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catena-Poly[[(dipyrido[3,2-*a*:2′,3′-*c*]-phenazine)cadmium(II)]-μ-biphenyl-2,2′-dicarboxylato]

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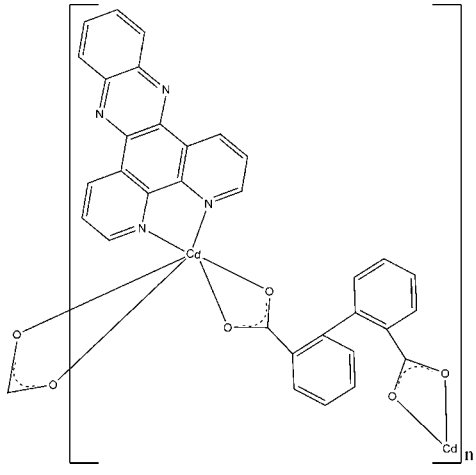
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.007 Å; R factor = 0.047; wR factor = 0.101; data-to-parameter ratio = 13.6.

In the title compound, $[Cd(C_{14}H_8O_4)(C_{18}H_{10}N_4)]_n$, the Cd^{II} atom is coordinated by four O atoms from two different biphenyl-2,2′-dicarboxylate (bdc) dianions and two N atoms from the bidentate dipyrido[3,2-*a*:2′,3′-*c*]phenazine (*L*) ligand, resulting in a very distorted *cis*-CdN_2O_4 octahedral geometry. The Cd^{II} ions are bridged by the bdc ligands to form a one-dimensional chain structure. Neighboring chains interact through π–π interactions [centroid-to-centroid separation = 3.496 (3) Å], resulting in a two-dimensional supramolecular network.

Related literature

For related literature, see: Li *et al.* (2006); Noveron *et al.* (2002). For the ligand synthesis, see: Dickeson & Summers (1970).



Experimental

Crystal data

$[Cd(C_{14}H_8O_4)(C_{18}H_{10}N_4)]$
M_r = 634.90
Monoclinic, $P2_1/n$
a = 9.4547 (10) Å
b = 12.4137 (13) Å
c = 22.015 (2) Å
β = 100.414 (2)°
V = 2541.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.91 mm^{-1}
T = 292 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.881, T_{max} = 0.915
13546 measured reflections
5027 independent reflections
2971 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.101
S = 0.95
5027 reflections
370 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.311 (4)	Cd1—O3^{i}	2.296 (3)
Cd1—N2	2.333 (4)	Cd1—O4^{i}	2.342 (3)
Cd1—O1	2.294 (4)	Cd1—O2	2.344 (3)
N1—Cd1—N2	71.16 (14)	O1—Cd1—O2	56.04 (12)
O3^{i}—Cd1—O4^{i}	56.27 (11)		

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: HB2577).

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supplementary materials

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catena-Poly[[(dipyrido[3,2-*a*:2',3'-*c*]phenazine)cadmium(II)]-μ-biphenyl-2,2'-dicarboxylato]

X.-J. Jin, W. Fang and X.-P. Li

Comment

The chelating ligand 1,10-phenanthroline (phen) and its derivatives have been widely used in the construction of metal–organic coordination polymers (Li *et al.*, 2006). Here, we reacted dipydo[3,2 − a:2',3'-c]phenazine (*L*) with Cd^{2+} and 2,6'-biphenyl dicarboxylic acid, resulting in the title polymeric complex, (I).

In compound (I) the Cd^{II} atom is coordinated by one *L* ligand and two 2,6'-biphenyl dicarboxylate (bdc) dianions (Fig. 1) to result in a substantially distorted *cis*-CdN_2O_4 octahedron. The ligand bite angles are all less than 72°. The mean Cd—O and Cd—N distances are 2.319 (3) and 2.318 (4) Å, respectively. The similar C—O bond lengths of the bdc carboxylate groups imply electronic delocalization of their negative charges.

Neighboring Cd^{II} atoms are bridged by the bdc ligands, forming a one-dimensional chain structure (Fig. 2). Then, neighbouring chains are connected by π–π interactions, generating a two-dimensional supramolecular structure (Fig. 3). The π–π stacking distances are 3.496 (3) Å between *L* ligands. Similar values occur in related structures (Noveron *et al.*, 2002).

Experimental

The *L* ligand was synthesized by the literature method of Dickeson & Summers (1970). A mixture of $CdCl_2{\cdot}2H_2O$ (0.3 mmol), *L* (0.1 mmol) and 2,6'-biphenyl dicarboxylic acid (0.3 mmol) in 30 ml of distilled water was stirred thoroughly for 1 h at room temperature. The pH value was adjusted to about 7.5 with NaOH aqueous solution. The suspension was sealed in a Teflon-lined stainless reaction vessel (40 ml) and heated at 443 K for 5 days. The vessel was cooled slowly to room temperature at a rate of 10 K h^{-1} before opening and yellow blocks of (I) were collected.

