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Poly[(μ_3-acetylenedicarboxylato-$\kappa^4O,O':O'':O'''$)(1,10-phenanthroline-κ^2N,N')cadmium(II)]

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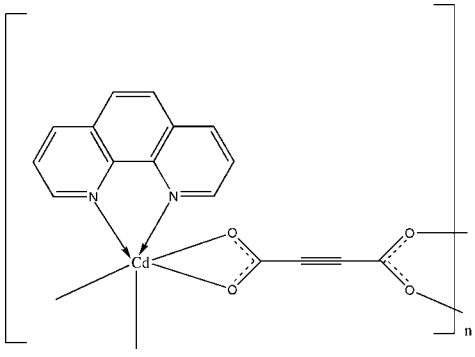
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.023; wR factor = 0.058; data-to-parameter ratio = 15.2.

In the title complex, $[Cd(C_4O_4)(C_{10}H_8N_2)]_n$, the Cd atom exists in a trigonal-prismatic geometry that is defined by the two N atoms of a 1,10-phenanthroline ligand and the four carboxylate O atoms of two different acetylenedicarboxylate dianions. Adjacent Cd atoms are bridged by acetylenedicarboxylate dianions, giving rise to a two-dimensional structure parallel to (100).

Related literature

The manganese(II) and cobalt(II) complexes of acetylenedicarboxylate have been characterized by X-ray crystallography (Wang *et al.*, 2006*a*,*b*).



Experimental

Crystal data

$[Cd(C_4O_4)(C_{10}H_8N_2)]$
M_r = 404.64
Monoclinic, $P2_1/c$
a = 9.6365 (19) Å
b = 17.140 (3) Å
c = 8.4144 (17) Å
β = 90.68 (3)°
V = 1389.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 293 (2) K
0.34 × 0.24 × 0.20 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.613, T_{max} = 0.741
13389 measured reflections
3168 independent reflections
2913 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.058
S = 1.12
3168 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O4^{i}	2.2219 (17)	Cd1—N1	2.339 (2)
Cd1—N2	2.3052 (19)	Cd1—O1	2.3386 (18)
Cd1—O3^{ii}	2.3227 (18)	Cd1—O2	2.4520 (18)
O4^{i}—Cd1—N2	125.44 (7)	O3^{ii}—Cd1—O1	111.25 (7)
O4^{i}—Cd1—O3^{ii}	81.99 (7)	N1—Cd1—O1	89.86 (7)
N2—Cd1—O3^{ii}	86.18 (7)	O4^{i}—Cd1—O2	141.24 (6)
O4^{i}—Cd1—N1	106.04 (7)	N2—Cd1—O2	92.40 (6)
N2—Cd1—N1	72.05 (7)	O3^{ii}—Cd1—O2	93.85 (6)
O3^{ii}—Cd1—N1	157.58 (7)	N1—Cd1—O2	92.37 (6)
O4^{i}—Cd1—O1	90.75 (7)	O1—Cd1—O2	54.79 (6)
N2—Cd1—O1	142.43 (6)		

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2365).

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supplementary materials

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Poly[(μ_3-acetylenedicarboxylato-$\kappa^4O,O':O'':O'''$)(1,10-phenanthroline-κ^2N,N')cadmium(II)]

H.-Y. Wang, S. Gao, L.-H. Huo and J.-G. Zhao

Comment

We are interested in the solid-state coordination chemistry of acetylenedicarboxylate acid, combining with specific transition metals to fabricate versatile coordination polymers. Some one-dimensional metal-organic frameworks have been reported (Wang *et al.*, 2006*a*; Wang *et al.*, 2006*b*). In order to further explore the behaviour of the acetylenedicarboxylate acid ligand, a new two-dimensional cadmium(II) complex had been obtained.

The molecular strucrure of the title compound is illustated in Fig. 1. Each Cd^{II} ion is a distorted trigonal prismatic geometry, defined by two N atoms of a 1,10-phenanthroline ligand and four carboxyl O atoms of two different acetylenedicarboxylate dianions. Adjacent Cd^{II} ions are bridged by tetradentate acetylenedicarboxylate dianions, giving rise to a two-dimensional structure parallel to (100) (Table 2 and Fig. 2).

