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catena-Poly[[[tetraaquacadmium(II)]-μ-4,4′-bipyridine] fumarate tetrahydrate]

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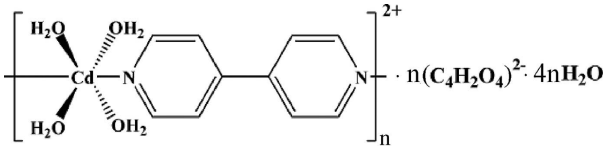
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.072; data-to-parameter ratio = 14.4.

In the crystal structure of the title compound, $[Cd(C_{10}H_8N_2)(H_2O)_4](C_4H_2O_4)\cdot 4H_2O$, the Cd^{II} atom, on an inversion centre, is six-coordinated by four O atoms from four water molecules and two N atoms from 4,4′-bpy molecules in a distorted octahedral coordination geometry. Weak C—H···O interactions between uncoordinated carboxylate O atoms of fumaric acid and water molecules contribute to the crystal packing stability.

Related literature

For related literature, see: Dai *et al.* (2003); Dalai *et al.* (2002); Devereux *et al.* (2000); Kang *et al.* (2004); Konar *et al.* (2003); Shen *et al.* (2004); Tao *et al.* (2000); Ying, Zheng & Zhang (2004); Ying, Zheng & Zhou (2004); Zheng *et al.* (2002).



Experimental

Crystal data

$[Cd(C_{10}H_8N_2)(H_2O)_4](C_4H_2O_4)\cdot 4H_2O$
M_r = 526.77
Triclinic, $P\overline{1}$
a = 7.183 (5) Å
b = 7.802 (5) Å
c = 10.038 (5) Å
α = 80.434 (5)°
β = 87.791 (5)°
γ = 73.288 (5)°
V = 531.3 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.09 mm^{-1}
T = 293 (2) K
0.21 × 0.19 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (Higashi, 1995)
T_{min} = 0.804, T_{max} = 0.854
3414 measured reflections
2378 independent reflections
2363 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.072
S = 1.08
2378 reflections
165 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −1.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O2W	2.259 (2)	Cd1—O1W	2.348 (2)
Cd1—N1	2.295 (2)		
O2W^i—Cd1—O2W	180	O2W^i—Cd1—O1W	86.81 (9)
O2W^i—Cd1—N1	91.00 (8)	O2W—Cd1—O1W	93.19 (9)
O2W—Cd1—N1	89.00 (8)	N1^i—Cd1—O1W	89.40 (8)
N1^i—Cd1—N1	180	N1—Cd1—O1W	90.60 (8)

Symmetry code: (i) $-x, -y, -z+2$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WB···O3W^{ii}	0.71 (4)	2.10 (4)	2.811 (3)	175 (4)
O1W—H1WA···O4W^{iii}	0.76 (5)	2.04 (5)	2.790 (3)	168 (5)
O4W—H4WB···O3W	0.77 (4)	2.16 (4)	2.929 (3)	173 (4)
O3W—H3WB···O1^{iv}	0.74 (4)	2.06 (4)	2.759 (3)	157 (4)
O4W—H4WA···O2	0.70 (4)	2.02 (4)	2.714 (3)	170 (4)
O3W—H3WA···O1^{v}	0.85 (4)	1.98 (4)	2.833 (3)	172 (3)
O2W—H2WB···O2^{vi}	0.72 (4)	1.91 (4)	2.615 (3)	168 (4)
O2W—H2WA···O4W^{vii}	0.73 (3)	2.02 (3)	2.748 (3)	175 (3)

Symmetry codes: (ii) $-x, -y+1, -z+1$; (iii) $x-1, y-1, z+1$; (iv) $x, y+1, z$; (v) $-x+1, -y+1, -z+1$; (vi) $-x+1, -y, -z+1$; (vii) $x, y-1, z+1$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); 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: BQ2045).