Refinement

All H atoms were placed geometrically (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}$(carrier).

Figures

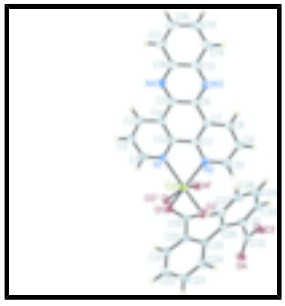

Fig. 1. The asymmetric unit of (I), together with additional atoms to complete the coordination of Cd1 with displacement ellipsoids drawn at the 30% probability level (H atoms omitted for clarity). Symmetry code: (i) 3/2 − *x*, *y* − 1/2, 3/2 − *z*.

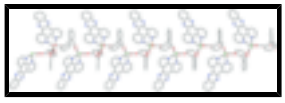

Fig. 2. A view of the chain structure of (I). H atoms have been omitted for clarity.

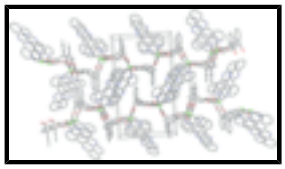

Fig. 3. View of the two-dimensional supramolecular structure of (I) generated by π–π interations. H atoms have been omitted for clarity.

catena-Poly[[(dipyrido[3,2 − a:2',3'-c]phenazine)cadmium(II)]- μ-biphenyl-2,2'-dicarboxylato]

Crystal data

$[Cd(C_{14}H_8O_4)(C_{18}H_{10}N_4)]$	F_{000} = 1272
M_r = 634.90	D_x = 1.660 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1258 reflections
a = 9.4547 (10) Å	θ = 2.3–26.0º
b = 12.4137 (13) Å	μ = 0.91 mm^{-1}
c = 22.015 (2) Å	T = 292 (2) K
β = 100.414 (2)º	Block, yellow
V = 2541.3 (5) Å^3	0.15 × 0.12 × 0.10 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	5027 independent reflections
Radiation source: fine-focus sealed tube	2971 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.070
Detector resolution: 0 pixels mm^{-1}	θ_{max} = 26.1º
T = 292(2) K	θ_{min} = 1.9º
ω scans	h = −10→11
Absorption correction: multi-scan (SADABS; Bruker, 2002)	k = −15→15
T_{min} = 0.881, T_{max} = 0.915	l = −27→23
13546 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
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.101	$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.95	$(\Delta/\sigma)_{max}$ = 0.002

5027 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
370 parameters	$\Delta\rho_{min} = -0.35$ 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	0.67647 (4)	0.27255 (3)	0.699658 (16)	0.04447 (14)
C15	0.9782 (7)	−0.0721 (5)	0.3188 (2)	0.0632 (17)
H15A	1.0326	−0.0774	0.2877	0.076*
N2	0.7908 (4)	0.2926 (3)	0.61487 (17)	0.0418 (10)
N3	0.9236 (4)	0.1112 (3)	0.44113 (17)	0.0463 (11)
N4	0.7425 (4)	−0.0625 (3)	0.45997 (18)	0.0451 (11)
N1	0.6417 (4)	0.1177 (3)	0.64049 (17)	0.0427 (10)
C14	0.8838 (7)	−0.1561 (5)	0.3274 (3)	0.0688 (18)
H14A	0.8764	−0.2153	0.3011	0.083*
C4	0.6869 (5)	0.0239 (4)	0.5504 (2)	0.0377 (12)
C6	0.8477 (5)	0.1110 (4)	0.4866 (2)	0.0413 (12)
C5	0.7600 (5)	0.0224 (4)	0.4971 (2)	0.0404 (12)
C7	0.8573 (5)	0.2064 (4)	0.5264 (2)	0.0395 (12)
C1	0.5694 (6)	0.0318 (4)	0.6544 (2)	0.0512 (14)
H1A	0.5293	0.0342	0.6900	0.061*
C3	0.7007 (5)	0.1139 (4)	0.5894 (2)	0.0374 (12)
C9	0.9368 (6)	0.2966 (4)	0.5169 (2)	0.0491 (14)
H9A	0.9854	0.2983	0.4838	0.059*
C2	0.6083 (5)	−0.0640 (4)	0.5661 (2)	0.0495 (14)
H2A	0.5948	−0.1245	0.5408	0.059*
C13	0.8032 (6)	−0.1541 (4)	0.3725 (2)	0.0572 (15)
H13A	0.7409	−0.2104	0.3770	0.069*
C11	0.9098 (6)	0.0230 (4)	0.4037 (2)	0.0466 (13)
C031	0.7855 (5)	0.2074 (4)	0.5766 (2)	0.0396 (12)
C10	0.8689 (6)	0.3771 (4)	0.6044 (2)	0.0526 (14)
H10A	0.8732	0.4355	0.6311	0.063*
C12	0.8165 (6)	−0.0637 (4)	0.4128 (2)	0.0461 (14)
O2	0.6178 (4)	0.4561 (3)	0.69209 (16)	0.0532 (10)