Experimental

The title complex was prepared by the addition of cadmium nitrate tetrahydrate(1 mmol) and 1,10-phenanthroline (1 mmol) to a DMF solution of acetylenedicarboxylate acid (1 mmol). The pH value of the solution was adjusted to 7 with 1.0 mol/*L* NaOH solution. After the mixture was stirred for 30 min, the residue was filtered. The filtrate was allowed to evaporate at room temperature and crystals were obtained after two weeks. Analysis calculated for $C_{16}H_8CdN_2O_4$: C 47.30, H 1.99, N 6.90%; found: C 47.32, H 1.96, N 6.91%.

Refinement

The H atoms were placed in calculated positions with C—H = 0.93 or 0.97Å and U_{iso}(H) = 1.2U_{eq} (C) and were included in the refinement in the riding model approximation.

Figures

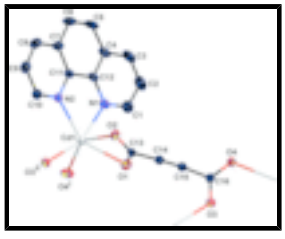


Fig. 1. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. [Symmetry code: (i) −*x*,*y* + 1/2,-*z* + 1/2, (ii) −*x*,-*y*,-*z* + 1]

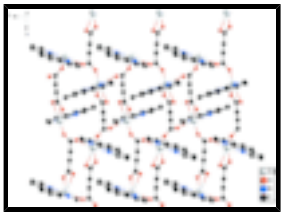


Fig. 2. The two-dimensional structure of the title complex. H atoms have been omitted for clarify

Poly[(μ$_3$-acetylenedicarboxylato-κ^4*O*,*O*':*O*'': *O*''')(1,10-phenanthroline-κ^2*N*,*N*')cadmium(II)]

Crystal data

$[Cd(C_4O_4)(C_{10}H_8N_2)]$	F_{000} = 792
M_r = 404.64	D_x = 1.934 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 11965 reflections
a = 9.6365 (19) Å	θ = 3.2–27.4º
b = 17.140 (3) Å	μ = 1.59 mm^{-1}
c = 8.4144 (17) Å	T = 293 (2) K
β = 90.68 (3)º	Block, colorless
V = 1389.7 (5) Å^3	0.34 × 0.24 × 0.20 mm
Z = 4	

Data collection

Rigaku RAXIS-RAPID diffractometer	3168 independent reflections
Radiation source: fine-focus sealed tube	2913 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.018
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.4º
T = 293(2) K	θ_{min} = 3.2º
ω scans	h = −12→12
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −22→21
T_{min} = 0.613, T_{max} = 0.741	l = −10→10
13389 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.023	H-atom parameters constrained
$wR(F^2)$ = 0.058	$w = 1/[\sigma^2(F_o^2) + (0.0262P)^2 + 0.9731P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max}$ = 0.002
3168 reflections	$\Delta\rho_{max}$ = 0.68 e Å^{-3}

208 parameters	$\Delta\rho_{min} = -0.28$ 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	0.216980 (16)	0.149141 (9)	0.29728 (2)	0.03198 (7)
O1	0.04393 (18)	0.05514 (11)	0.2587 (2)	0.0491 (4)
O2	0.22377 (18)	0.01572 (10)	0.4022 (2)	0.0426 (4)
O3	−0.20190 (18)	−0.20600 (10)	0.4529 (2)	0.0419 (4)
O4	−0.06832 (19)	−0.25630 (11)	0.2651 (2)	0.0498 (5)
N1	0.3193 (2)	0.11138 (11)	0.0587 (2)	0.0357 (4)
N2	0.45379 (19)	0.16375 (11)	0.3256 (2)	0.0327 (4)
C1	0.2543 (3)	0.08390 (16)	−0.0704 (3)	0.0477 (6)
H1	0.1581	0.0797	−0.0696	0.057*
C2	0.3253 (4)	0.06101 (18)	−0.2075 (3)	0.0550 (7)
H2	0.2767	0.0420	−0.2954	0.066*
C3	0.4649 (3)	0.06691 (16)	−0.2103 (3)	0.0521 (7)
H3	0.5130	0.0520	−0.3006	0.062*
C4	0.5380 (3)	0.09571 (14)	−0.0763 (3)	0.0431 (6)
C5	0.6862 (3)	0.10271 (18)	−0.0697 (4)	0.0568 (8)
H5	0.7373	0.0912	−0.1599	0.068*
C6	0.7533 (3)	0.12547 (19)	0.0633 (4)	0.0565 (7)
H6	0.8497	0.1287	0.0648	0.068*
C7	0.6766 (3)	0.14488 (14)	0.2034 (3)	0.0433 (6)
C8	0.7421 (3)	0.16644 (18)	0.3470 (4)	0.0529 (7)
H8	0.8384	0.1681	0.3543	0.063*
C9	0.6646 (3)	0.18468 (17)	0.4740 (4)	0.0511 (7)
H9	0.7070	0.1975	0.5703	0.061*
C10	0.5198 (3)	0.18415 (14)	0.4597 (3)	0.0409 (5)
H10	0.4675	0.1986	0.5470	0.049*
C11	0.5307 (2)	0.14312 (12)	0.1989 (3)	0.0332 (5)
C12	0.4596 (2)	0.11687 (13)	0.0562 (3)	0.0336 (5)
C13	0.1090 (2)	0.00483 (13)	0.3364 (3)	0.0352 (5)
C14	0.0436 (2)	−0.07199 (14)	0.3495 (3)	0.0352 (5)
C15	−0.0146 (2)	−0.13369 (14)	0.3593 (3)	0.0355 (5)

