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catena-Poly[[diaquacadmium(II)]-μ-3,3′-(*p*-phenylene)diacrylato]

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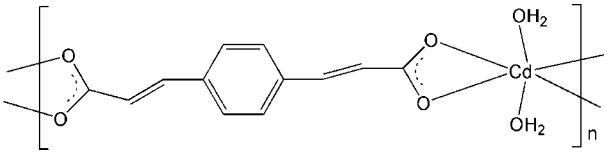
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.020; wR factor = 0.046; data-to-parameter ratio = 13.0.

In the title compound, $[Cd(C_{12}H_{10}O_4)(H_2O)_2]$, each Cd^{II} atom lies on a crystallographic twofold rotation axis and is six-coordinated by four carboxylate O atoms from two different 3,3′-(*p*-phenylene)diacrylate ligands, and two *cis* water molecules in a very distorted octahedral CdO_6 environment. Each 3,3′-(*p*-phenylene)diacrylate dianion is centrosymmetric and acts as a bis-chelating ligand that binds two Cd^{II} atoms, thus forming a zigzag chain. The chain is decorated with water molecules and O—H···O hydrogen bonds link the chains together, forming a three-dimensional supramolecular structure.

Related literature

For a related structure, see: Fang *et al.* (2006). For background, see: Qi *et al.* (2003).



Experimental

Crystal data

$[Cd(C_{12}H_{10}O_4)(H_2O)_2]$
M_r = 364.62
Monoclinic, $C2/c$
a = 11.857 (3) Å
b = 5.3296 (14) Å
c = 20.030 (5) Å
β = 94.983 (4)°
V = 1261.0 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.75 mm^{-1}
T = 293 (2) K
0.31 × 0.21 × 0.19 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.574, T_{max} = 0.716
3315 measured reflections
1235 independent reflections
1199 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.046
S = 1.11
1235 reflections
95 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.3251 (16)	Cd1—O1*W*	2.2044 (18)
Cd1—O2	2.3846 (16)		
O1—Cd1—O2	55.50 (5)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H*W*12···O1^{i}	0.77 (3)	1.95 (3)	2.703 (3)	170 (3)
O1*W*—H*W*11···O2^{ii}	0.83 (4)	1.85 (4)	2.675 (3)	174 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: HB2555).

References

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supplementary materials

Acta Cryst. (2007). E**63**, m2595 [**doi:10.1107/S1600536807046909**]

catena-Poly[[diaquacadmium(II)]-μ-3,3'-(*p*-phenylene)diacrylato]

C.-B. Liu, L. Lu, Z.-L. Xu and Q.-W. Wang

Comment

The supramolecular networks formed by metal 1,4-benzenedicarboxylates (1,4-bdc) have been widely studied (Qi *et al.*, 2003). However, so far, less attention has been given to the participation of *p*-phenylenediacrylic acid (H_2pda) in such networks. The pda dianion, as an important analogue of 1,4-bdc may be a good candidate for the construction of metal–organic helical architectures. We selected pda as a bridging ligand and Cd^{II} as a central metal, generating a new zigzag chain coordination polymer, [Cd(pda)(H_2O)$_2$], (I), which is reported here.

In compound (I), the Cd^{II} atom is six-coordinated by four carboxylate atoms from two different pda ligands, and two water molecules in a very distorted octahedral environment (Fig. 1). The O1, O2, O2^{i} and O1W^{i} atoms comprise the basal plane, whereas O1W and O1^{i} occupy the axial positions of the octahedron. The Cd—*O*(carboxylate) distances range from 2.3251 (16) to 2.3846 (16) Å (Table 1).

As shown in Fig. 2, each pda acts as a bis-chelating ligand that binds two Cd^{II} atoms, forming a zigzag chain. The chain is decorated with water molecules which participate in O—H···O hydrogen bonds (Table 2) to link the chains together, thus forming a three-dimensional supramolecular structure (Fig. 3).

Experimental

A mixture of $CdCl_2 \cdot 2H_2O$ (0.5 mmol), H_2pda (0.5 mmol), and H_2O (500 mmol) was adjusted to pH = 7 by addition of aqueous NaOH solution, and heated at 453 K for 6 days. After the mixture was slowly cooled to room temperature, colorless blocks of (I) resulted (38% yield).

Refinement

All the C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C). The water H-atoms were located in a difference Fourier map, and were refined freely.

Figures

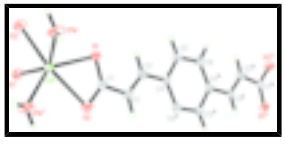

Fig. 1. The structure of (I), with displacement ellipsoids drawn at the 30% probability level. (H atoms have been omitted). Symmetry codes: (i) 2 − *x*, *y*, 1.5 − *z*; (ii) 2.5 − *x*, 0.5 − *y*, 2 − *z*.

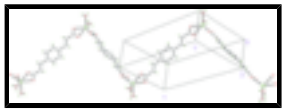

Fig. 2. View of the chain structure of (I).