O1	0.4465 (4)	0.3370 (3)	0.67188 (17)	0.0620 (10)
C19	0.4883 (6)	0.4330 (4)	0.6775 (2)	0.0401 (12)
C17	0.9447 (6)	0.3836 (5)	0.5560 (2)	0.0574 (15)
H17A	0.9985	0.4443	0.5503	0.069*
C16	0.5510 (6)	−0.0602 (4)	0.6192 (3)	0.0579 (15)
H16A	0.5008	−0.1187	0.6310	0.069*
C18	0.9907 (6)	0.0171 (5)	0.3557 (2)	0.0542 (15)
H18A	1.0515	0.0732	0.3493	0.065*
C21	0.2513 (6)	0.5003 (4)	0.6936 (2)	0.0469 (13)
H21A	0.2387	0.4336	0.7111	0.056*
C20	0.3766 (5)	0.5201 (4)	0.6692 (2)	0.0375 (12)
C22	0.3937 (5)	0.6185 (4)	0.6406 (2)	0.0361 (11)
C25	0.2847 (5)	0.6948 (4)	0.6400 (2)	0.0486 (14)
H25A	0.2937	0.7612	0.6214	0.058*
C23	0.1473 (6)	0.5785 (5)	0.6919 (2)	0.0565 (15)
H23A	0.0654	0.5650	0.7086	0.068*
C24	0.1654 (6)	0.6760 (5)	0.6655 (2)	0.0559 (15)
H24A	0.0965	0.7296	0.6649	0.067*
C26	0.5065 (5)	0.6380 (3)	0.6024 (2)	0.0353 (11)
C27	0.6490 (5)	0.6666 (4)	0.6241 (2)	0.0368 (11)
C28	0.4606 (6)	0.6254 (4)	0.5388 (2)	0.0484 (13)
H28A	0.3653	0.6068	0.5238	0.058*
C30	0.6930 (6)	0.6629 (4)	0.5189 (2)	0.0533 (14)
H30A	0.7563	0.6699	0.4914	0.064*
C31	0.5529 (6)	0.6397 (4)	0.4978 (2)	0.0551 (15)
H31A	0.5191	0.6333	0.4555	0.066*
C29	0.7421 (6)	0.6764 (4)	0.5818 (2)	0.0498 (14)
H29A	0.8385	0.6922	0.5960	0.060*
C32	0.7076 (5)	0.6971 (4)	0.6900 (2)	0.0401 (12)
O4	0.6252 (3)	0.7352 (3)	0.72288 (14)	0.0451 (8)
O3	0.8404 (4)	0.6899 (3)	0.70860 (15)	0.0634 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0506 (3)	0.0467 (2)	0.0365 (2)	0.0082 (2)	0.00888 (17)	0.00026 (19)
C15	0.070 (5)	0.086 (5)	0.033 (3)	0.038 (4)	0.011 (3)	0.006 (3)
N2	0.048 (3)	0.043 (3)	0.034 (2)	0.000 (2)	0.006 (2)	0.0001 (19)
N3	0.050 (3)	0.056 (3)	0.032 (2)	0.013 (2)	0.006 (2)	0.004 (2)
N4	0.044 (3)	0.046 (3)	0.042 (2)	0.003 (2)	−0.002 (2)	−0.010 (2)
N1	0.047 (3)	0.049 (3)	0.035 (2)	0.002 (2)	0.014 (2)	−0.0008 (19)
C14	0.082 (5)	0.073 (5)	0.046 (4)	0.030 (4)	−0.004 (3)	−0.018 (3)
C4	0.033 (3)	0.039 (3)	0.039 (3)	0.006 (2)	0.001 (2)	0.001 (2)
C6	0.042 (3)	0.046 (3)	0.034 (3)	0.007 (2)	0.002 (2)	0.002 (2)
C5	0.038 (3)	0.044 (3)	0.037 (3)	0.007 (2)	0.000 (2)	−0.001 (2)
C7	0.044 (3)	0.039 (3)	0.035 (3)	0.006 (2)	0.007 (2)	0.000 (2)
C1	0.056 (4)	0.051 (4)	0.048 (3)	0.002 (3)	0.014 (3)	0.002 (3)
C3	0.036 (3)	0.038 (3)	0.037 (3)	0.011 (2)	0.005 (2)	0.004 (2)