C16	−0.1001 (2)	−0.20456 (13)	0.3621 (3)	0.0328 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02869 (9)	0.02783 (9)	0.03960 (10)	0.00070 (6)	0.00744 (6)	−0.00041 (6)
O1	0.0420 (9)	0.0378 (9)	0.0677 (12)	−0.0010 (8)	0.0037 (9)	0.0061 (9)
O2	0.0401 (9)	0.0395 (9)	0.0482 (10)	−0.0113 (7)	0.0029 (8)	−0.0053 (8)
O3	0.0419 (9)	0.0367 (9)	0.0474 (10)	−0.0073 (7)	0.0138 (7)	−0.0062 (7)
O4	0.0443 (10)	0.0418 (10)	0.0636 (12)	−0.0123 (8)	0.0195 (9)	−0.0213 (9)
N1	0.0396 (10)	0.0336 (10)	0.0340 (10)	0.0042 (8)	0.0032 (8)	0.0024 (8)
N2	0.0316 (9)	0.0272 (9)	0.0392 (10)	−0.0005 (7)	0.0060 (8)	−0.0004 (8)
C1	0.0539 (15)	0.0504 (15)	0.0385 (13)	0.0049 (12)	−0.0078 (11)	−0.0003 (11)
C2	0.081 (2)	0.0500 (16)	0.0342 (13)	0.0111 (15)	−0.0083 (13)	−0.0006 (11)
C3	0.077 (2)	0.0434 (14)	0.0361 (13)	0.0170 (13)	0.0138 (13)	0.0027 (11)
C4	0.0551 (15)	0.0342 (12)	0.0403 (13)	0.0119 (11)	0.0146 (11)	0.0045 (10)
C5	0.0513 (16)	0.0576 (17)	0.0621 (18)	0.0172 (13)	0.0323 (14)	0.0043 (14)
C6	0.0362 (13)	0.0643 (18)	0.069 (2)	0.0104 (13)	0.0206 (13)	0.0025 (16)
C7	0.0326 (12)	0.0388 (13)	0.0588 (16)	0.0046 (10)	0.0095 (11)	0.0059 (11)
C8	0.0318 (12)	0.0570 (17)	0.0698 (19)	0.0000 (12)	−0.0037 (12)	0.0018 (15)
C9	0.0452 (14)	0.0486 (15)	0.0593 (17)	−0.0022 (12)	−0.0114 (13)	−0.0034 (13)
C10	0.0425 (13)	0.0368 (12)	0.0433 (13)	−0.0017 (10)	0.0019 (10)	−0.0034 (10)
C11	0.0334 (11)	0.0250 (10)	0.0413 (12)	0.0028 (8)	0.0077 (9)	0.0042 (9)
C12	0.0385 (11)	0.0265 (10)	0.0360 (11)	0.0079 (9)	0.0076 (9)	0.0038 (9)
C13	0.0356 (11)	0.0319 (11)	0.0384 (12)	−0.0065 (9)	0.0155 (9)	−0.0089 (9)
C14	0.0310 (10)	0.0350 (12)	0.0398 (12)	−0.0010 (9)	0.0032 (9)	−0.0069 (9)
C15	0.0325 (11)	0.0360 (12)	0.0381 (12)	−0.0028 (9)	0.0060 (9)	−0.0057 (9)
C16	0.0284 (10)	0.0311 (11)	0.0387 (12)	−0.0023 (8)	0.0005 (9)	−0.0037 (9)

