
C7	0.041 (2)	0.0253 (16)	0.029 (2)	0.0159 (15)	0.0035 (16)	0.0020 (14)
C8	0.043 (2)	0.0264 (16)	0.0231 (19)	0.0208 (15)	0.0025 (15)	0.0031 (14)
C9	0.042 (2)	0.0247 (16)	0.024 (2)	0.0134 (15)	0.0034 (16)	0.0008 (14)
C10	0.0374 (19)	0.0318 (17)	0.0236 (19)	0.0159 (15)	0.0063 (15)	0.0007 (14)
C11	0.0329 (18)	0.0315 (17)	0.0247 (19)	0.0164 (15)	0.0010 (15)	−0.0008 (14)
C12	0.0355 (19)	0.0428 (19)	0.027 (2)	0.0245 (16)	0.0076 (16)	0.0031 (15)
C13	0.0299 (17)	0.0306 (17)	0.028 (2)	0.0145 (14)	0.0065 (15)	0.0121 (15)
C14	0.0363 (19)	0.0346 (18)	0.028 (2)	0.0177 (15)	0.0081 (16)	0.0082 (15)
C15	0.038 (2)	0.0413 (19)	0.030 (2)	0.0211 (17)	−0.0032 (16)	0.0042 (16)
C16	0.0314 (18)	0.0425 (19)	0.039 (2)	0.0221 (16)	0.0070 (17)	0.0140 (17)
C17	0.0367 (19)	0.0299 (17)	0.030 (2)	0.0175 (15)	0.0113 (16)	0.0138 (15)
C18	0.0331 (18)	0.0315 (17)	0.026 (2)	0.0135 (15)	0.0033 (15)	0.0097 (15)
C19	0.0284 (17)	0.0367 (18)	0.031 (2)	0.0137 (15)	0.0060 (15)	0.0119 (15)

C20	0.0279 (17)	0.0261 (15)	0.0211 (18)	0.0148 (14)	0.0042 (14)	0.0035 (13)
C21	0.041 (2)	0.0321 (17)	0.031 (2)	0.0188 (16)	0.0109 (17)	0.0094 (15)
C22	0.0338 (18)	0.0285 (16)	0.0193 (18)	0.0177 (15)	0.0052 (15)	−0.0010 (13)

Geometric parameters (Å, °)

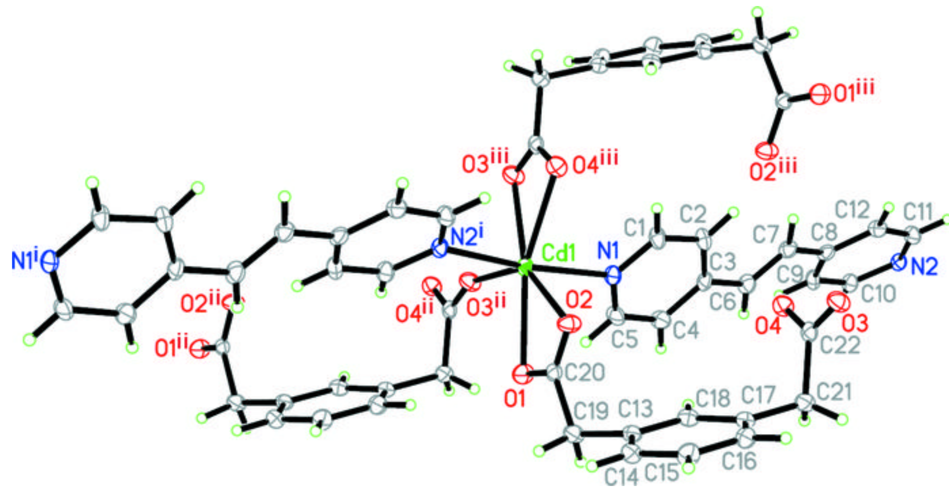
Cd1—N1	2.327 (3)	C6—H6	0.9400
Cd1—N2^{i}	2.332 (3)	C7—C8	1.474 (5)
Cd1—O3^{ii}	2.351 (2)	C7—H7	0.9400
Cd1—O2	2.398 (2)	C8—C9	1.386 (5)
Cd1—O3^{iii}	2.402 (2)	C8—C12	1.390 (5)
Cd1—O1	2.413 (2)	C9—C10	1.378 (5)
Cd1—O4^{iii}	2.470 (2)	C9—H9	0.9400
Cd1—C20	2.729 (3)	C10—H10	0.9400
Cd1—C22^{iii}	2.781 (3)	C11—C12	1.380 (5)
N1—C5	1.331 (4)	C11—H11	0.9400
N1—C1	1.340 (4)	C12—H12	0.9400
N2—C10	1.337 (4)	C13—C18	1.387 (5)
N2—C11	1.338 (4)	C13—C14	1.395 (5)
N2—Cd1^{iv}	2.331 (3)	C13—C19	1.513 (5)
O1—C20	1.249 (4)	C14—C15	1.382 (5)
O2—C20	1.247 (4)	C14—H14	0.9400
O3—C22	1.267 (4)	C15—C16	1.376 (5)
O3—Cd1^{v}	2.351 (2)	C15—H15	0.9400
O3—Cd1^{iii}	2.402 (2)	C16—C17	1.399 (5)
O4—C22	1.235 (4)	C16—H16	0.9400
O4—Cd1^{iii}	2.470 (2)	C17—C18	1.392 (5)
C1—C2	1.376 (5)	C17—C21	1.507 (5)
C1—H1	0.9400	C18—H18	0.9400
C2—C3	1.400 (4)	C19—C20	1.522 (5)
C2—H2	0.9400	C19—H19A	0.9800
C3—C4	1.385 (5)	C19—H19B	0.9800
C3—C6	1.469 (5)	C21—C22	1.529 (5)
C4—C5	1.380 (5)	C21—H21A	0.9800
C4—H4	0.9400	C21—H21B	0.9800
C5—H5	0.9400	C22—Cd1^{iii}	2.781 (3)
C6—C7	1.323 (5)		
N1—Cd1—N2^{i}	172.12 (9)	C3—C4—H4	120.1
N1—Cd1—O3^{ii}	92.92 (10)	N1—C5—C4	123.3 (3)
N2^{i}—Cd1—O3^{ii}	93.60 (10)	N1—C5—H5	118.4
N1—Cd1—O2	88.91 (10)	C4—C5—H5	118.4
N2^{i}—Cd1—O2	88.96 (10)	C7—C6—C3	126.8 (3)
O3^{ii}—Cd1—O2	139.86 (8)	C7—C6—H6	116.6
N1—Cd1—O3^{iii}	86.43 (9)	C3—C6—H6	116.6
N2^{i}—Cd1—O3^{iii}	91.45 (9)	C6—C7—C8	125.0 (3)