C9	0.051 (4)	0.058 (4)	0.041 (3)	0.001 (3)	0.015 (3)	0.004 (3)
C2	0.050 (4)	0.041 (3)	0.054 (3)	0.001 (3)	0.001 (3)	−0.007 (3)
C13	0.068 (4)	0.050 (4)	0.049 (3)	0.018 (3)	0.001 (3)	−0.010 (3)
C11	0.043 (3)	0.056 (4)	0.038 (3)	0.016 (3)	−0.001 (3)	0.003 (3)
C031	0.038 (3)	0.044 (3)	0.035 (3)	0.009 (2)	0.003 (2)	0.004 (2)
C10	0.060 (4)	0.041 (3)	0.055 (3)	−0.008 (3)	0.006 (3)	−0.011 (3)
C12	0.045 (3)	0.057 (4)	0.034 (3)	0.018 (3)	0.001 (3)	−0.005 (3)
O2	0.039 (2)	0.044 (2)	0.077 (3)	0.0016 (17)	0.009 (2)	0.0000 (18)
O1	0.053 (2)	0.041 (2)	0.089 (3)	−0.0031 (19)	0.005 (2)	0.001 (2)
C19	0.046 (3)	0.045 (3)	0.031 (3)	0.001 (3)	0.012 (3)	0.001 (2)
C17	0.059 (4)	0.061 (4)	0.056 (4)	−0.009 (3)	0.021 (3)	0.001 (3)
C16	0.055 (4)	0.053 (4)	0.070 (4)	0.000 (3)	0.023 (3)	0.002 (3)
C18	0.051 (4)	0.071 (4)	0.040 (3)	0.024 (3)	0.007 (3)	0.003 (3)
C21	0.046 (3)	0.051 (4)	0.047 (3)	−0.006 (3)	0.016 (3)	0.001 (3)
C20	0.035 (3)	0.047 (3)	0.031 (3)	0.001 (2)	0.007 (2)	−0.008 (2)
C22	0.031 (3)	0.036 (3)	0.040 (3)	−0.003 (2)	0.002 (2)	0.001 (2)
C25	0.039 (3)	0.048 (3)	0.058 (3)	0.011 (3)	0.007 (3)	0.008 (3)
C23	0.036 (3)	0.080 (4)	0.056 (4)	0.002 (3)	0.015 (3)	0.002 (3)
C24	0.036 (3)	0.067 (4)	0.065 (4)	0.013 (3)	0.011 (3)	−0.002 (3)
C26	0.035 (3)	0.040 (3)	0.032 (3)	0.005 (2)	0.010 (2)	0.001 (2)
C27	0.035 (3)	0.044 (3)	0.033 (3)	0.001 (2)	0.008 (2)	0.007 (2)
C28	0.044 (3)	0.054 (4)	0.045 (3)	−0.001 (3)	0.001 (3)	−0.004 (3)
C30	0.058 (4)	0.070 (4)	0.036 (3)	0.001 (3)	0.018 (3)	0.004 (3)
C31	0.057 (4)	0.074 (4)	0.033 (3)	0.002 (3)	0.002 (3)	−0.008 (3)
C29	0.039 (3)	0.065 (4)	0.045 (3)	−0.005 (3)	0.008 (3)	0.003 (3)
C32	0.033 (3)	0.046 (3)	0.041 (3)	−0.005 (2)	0.006 (3)	0.004 (2)
O4	0.037 (2)	0.062 (2)	0.0364 (18)	0.0003 (17)	0.0090 (16)	−0.0078 (16)
O3	0.030 (2)	0.113 (3)	0.047 (2)	0.002 (2)	0.0054 (18)	−0.016 (2)

Geometric parameters (Å, °)

Cd1—N1	2.311 (4)	C11—C12	1.429 (7)
Cd1—N2	2.333 (4)	C10—C17	1.390 (6)
Cd1—O1	2.294 (4)	C10—H10A	0.9300
Cd1—O3^{i}	2.296 (3)	O2—C19	1.242 (5)
Cd1—O4^{i}	2.342 (3)	O1—C19	1.255 (5)
Cd1—O2	2.344 (3)	C19—C20	1.499 (6)
C15—C18	1.366 (7)	C17—H17A	0.9300
C15—C14	1.408 (8)	C16—H16A	0.9300
C15—H15A	0.9300	C18—H18A	0.9300
N2—C10	1.326 (6)	C21—C23	1.377 (7)
N2—C031	1.348 (6)	C21—C20	1.408 (6)
N3—C6	1.333 (5)	C21—H21A	0.9300
N3—C11	1.362 (6)	C20—C22	1.396 (6)
N4—C5	1.325 (6)	C22—C25	1.398 (6)
N4—C12	1.353 (6)	C22—C26	1.492 (6)
N1—C1	1.333 (6)	C25—C24	1.368 (6)
N1—C3	1.343 (5)	C25—H25A	0.9300
C14—C13	1.358 (7)	C23—C24	1.367 (7)