Geometric parameters (Å, °)

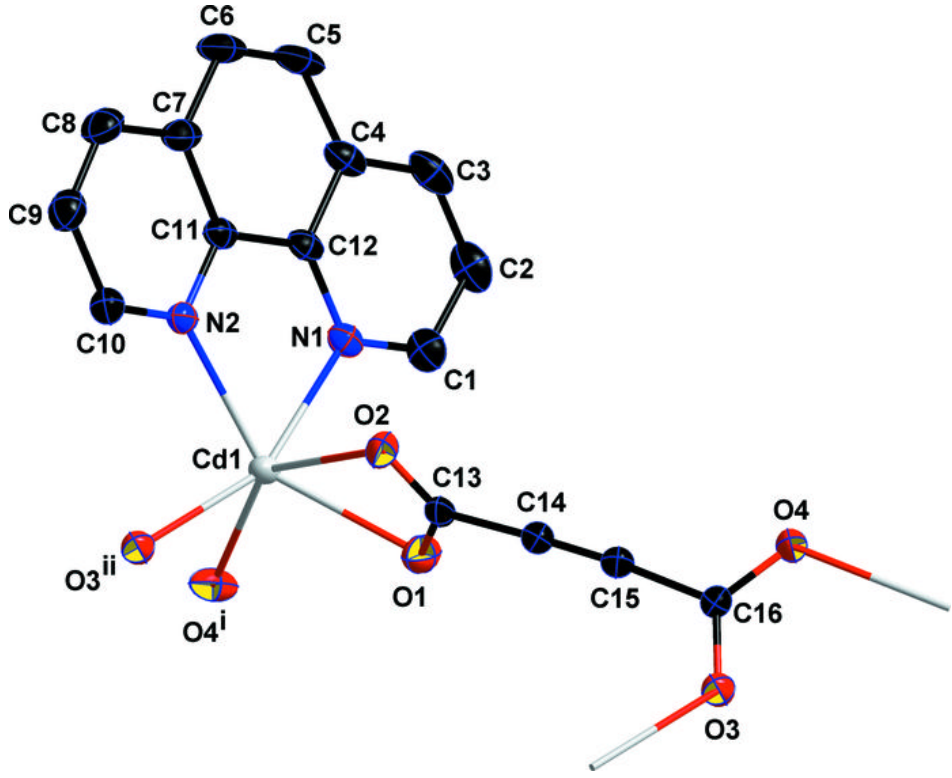
Cd1—O4^{i}	2.2219 (17)	C2—H2	0.9300
Cd1—N2	2.3052 (19)	C3—C4	1.412 (4)
Cd1—O3^{ii}	2.3227 (18)	C3—H3	0.9300
Cd1—N1	2.339 (2)	C4—C12	1.402 (3)
Cd1—O1	2.3386 (18)	C4—C5	1.433 (4)
Cd1—O2	2.4520 (18)	C5—C6	1.344 (5)
Cd1—C13	2.705 (2)	C5—H5	0.9300
O1—C13	1.246 (3)	C6—C7	1.438 (4)
O2—C13	1.246 (3)	C6—H6	0.9300
O3—C16	1.251 (3)	C7—C11	1.406 (3)
O3—Cd1^{ii}	2.3227 (18)	C7—C8	1.405 (4)
O4—C16	1.246 (3)	C8—C9	1.348 (4)
O4—Cd1^{iii}	2.2219 (17)	C8—H8	0.9300
N1—C1	1.334 (3)	C9—C10	1.399 (4)
N1—C12	1.355 (3)	C9—H9	0.9300
N2—C10	1.335 (3)	C10—H10	0.9300
N2—C11	1.352 (3)	C11—C12	1.448 (3)