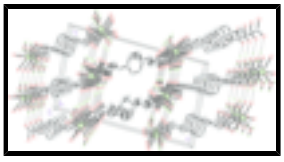

Fig. 3. View of the three-dimensional supramolecular structure of (I).

catena-Poly[[diaquacadmium(II)]-μ-3,3'-(_p_-phenylene)diacrylato]

Crystal data

$[Cd(C_{12}H_{10}O_4)(H_2O)_2]$	F_{000} = 720
M_r = 364.62	D_x = 1.921 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1235 reflections
a = 11.857 (3) Å	θ = 2.0–26.1º
b = 5.3296 (14) Å	μ = 1.75 mm^{-1}
c = 20.030 (5) Å	*T* = 293 (2) K
β = 94.983 (4)º	Block, colourless
V = 1261.0 (6) Å^3	0.31 × 0.21 × 0.19 mm
Z = 4	

Data collection

Bruker APEX CCD diffractometer	1235 independent reflections
Radiation source: fine-focus sealed tube	1199 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.016
T = 293(2) K	θ_{max} = 26.1º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	*h* = −14→11
T_{min} = 0.574, T_{max} = 0.716	*k* = −6→5
3315 measured reflections	*l* = −24→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap (O-H) and geom (C-H)
$R[F^2 > 2\sigma(F^2)]$ = 0.020	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.046	$w = 1/[\sigma^2(F_o^2) + (0.0216P)^2 + 1.4532P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.11	$(\Delta/\sigma)_{max} < 0.001$
1235 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
95 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}
C1	1.12499 (19)	−0.4749 (4)	0.83239 (11)	0.0287 (5)
C2	1.1910 (2)	−0.2843 (4)	0.87299 (13)	0.0362 (6)
H2	1.2691	−0.2784	0.8712	0.043*
C3	1.1430 (2)	−0.1220 (5)	0.91177 (11)	0.0320 (5)
H3	1.0646	−0.1300	0.9113	0.038*
C4	1.1997 (2)	0.0689 (4)	0.95542 (11)	0.0302 (5)
C5	1.1344 (2)	0.2195 (5)	0.99437 (13)	0.0359 (6)
H5	1.0562	0.2002	0.9906	0.043*
C6	1.1833 (2)	0.3962 (5)	1.03827 (12)	0.0356 (5)
H6	1.1379	0.4927	1.0638	0.043*
O1	1.01914 (13)	−0.4967 (3)	0.83570 (8)	0.0305 (4)
O2	1.17575 (13)	−0.6158 (3)	0.79418 (8)	0.0360 (4)
O1W	0.90126 (17)	−1.0774 (4)	0.79925 (11)	0.0429 (5)
Cd1	1.0000	−0.79192 (4)	0.7500	0.02670 (9)
HW11	0.832 (3)	−1.093 (6)	0.7946 (15)	0.057 (9)*
HW12	0.928 (3)	−1.205 (5)	0.8085 (15)	0.035 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0313 (12)	0.0234 (11)	0.0303 (11)	−0.0003 (9)	−0.0036 (9)	−0.0007 (9)
C2	0.0289 (13)	0.0363 (13)	0.0426 (14)	−0.0034 (10)	−0.0014 (11)	−0.0108 (11)
C3	0.0330 (12)	0.0327 (12)	0.0299 (12)	−0.0052 (10)	0.0008 (9)	−0.0040 (10)
C4	0.0365 (13)	0.0274 (12)	0.0263 (11)	−0.0041 (10)	0.0010 (9)	−0.0029 (9)
C5	0.0310 (12)	0.0379 (14)	0.0391 (13)	−0.0065 (10)	0.0043 (10)	−0.0091 (10)
C6	0.0360 (13)	0.0378 (13)	0.0333 (12)	−0.0020 (11)	0.0055 (10)	−0.0115 (10)
O1	0.0277 (8)	0.0273 (8)	0.0361 (9)	−0.0020 (7)	−0.0002 (7)	−0.0048 (6)
O2	0.0280 (8)	0.0336 (9)	0.0458 (10)	−0.0003 (7)	−0.0008 (7)	−0.0144 (8)
O1W	0.0250 (10)	0.0301 (11)	0.0739 (13)	0.0023 (8)	0.0060 (9)	0.0139 (9)
Cd1	0.02628 (14)	0.02161 (13)	0.03127 (14)	0.000	−0.00282 (9)	0.000

Geometric parameters (Å, °)