C14—H14A	0.9300	C23—H23A	0.9300
C4—C2	1.398 (6)	C24—H24A	0.9300
C4—C3	1.401 (6)	C26—C27	1.392 (6)
C4—C5	1.466 (6)	C26—C28	1.399 (6)
C6—C5	1.421 (6)	C27—C29	1.397 (6)
C6—C7	1.466 (6)	C27—C32	1.504 (6)
C7—C9	1.385 (6)	C28—C31	1.376 (6)
C7—C031	1.397 (6)	C28—H28A	0.9300
C1—C16	1.373 (7)	C30—C31	1.353 (7)
C1—H1A	0.9300	C30—C29	1.388 (6)
C3—C031	1.468 (6)	C30—H30A	0.9300
C9—C17	1.375 (7)	C31—H31A	0.9300
C9—H9A	0.9300	C29—H29A	0.9300
C2—C16	1.376 (6)	C32—O4	1.249 (5)
C2—H2A	0.9300	C32—O3	1.252 (5)
C13—C12	1.421 (6)	C32—Cd1^{ii}	2.649 (5)
C13—H13A	0.9300	O4—Cd1^{ii}	2.342 (3)
C11—C18	1.414 (6)	O3—Cd1^{ii}	2.296 (3)
O1—Cd1—O3^{i}	100.21 (13)	N4—C12—C13	119.2 (5)
O1—Cd1—N1	96.23 (14)	N4—C12—C11	121.1 (5)
O3^{i}—Cd1—N1	95.66 (14)	C13—C12—C11	119.7 (5)
O1—Cd1—N2	107.66 (13)	C19—O2—Cd1	90.2 (3)
O3^{i}—Cd1—N2	150.11 (13)	C19—O1—Cd1	92.2 (3)
N1—Cd1—N2	71.16 (14)	O2—C19—O1	121.5 (5)
O1—Cd1—O4^{i}	149.20 (12)	O2—C19—C20	120.3 (5)
O3^{i}—Cd1—O4^{i}	56.27 (11)	O1—C19—C20	118.1 (5)
N1—Cd1—O4^{i}	105.02 (12)	O2—C19—Cd1	61.9 (3)
N2—Cd1—O4^{i}	100.25 (12)	O1—C19—Cd1	59.6 (3)
O1—Cd1—O2	56.04 (12)	C20—C19—Cd1	175.3 (3)
O3^{i}—Cd1—O2	116.36 (13)	C9—C17—C10	117.2 (5)
N1—Cd1—O2	139.51 (13)	C9—C17—H17A	121.4
N2—Cd1—O2	88.69 (13)	C10—C17—H17A	121.4
O4^{i}—Cd1—O2	113.09 (12)	C1—C16—C2	118.7 (5)
C18—C15—C14	120.7 (6)	C1—C16—H16A	120.7
C18—C15—H15A	119.7	C2—C16—H16A	120.7
C14—C15—H15A	119.7	C15—C18—C11	119.1 (6)
C10—N2—C031	118.1 (4)	C15—C18—H18A	120.5
C10—N2—Cd1	125.2 (3)	C11—C18—H18A	120.5
C031—N2—Cd1	116.6 (3)	C23—C21—C20	120.8 (5)
C6—N3—C11	116.6 (4)	C23—C21—H21A	119.6
C5—N4—C12	117.3 (4)	C20—C21—H21A	119.6
C1—N1—C3	118.1 (4)	C22—C20—C21	119.9 (4)
C1—N1—Cd1	124.2 (3)	C22—C20—C19	123.3 (4)
C3—N1—Cd1	117.6 (3)	C21—C20—C19	116.8 (4)
C13—C14—C15	122.5 (6)	C20—C22—C25	116.9 (4)
C13—C14—H14A	118.7	C20—C22—C26	123.3 (4)