C1—C2	1.404 (4)	C13—C14	1.464 (3)
C1—H1	0.9300	C14—C15	1.200 (3)
C2—C3	1.350 (4)	C15—C16	1.468 (3)
O4^{i}—Cd1—N2	125.44 (7)	C4—C3—H3	120.0
O4^{i}—Cd1—O3^{ii}	81.99 (7)	C12—C4—C3	117.2 (3)
N2—Cd1—O3^{ii}	86.18 (7)	C12—C4—C5	119.6 (3)
O4^{i}—Cd1—N1	106.04 (7)	C3—C4—C5	123.2 (3)
N2—Cd1—N1	72.05 (7)	C6—C5—C4	121.7 (3)
O3^{ii}—Cd1—N1	157.58 (7)	C6—C5—H5	119.2
O4^{i}—Cd1—O1	90.75 (7)	C4—C5—H5	119.2
N2—Cd1—O1	142.43 (6)	C5—C6—C7	120.2 (3)
O3^{ii}—Cd1—O1	111.25 (7)	C5—C6—H6	119.9
N1—Cd1—O1	89.86 (7)	C7—C6—H6	119.9
O4^{i}—Cd1—O2	141.24 (6)	C11—C7—C8	117.9 (3)
N2—Cd1—O2	92.40 (6)	C11—C7—C6	119.8 (3)
O3^{ii}—Cd1—O2	93.85 (6)	C8—C7—C6	122.4 (3)
N1—Cd1—O2	92.37 (6)	C9—C8—C7	119.7 (3)
O1—Cd1—O2	54.79 (6)	C9—C8—H8	120.2
O4^{i}—Cd1—C13	116.60 (7)	C7—C8—H8	120.2
N2—Cd1—C13	117.95 (7)	C8—C9—C10	119.5 (3)
O3^{ii}—Cd1—C13	104.21 (6)	C8—C9—H9	120.3
N1—Cd1—C13	91.03 (7)	C10—C9—H9	120.3
O1—Cd1—C13	27.40 (7)	N2—C10—C9	122.6 (2)
O2—Cd1—C13	27.39 (7)	N2—C10—H10	118.7
C13—O1—Cd1	92.90 (14)	C9—C10—H10	118.7
C13—O2—Cd1	87.69 (14)	N2—C11—C7	122.0 (2)
C16—O3—Cd1^{ii}	127.05 (15)	N2—C11—C12	118.5 (2)
C16—O4—Cd1^{iii}	120.75 (15)	C7—C11—C12	119.5 (2)
C1—N1—C12	118.1 (2)	N1—C12—C4	122.8 (2)
C1—N1—Cd1	126.75 (18)	N1—C12—C11	118.1 (2)
C12—N1—Cd1	115.14 (15)	C4—C12—C11	119.0 (2)
C10—N2—C11	118.3 (2)	O2—C13—O1	124.6 (2)
C10—N2—Cd1	125.24 (16)	O2—C13—C14	118.8 (2)
C11—N2—Cd1	116.20 (15)	O1—C13—C14	116.6 (2)
N1—C1—C2	122.6 (3)	O2—C13—Cd1	64.92 (12)
N1—C1—H1	118.7	O1—C13—Cd1	59.70 (12)
C2—C1—H1	118.7	C14—C13—Cd1	176.22 (18)
C3—C2—C1	119.3 (3)	C15—C14—C13	177.6 (3)
C3—C2—H2	120.4	C14—C15—C16	173.2 (3)
C1—C2—H2	120.4	O4—C16—O3	125.9 (2)
C2—C3—C4	120.0 (2)	O4—C16—C15	115.9 (2)
C2—C3—H3	120.0	O3—C16—C15	118.0 (2)
O4^{i}—Cd1—O1—C13	−161.44 (15)	C11—C7—C8—C9	−0.1 (4)
N2—Cd1—O1—C13	33.1 (2)	C6—C7—C8—C9	179.4 (3)
O3^{ii}—Cd1—O1—C13	−79.74 (15)	C7—C8—C9—C10	−1.9 (4)