O3^{ii}—Cd1—O3^{iii}	71.46 (9)	C6—C7—H7	117.5
O2—Cd1—O3^{iii}	148.59 (8)	C8—C7—H7	117.5
N1—Cd1—O1	88.59 (9)	C9—C8—C12	116.8 (3)
N2^{i}—Cd1—O1	96.33 (9)	C9—C8—C7	120.0 (3)
O3^{ii}—Cd1—O1	85.54 (8)	C12—C8—C7	123.1 (3)
O2—Cd1—O1	54.39 (8)	C10—C9—C8	119.7 (3)
O3^{iii}—Cd1—O1	156.16 (8)	C10—C9—H9	120.1
N1—Cd1—O4^{iii}	89.83 (9)	C8—C9—H9	120.1
N2^{i}—Cd1—O4^{iii}	82.82 (9)	N2—C10—C9	123.3 (3)
O3^{ii}—Cd1—O4^{iii}	124.49 (8)	N2—C10—H10	118.4
O2—Cd1—O4^{iii}	95.59 (8)	C9—C10—H10	118.4
O3^{iii}—Cd1—O4^{iii}	53.40 (8)	N2—C11—C12	122.8 (3)
O1—Cd1—O4^{iii}	149.96 (8)	N2—C11—H11	118.6
N1—Cd1—C20	87.53 (10)	C12—C11—H11	118.6
N2^{i}—Cd1—C20	94.02 (10)	C11—C12—C8	120.0 (3)
O3^{ii}—Cd1—C20	112.79 (9)	C11—C12—H12	120.0
O2—Cd1—C20	27.18 (8)	C8—C12—H12	120.0
O3^{iii}—Cd1—C20	172.80 (8)	C18—C13—C14	118.6 (3)
O1—Cd1—C20	27.25 (8)	C18—C13—C19	120.1 (3)
O4^{iii}—Cd1—C20	122.72 (9)	C14—C13—C19	121.3 (3)
N1—Cd1—C22^{iii}	88.67 (9)	C15—C14—C13	120.6 (3)
N2^{i}—Cd1—C22^{iii}	86.02 (9)	C15—C14—H14	119.7
O3^{ii}—Cd1—C22^{iii}	98.26 (10)	C13—C14—H14	119.7
O2—Cd1—C22^{iii}	121.88 (9)	C16—C15—C14	120.2 (4)
O3^{iii}—Cd1—C22^{iii}	27.06 (9)	C16—C15—H15	119.9
O1—Cd1—C22^{iii}	175.42 (8)	C14—C15—H15	119.9
O4^{iii}—Cd1—C22^{iii}	26.36 (9)	C15—C16—C17	120.6 (3)
C20—Cd1—C22^{iii}	148.87 (10)	C15—C16—H16	119.7
N1—Cd1—Cd1^{vi}	89.56 (8)	C17—C16—H16	119.7
N2^{i}—Cd1—Cd1^{vi}	93.09 (8)	C18—C17—C16	118.3 (3)
O3^{ii}—Cd1—Cd1^{vi}	36.17 (6)	C18—C17—C21	120.9 (3)
O2—Cd1—Cd1^{vi}	175.62 (5)	C16—C17—C21	120.7 (3)
O3^{iii}—Cd1—Cd1^{vi}	35.29 (6)	C13—C18—C17	121.6 (3)
O1—Cd1—Cd1^{vi}	121.47 (6)	C13—C18—H18	119.2
O4^{iii}—Cd1—Cd1^{vi}	88.51 (6)	C17—C18—H18	119.2
C20—Cd1—Cd1^{vi}	148.61 (7)	C13—C19—C20	116.1 (3)
C22^{iii}—Cd1—Cd1^{vi}	62.17 (8)	C13—C19—H19A	108.3
C5—N1—C1	117.3 (3)	C20—C19—H19A	108.3
C5—N1—Cd1	118.4 (2)	C13—C19—H19B	108.3
C1—N1—Cd1	124.0 (2)	C20—C19—H19B	108.3
C10—N2—C11	117.2 (3)	H19A—C19—H19B	107.4
C10—N2—Cd1^{iv}	118.7 (2)	O2—C20—O1	123.5 (3)