C15—C14—H14A	118.7	C25—C22—C26	119.0 (4)
C2—C4—C3	117.8 (5)	C24—C25—C22	122.8 (5)
C2—C4—C5	122.5 (5)	C24—C25—H25A	118.6
C3—C4—C5	119.7 (4)	C22—C25—H25A	118.6
N3—C6—C5	122.2 (4)	C24—C23—C21	119.4 (5)
N3—C6—C7	117.6 (5)	C24—C23—H23A	120.3
C5—C6—C7	120.2 (5)	C21—C23—H23A	120.3
N4—C5—C6	121.8 (5)	C23—C24—C25	120.1 (5)
N4—C5—C4	118.6 (5)	C23—C24—H24A	119.9
C6—C5—C4	119.6 (4)	C25—C24—H24A	119.9
C9—C7—C031	117.8 (4)	C27—C26—C28	118.6 (4)
C9—C7—C6	122.7 (5)	C27—C26—C22	126.4 (4)
C031—C7—C6	119.6 (4)	C28—C26—C22	115.0 (4)
N1—C1—C16	123.6 (5)	C26—C27—C29	118.7 (4)
N1—C1—H1A	118.2	C26—C27—C32	124.0 (4)
C16—C1—H1A	118.2	C29—C27—C32	117.0 (4)
N1—C3—C4	122.4 (4)	C31—C28—C26	121.6 (5)
N1—C3—C031	117.2 (4)	C31—C28—H28A	119.2
C4—C3—C031	120.4 (4)	C26—C28—H28A	119.2
C17—C9—C7	120.7 (5)	C31—C30—C29	119.9 (5)
C17—C9—H9A	119.7	C31—C30—H30A	120.0
C7—C9—H9A	119.7	C29—C30—H30A	120.0
C16—C2—C4	119.4 (5)	C30—C31—C28	119.9 (5)
C16—C2—H2A	120.3	C30—C31—H31A	120.0
C4—C2—H2A	120.3	C28—C31—H31A	120.0
C14—C13—C12	118.2 (6)	C30—C29—C27	121.1 (5)
C14—C13—H13A	120.9	C30—C29—H29A	119.4
C12—C13—H13A	120.9	C27—C29—H29A	119.4
N3—C11—C18	119.2 (5)	O4—C32—O3	122.1 (4)
N3—C11—C12	121.0 (5)	O4—C32—C27	119.7 (4)
C18—C11—C12	119.8 (5)	O3—C32—C27	118.1 (4)
N2—C031—C7	122.3 (4)	O4—C32—Cd1^{ii}	62.1 (2)
N2—C031—C3	117.4 (4)	O3—C32—Cd1^{ii}	60.0 (2)
C7—C031—C3	120.4 (4)	C27—C32—Cd1^{ii}	172.9 (3)
N2—C10—C17	124.0 (5)	C32—O4—Cd1^{ii}	89.8 (3)
N2—C10—H10A	118.0	C32—O3—Cd1^{ii}	91.8 (3)
C17—C10—H10A	118.0		
O1—Cd1—N2—C10	92.5 (4)	C4—C3—C031—C7	−2.0 (7)
O3^{i}—Cd1—N2—C10	−109.5 (4)	C031—N2—C10—C17	0.6 (8)
N1—Cd1—N2—C10	−176.8 (4)	Cd1—N2—C10—C17	175.0 (4)
O4^{i}—Cd1—N2—C10	−74.3 (4)	C5—N4—C12—C13	178.7 (4)
O2—Cd1—N2—C10	38.9 (4)	C5—N4—C12—C11	0.2 (7)
C32^{i}—Cd1—N2—C10	−85.1 (4)	C14—C13—C12—N4	−176.8 (4)
C19—Cd1—N2—C10	64.7 (4)	C14—C13—C12—C11	1.8 (7)
O1—Cd1—N2—C031	−93.0 (3)	N3—C11—C12—N4	−2.1 (7)
O3^{i}—Cd1—N2—C031	65.0 (4)	C18—C11—C12—N4	177.1 (4)
N1—Cd1—N2—C031	−2.4 (3)	N3—C11—C12—C13	179.3 (4)