N1—Cd1—O1—C13	92.52 (15)	C11—N2—C10—C9	−0.2 (4)
O2—Cd1—O1—C13	−0.48 (13)	Cd1—N2—C10—C9	173.54 (19)
O4^{i}—Cd1—O2—C13	31.88 (18)	C8—C9—C10—N2	2.2 (4)
N2—Cd1—O2—C13	−159.79 (14)	C10—N2—C11—C7	−1.9 (3)
O3^{ii}—Cd1—O2—C13	113.87 (14)	Cd1—N2—C11—C7	−176.29 (17)
N1—Cd1—O2—C13	−87.67 (14)	C10—N2—C11—C12	176.7 (2)
O1—Cd1—O2—C13	0.48 (13)	Cd1—N2—C11—C12	2.3 (2)
O4^{i}—Cd1—N1—C1	−59.1 (2)	C8—C7—C11—N2	2.2 (4)
N2—Cd1—N1—C1	178.1 (2)	C6—C7—C11—N2	−177.4 (2)
O3^{ii}—Cd1—N1—C1	−167.56 (19)	C8—C7—C11—C12	−176.4 (2)
O1—Cd1—N1—C1	31.6 (2)	C6—C7—C11—C12	4.0 (4)
O2—Cd1—N1—C1	86.4 (2)	C1—N1—C12—C4	0.7 (3)
C13—Cd1—N1—C1	59.0 (2)	Cd1—N1—C12—C4	179.14 (17)
O4^{i}—Cd1—N1—C12	122.60 (16)	C1—N1—C12—C11	−177.1 (2)
N2—Cd1—N1—C12	−0.16 (15)	Cd1—N1—C12—C11	1.4 (2)
O3^{ii}—Cd1—N1—C12	14.1 (3)	C3—C4—C12—N1	−0.7 (3)
O1—Cd1—N1—C12	−146.67 (16)	C5—C4—C12—N1	−179.6 (2)
O2—Cd1—N1—C12	−91.92 (16)	C3—C4—C12—C11	177.0 (2)
C13—Cd1—N1—C12	−119.29 (16)	C5—C4—C12—C11	−1.9 (3)
O4^{i}—Cd1—N2—C10	87.7 (2)	N2—C11—C12—N1	−2.5 (3)
O3^{ii}—Cd1—N2—C10	10.37 (19)	C7—C11—C12—N1	176.1 (2)
N1—Cd1—N2—C10	−175.0 (2)	N2—C11—C12—C4	179.7 (2)
O1—Cd1—N2—C10	−110.2 (2)	C7—C11—C12—C4	−1.7 (3)
O2—Cd1—N2—C10	−83.33 (19)	Cd1—O2—C13—O1	−0.9 (2)
C13—Cd1—N2—C10	−93.70 (19)	Cd1—O2—C13—C14	179.21 (18)
O4^{i}—Cd1—N2—C11	−98.38 (16)	Cd1—O1—C13—O2	0.9 (3)
O3^{ii}—Cd1—N2—C11	−175.73 (16)	Cd1—O1—C13—C14	−179.17 (17)
N1—Cd1—N2—C11	−1.15 (15)	O4^{i}—Cd1—C13—O2	−158.30 (13)
O1—Cd1—N2—C11	63.7 (2)	N2—Cd1—C13—O2	23.00 (15)
O2—Cd1—N2—C11	90.56 (15)	O3^{ii}—Cd1—C13—O2	−70.25 (14)
C13—Cd1—N2—C11	80.20 (16)	N1—Cd1—C13—O2	93.15 (14)
C12—N1—C1—C2	−0.3 (4)	O1—Cd1—C13—O2	−179.2 (2)
Cd1—N1—C1—C2	−178.5 (2)	O4^{i}—Cd1—C13—O1	20.85 (17)
N1—C1—C2—C3	−0.1 (4)	N2—Cd1—C13—O1	−157.85 (14)
C1—C2—C3—C4	0.1 (4)	O3^{ii}—Cd1—C13—O1	108.90 (15)
C2—C3—C4—C12	0.3 (4)	N1—Cd1—C13—O1	−87.69 (15)
C2—C3—C4—C5	179.2 (3)	O2—Cd1—C13—O1	179.2 (2)
C12—C4—C5—C6	3.4 (4)	Cd1^{iii}—O4—C16—O3	13.0 (4)
C3—C4—C5—C6	−175.5 (3)	Cd1^{iii}—O4—C16—C15	−162.39 (16)
C4—C5—C6—C7	−1.1 (5)	Cd1^{ii}—O3—C16—O4	149.4 (2)
C5—C6—C7—C11	−2.6 (4)	Cd1^{ii}—O3—C16—C15	−35.3 (3)
C5—C6—C7—C8	177.8 (3)		

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

Fig. 1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C16
O4i
O3

Fig. 2