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supplementary materials

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catena-Poly[[[tetraaquacadmium(II)]-μ-4,4'-bipyridine] fumarate tetrahydrate]

Y.-R. Pan

Comment

Recently, 4,4'-bipyridine (bpy) hve been used to construct coordination polymers (Tao *et al.*, 2000; Dai *et al.*, 2003). A few structures of copper (Dalai *et al.*, 2002; Ying, Zheng & Zhou, 2004; Kang *et al.*, 2004), manganese (Devereux *et al.*, 2000; Ying, Zheng & Zhang, 2004), nickel (Zheng *et al.*, 2002) and cobalt (Shen *et al.*, 2004; Konar *et al.*, 2003] fumarate complexes with 4,4'-bpy are known. Herein, we report the structure of the title complex with 4,4'-bpy and fumaric acid, $[Cd(4,4'\text{-bpy})(H_2O)_4](C_4H_2O_4)(H_2O)_4$ (I).

The structure of the title compound, shown in Fig. 1, consists of one $[Cd(4,4'\text{-bpy})(H_2O)_4]^{2+}$ cation, one uncoordination fumarate anion and four water molecules. The CdII ion is coordinated by one bpy and four water molecules in a distorted octahedral geometry to form a one-dimensional chain. Table 1 gives a listing of selected bond lengths and bond angles, which are comparable to those values found in other such complexes.

There are weak C—H···O hydrogen bonds between uncoordinated carboxylate O atoms of fumaric acid and lattice water molecules, which extend one-dimensional chain into three-dimensional supramolecular packing structure (Fig. 2, Table 2).

Experimental

Cadmium(II) acetate dihydrate (0.080 g, 0.3 mol), 4,4'-bipyridine (0.039 g, 0.2 mmol), fumaric acid (0.232 g, 0.2 mmol), sodium hydroxide (0.024 g, 0.4 mmol) and water (14 ml) were placed in a 23 ml Teflon-lined autoclave, and the autoclave was heated at 423 K for 3 d. After cooling slowly to room temperature at a rate of 10 K h^{-1}, colorless crystals of (I) were obtained. Analysis found: C 31.78, H 5.02, N 5.29%; calculated for $C_{14}H_{26}N_2O_{12}Cd$: C 31.89, H 4.94, N 5.34%.

Refinement

Water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions; U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were placed at calculated positions with C—H = 0.93Å and refined in riding mode;U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

Fig. 1. View of the local coordination of Cd(II) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Symmetry code: (i) -*x*,-*y*,-*z* + 2.

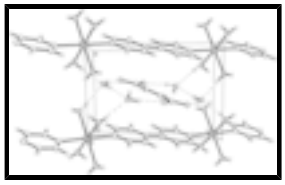

Fig. 2. A packing diagram for the two-dimensional supramolecular hydrogen-bonding framework *via* C—H···O interactions. The view shows a layer parallel to the *ac* plane; the view direction is parallel to the *b* axis. Hydrogen bonds are indicated by dashed lines.

catena-Poly[[[tetraaquacadmium(II)]-μ-4,4'-bipyridine] fumarate tetrahydrate]

Crystal data

$[Cd(C_{10}H_8N_2)(H_2O)_4](C_4H_2O_4)\cdot 4H_2O$	$Z = 1$
$M_r = 526.77$	$F_{000} = 268$
Triclinic, $P\overline{1}$	$D_x = 1.646$ Mg m^{-3}
Hall symbol: -p 1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 7.183$ (5) Å	Cell parameters from 3394 reflections
$b = 7.802$ (5) Å	$\theta = 2.1$–28.0º
$c = 10.038$ (5) Å	$\mu = 1.09$ mm^{-1}
$\alpha = 80.434$ (5)º	$T = 293$ (2) K
$\beta = 87.791$ (5)º	Block, colorless
$\gamma = 73.288$ (5)º	0.21 × 0.19 × 0.15 mm
$V = 531.3$ (6) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	2378 independent reflections
Radiation source: fine-focus sealed tube	2363 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.045$
Detector resolution: 10 pixels mm^{-1}	$\theta_{max} = 28.2$º
$T = 293$(2) K	$\theta_{min} = 2.1$º
ω scan	$h = -9\rightarrow 9$
Absorption correction: multi-scan (Higashi, 1995)	$k = -10\rightarrow 10$
$T_{min} = 0.804$, $T_{max} = 0.854$	$l = -13\rightarrow 10$
3414 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
$R[F^2 > 2\sigma(F^2)] = 0.028$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.072$	$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$