O4^{i}—Cd1—N2—C031	100.1 (3)	C18—C11—C12—C13	−1.4 (7)
O2—Cd1—N2—C031	−146.6 (3)	O1—Cd1—O2—C19	0.9 (3)
C32^{i}—Cd1—N2—C031	89.4 (3)	O3^{i}—Cd1—O2—C19	−83.7 (3)
C19—Cd1—N2—C031	−120.8 (3)	N1—Cd1—O2—C19	54.9 (4)
O1—Cd1—N1—C1	−74.4 (4)	N2—Cd1—O2—C19	113.3 (3)
O3^{i}—Cd1—N1—C1	26.6 (4)	O4^{i}—Cd1—O2—C19	−146.1 (3)
N2—Cd1—N1—C1	179.0 (4)	C32^{i}—Cd1—O2—C19	−115.3 (3)
O4^{i}—Cd1—N1—C1	83.1 (4)	O3^{i}—Cd1—O1—C19	114.1 (3)
O2—Cd1—N1—C1	−116.9 (4)	N1—Cd1—O1—C19	−149.0 (3)
C32^{i}—Cd1—N1—C1	54.3 (4)	N2—Cd1—O1—C19	−76.8 (3)
C19—Cd1—N1—C1	−90.7 (4)	O4^{i}—Cd1—O1—C19	77.2 (4)
O1—Cd1—N1—C3	106.9 (3)	O2—Cd1—O1—C19	−0.9 (3)
O3^{i}—Cd1—N1—C3	−152.2 (3)	C32^{i}—Cd1—O1—C19	100.8 (3)
N2—Cd1—N1—C3	0.3 (3)	Cd1—O2—C19—O1	−1.6 (5)
O4^{i}—Cd1—N1—C3	−95.6 (3)	Cd1—O2—C19—C20	175.3 (4)
O2—Cd1—N1—C3	64.4 (4)	Cd1—O1—C19—O2	1.6 (5)
C32^{i}—Cd1—N1—C3	−124.5 (3)	Cd1—O1—C19—C20	−175.3 (3)
C19—Cd1—N1—C3	90.6 (3)	C7—C9—C17—C10	−0.6 (8)
C18—C15—C14—C13	−1.1 (9)	N2—C10—C17—C9	0.2 (8)
C11—N3—C6—C5	1.9 (6)	N1—C1—C16—C2	−0.9 (8)
C11—N3—C6—C7	−178.2 (4)	C4—C2—C16—C1	1.9 (8)
C12—N4—C5—C6	2.7 (7)	C14—C15—C18—C11	1.5 (8)
C12—N4—C5—C4	−177.1 (4)	N3—C11—C18—C15	179.0 (4)
N3—C6—C5—N4	−3.9 (7)	C12—C11—C18—C15	−0.2 (7)
C7—C6—C5—N4	176.1 (4)	C23—C21—C20—C22	−2.6 (7)
N3—C6—C5—C4	175.8 (4)	C23—C21—C20—C19	175.6 (5)
C7—C6—C5—C4	−4.1 (7)	O2—C19—C20—C22	40.2 (7)
C2—C4—C5—N4	4.8 (7)	O1—C19—C20—C22	−142.9 (5)
C3—C4—C5—N4	−178.3 (4)	O2—C19—C20—C21	−137.9 (5)
C2—C4—C5—C6	−174.9 (5)	O1—C19—C20—C21	39.0 (6)
C3—C4—C5—C6	1.9 (7)	C21—C20—C22—C25	2.3 (7)
N3—C6—C7—C9	2.4 (7)	C19—C20—C22—C25	−175.8 (4)
C5—C6—C7—C9	−177.6 (5)	C21—C20—C22—C26	−166.9 (4)
N3—C6—C7—C031	−176.7 (4)	C19—C20—C22—C26	15.0 (7)
C5—C6—C7—C031	3.3 (7)	C20—C22—C25—C24	−0.3 (7)
C3—N1—C1—C16	−0.5 (8)	C26—C22—C25—C24	169.4 (5)
Cd1—N1—C1—C16	−179.3 (4)	C20—C21—C23—C24	0.8 (8)
C1—N1—C3—C4	0.9 (7)	C21—C23—C24—C25	1.2 (8)
Cd1—N1—C3—C4	179.7 (3)	C22—C25—C24—C23	−1.5 (8)
C1—N1—C3—C031	−177.2 (4)	C20—C22—C26—C27	−83.7 (6)
Cd1—N1—C3—C031	1.6 (5)	C25—C22—C26—C27	107.3 (6)
C2—C4—C3—N1	0.2 (7)	C20—C22—C26—C28	96.1 (5)
C5—C4—C3—N1	−176.8 (4)	C25—C22—C26—C28	−72.9 (6)
C2—C4—C3—C031	178.1 (4)	C28—C26—C27—C29	−3.0 (7)
C5—C4—C3—C031	1.1 (7)	C22—C26—C27—C29	176.8 (4)
C031—C7—C9—C17	0.2 (7)	C28—C26—C27—C32	171.6 (4)
C6—C7—C9—C17	−178.9 (5)	C22—C26—C27—C32	−8.6 (7)

C3—C4—C2—C16	−1.6 (7)	C27—C26—C28—C31	0.5 (7)
C5—C4—C2—C16	175.3 (4)	C22—C26—C28—C31	−179.3 (4)
C15—C14—C13—C12	−0.6 (8)	C29—C30—C31—C28	−2.5 (8)
C6—N3—C11—C18	−178.2 (4)	C26—C28—C31—C30	2.3 (8)
C6—N3—C11—C12	1.0 (6)	C31—C30—C29—C27	−0.2 (8)
C10—N2—C031—C7	−1.0 (7)	C26—C27—C29—C30	2.9 (7)
Cd1—N2—C031—C7	−175.9 (3)	C32—C27—C29—C30	−172.0 (5)
C10—N2—C031—C3	179.0 (4)	C26—C27—C32—O4	−25.8 (7)
Cd1—N2—C031—C3	4.1 (5)	C29—C27—C32—O4	148.9 (4)
C9—C7—C031—N2	0.6 (7)	C26—C27—C32—O3	159.0 (5)
C6—C7—C031—N2	179.7 (4)	C29—C27—C32—O3	−26.3 (7)
C9—C7—C031—C3	−179.4 (4)	O3—C32—O4—Cd1^{ii}	2.9 (5)
C6—C7—C031—C3	−0.2 (7)	C27—C32—O4—Cd1^{ii}	−172.1 (4)
N1—C3—C031—N2	−3.9 (6)	O4—C32—O3—Cd1^{ii}	−3.0 (5)
C4—C3—C031—N2	178.1 (4)	C27—C32—O3—Cd1^{ii}	172.1 (4)
N1—C3—C031—C7	176.1 (4)		

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+3/2, *y*+1/2, −*z*+3/2.