Cd1—O1	2.3251 (16)	C3—C4	1.466 (3)
Cd1—O2	2.3846 (16)	C3—H3	0.9300
Cd1—O1W	2.2044 (18)	C4—C6^{ii}	1.394 (3)
Cd1—O1W^{i}	2.2044 (18)	C4—C5	1.399 (3)
Cd1—O1^{i}	2.3251 (16)	C5—C6	1.381 (3)
Cd1—O2^{i}	2.3846 (16)	C5—H5	0.9300
C1—O2	1.262 (3)	C6—C4^{ii}	1.394 (3)
C1—O1	1.268 (3)	C6—H6	0.9300
C1—C2	1.482 (3)	O1W—HW11	0.83 (4)
C2—C3	1.324 (3)	O1W—HW12	0.77 (3)
C2—H2	0.9300		
O1W^{i}—Cd1—O1W	92.72 (11)	C3—C2—C1	122.4 (2)
O1W^{i}—Cd1—O1	140.88 (7)	C3—C2—H2	118.8
O1W—Cd1—O1	99.10 (7)	C1—C2—H2	118.8
O1W^{i}—Cd1—O1^{i}	99.10 (7)	C2—C3—C4	127.2 (2)
O1W—Cd1—O1^{i}	140.88 (7)	C2—C3—H3	116.4
O1—Cd1—O1^{i}	94.82 (8)	C4—C3—H3	116.4
O1W^{i}—Cd1—O2	87.52 (7)	C6^{ii}—C4—C5	117.9 (2)
O1W—Cd1—O2	125.91 (7)	C6^{ii}—C4—C3	123.2 (2)
O1—Cd1—O2	55.50 (5)	C5—C4—C3	118.9 (2)
O1^{i}—Cd1—O2	91.93 (6)	C6—C5—C4	121.6 (2)
O1W^{i}—Cd1—O2^{i}	125.91 (7)	C6—C5—H5	119.2
O1W—Cd1—O2^{i}	87.52 (7)	C4—C5—H5	119.2
O1—Cd1—O2^{i}	91.93 (6)	C5—C6—C4^{ii}	120.5 (2)
O1^{i}—Cd1—O2^{i}	55.50 (5)	C5—C6—H6	119.7
O2—Cd1—O2^{i}	133.64 (9)	C4^{ii}—C6—H6	119.7
O2—C1—O1	120.3 (2)	C1—O1—Cd1	93.27 (13)
O2—C1—C2	118.9 (2)	C1—O2—Cd1	90.68 (13)
O1—C1—C2	120.8 (2)	Cd1—O1W—HW11	126 (2)
O2—C1—Cd1	61.59 (11)	Cd1—O1W—HW12	120 (2)
O1—C1—Cd1	58.90 (11)	HW11—O1W—HW12	109 (3)
C2—C1—Cd1	174.99 (17)		

Symmetry codes: (i) −*x*+2, *y*, −*z*+3/2; (ii) −*x*+5/2, −*y*+1/2, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—HW12···O1^{iii}	0.77 (3)	1.95 (3)	2.703 (3)	170 (3)
O1W—HW11···O2^{iv}	0.83 (4)	1.85 (4)	2.675 (3)	174 (3)

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

Fig. 1

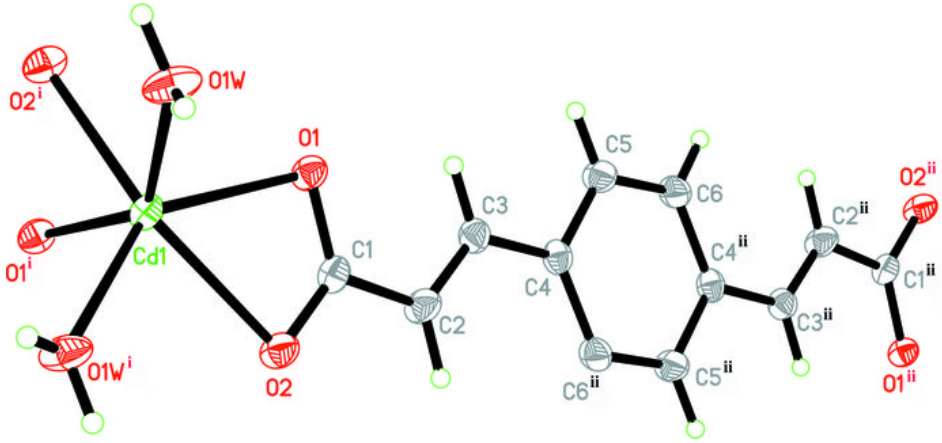
O2i
O1W
O1
O1i
Cd1
C1
C3
C5
C6
O2ii
C2ii
C4ii
C1ii
C2
C4
C3ii
O1W i
O2
C6ii
C5ii
O1ii

Fig. 2

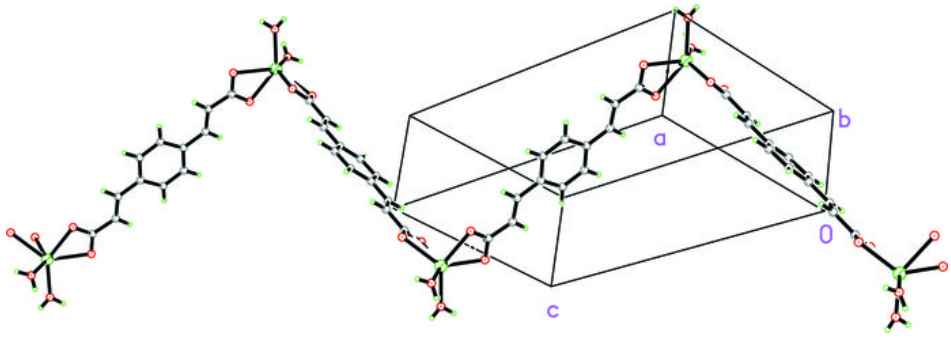

Fig. 3