C11—N2—Cd1^{iv}	123.5 (2)	O2—C20—C19	119.4 (3)
C20—O1—Cd1	90.57 (19)	O1—C20—C19	117.1 (3)
C20—O2—Cd1	91.3 (2)	O2—C20—Cd1	61.47 (17)
C22—O3—Cd1^{v}	156.6 (2)	O1—C20—Cd1	62.18 (17)
C22—O3—Cd1^{iii}	93.4 (2)	C19—C20—Cd1	176.6 (2)
Cd1^{v}—O3—Cd1^{iii}	108.54 (9)	C17—C21—C22	109.4 (3)
C22—O4—Cd1^{iii}	91.02 (19)	C17—C21—H21A	109.8
N1—C1—C2	123.2 (3)	C22—C21—H21A	109.8
N1—C1—H1	118.4	C17—C21—H21B	109.8
C2—C1—H1	118.4	C22—C21—H21B	109.8
C1—C2—C3	119.4 (3)	H21A—C21—H21B	108.2
C1—C2—H2	120.3	O4—C22—O3	122.1 (3)
C3—C2—H2	120.3	O4—C22—C21	120.0 (3)
C4—C3—C2	116.9 (3)	O3—C22—C21	117.7 (3)
C4—C3—C6	118.5 (3)	O4—C22—Cd1^{iii}	62.63 (17)
C2—C3—C6	124.5 (3)	O3—C22—Cd1^{iii}	59.56 (17)
C5—C4—C3	119.8 (3)	C21—C22—Cd1^{iii}	177.3 (3)
C5—C4—H4	120.1		

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

Fig. 1


O1iii
O3iii
O4iii
O2iii
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N2i
Cd1
N1
C1
C2
C3
C7
C8
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C11
N2
C9
C10
C6
O2
O4ii
O3ii
O2ii
O1ii
O4
O3
C22
C5
C4
C20
O1
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C14
C15

Fig. 2

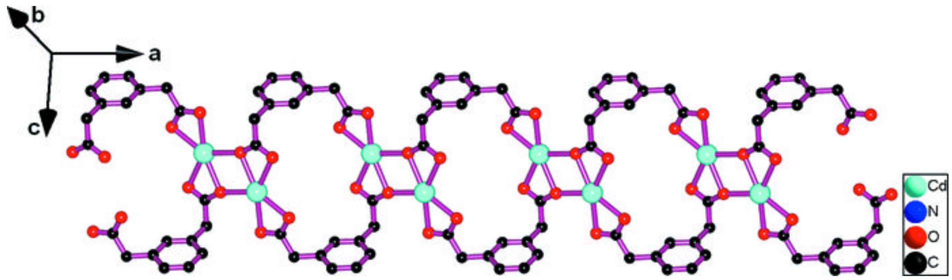

Fig. 3