Fig. 1

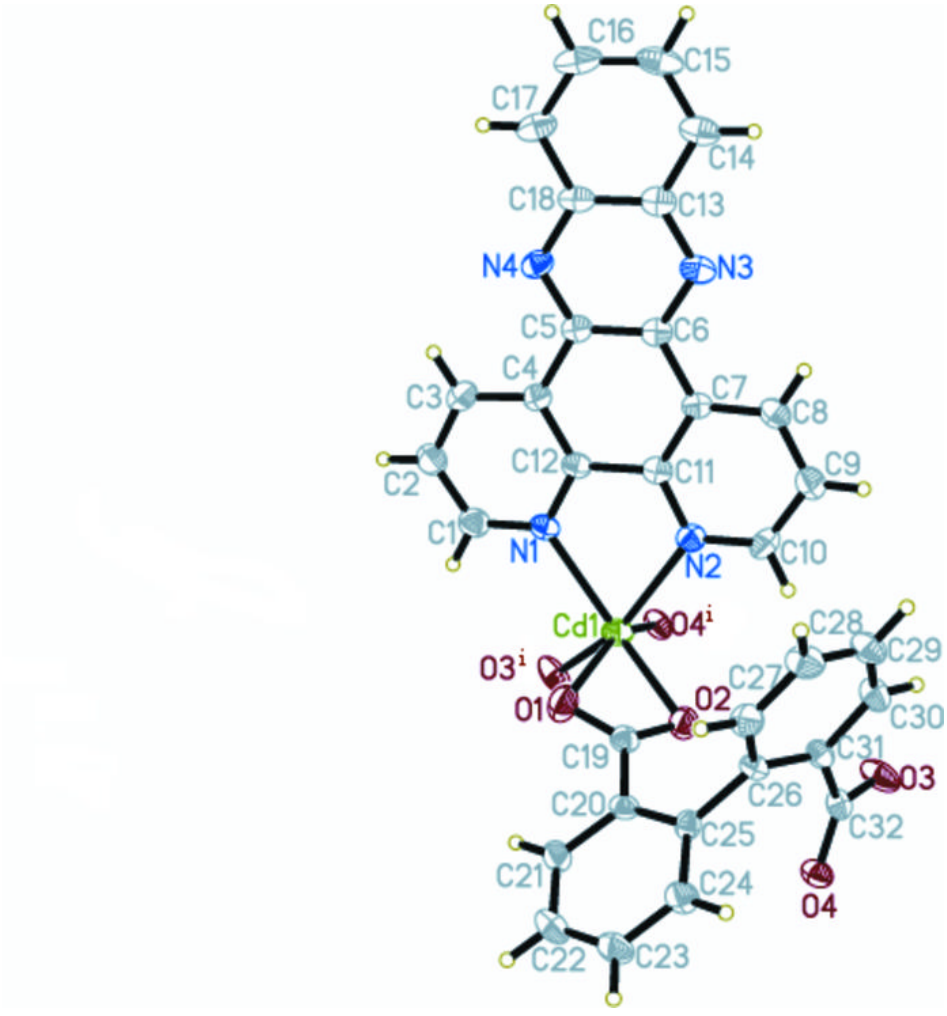
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Fig. 2

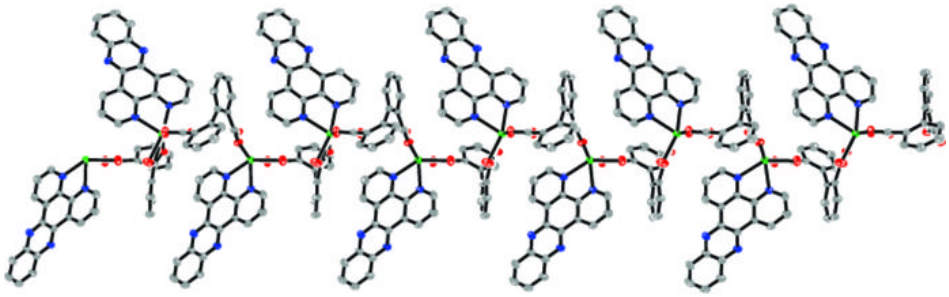

Fig. 3