2378 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
165 parameters	$\Delta\rho_{min} = -1.30$ 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	0.0000	0.0000	1.0000	0.03262 (9)
O1W	−0.1754 (3)	−0.1628 (3)	0.9055 (2)	0.0469 (4)
O2W	0.2890 (3)	−0.1665 (3)	0.9317 (2)	0.0554 (5)
O3W	0.4251 (4)	0.9783 (3)	0.3137 (2)	0.0540 (5)
O4W	0.5895 (3)	0.7407 (3)	0.1154 (2)	0.0492 (4)
O1	0.6065 (3)	0.1946 (3)	0.4185 (2)	0.0531 (4)
O2	0.6400 (4)	0.3942 (3)	0.2406 (2)	0.0606 (5)
N1	−0.0243 (3)	0.1980 (2)	0.80060 (18)	0.0371 (4)
C1	0.5988 (3)	0.3514 (3)	0.3622 (2)	0.0387 (4)
C2	0.5375 (4)	0.5053 (3)	0.4404 (2)	0.0424 (5)
H2	0.5545	0.6162	0.4007	0.051*
C3	0.0421 (4)	0.1372 (3)	0.6866 (2)	0.0465 (5)
H3	0.0823	0.0126	0.6873	0.056*
C4	0.0540 (4)	0.2496 (3)	0.5679 (2)	0.0468 (5)
H4	0.1014	0.2005	0.4907	0.056*
C5	−0.0050 (3)	0.4372 (3)	0.56279 (19)	0.0317 (4)
C6	−0.0735 (4)	0.4991 (3)	0.6825 (2)	0.0438 (5)
H6	−0.1135	0.6229	0.6852	0.053*
C7	−0.0823 (4)	0.3778 (3)	0.7969 (2)	0.0449 (5)
H7	−0.1307	0.4227	0.8754	0.054*
H1WA	−0.248 (6)	−0.192 (6)	0.955 (5)	0.087 (15)*
H1WB	−0.233 (5)	−0.117 (5)	0.847 (4)	0.052 (10)*
H2WA	0.366 (4)	−0.196 (4)	0.983 (3)	0.036 (7)*
H2WB	0.300 (5)	−0.218 (5)	0.877 (4)	0.058 (10)*
H3WA	0.406 (5)	0.923 (5)	0.392 (4)	0.058 (9)*
H3WB	0.493 (6)	1.030 (6)	0.324 (4)	0.081 (13)*
H4WA	0.615 (5)	0.651 (5)	0.147 (4)	0.053 (10)*
H4WB	0.555 (6)	0.805 (6)	0.167 (5)	0.076 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04199 (14)	0.02980 (13)	0.02433 (12)	−0.00900 (8)	0.00253 (8)	−0.00217 (7)
O1W	0.0558 (10)	0.0477 (10)	0.0416 (10)	−0.0201 (8)	−0.0010 (9)	−0.0096 (8)
O2W	0.0517 (10)	0.0647 (12)	0.0434 (10)	0.0051 (9)	−0.0049 (8)	−0.0284 (9)
O3W	0.0781 (13)	0.0511 (11)	0.0409 (10)	−0.0323 (10)	−0.0092 (9)	−0.0037 (8)
O4W	0.0629 (11)	0.0454 (11)	0.0406 (10)	−0.0186 (9)	−0.0017 (8)	−0.0044 (8)
O1	0.0835 (13)	0.0395 (9)	0.0421 (9)	−0.0222 (9)	0.0074 (9)	−0.0167 (7)
O2	0.0999 (15)	0.0437 (10)	0.0431 (10)	−0.0239 (10)	0.0203 (10)	−0.0195 (8)
N1	0.0459 (9)	0.0343 (9)	0.0284 (8)	−0.0105 (7)	0.0014 (7)	0.0002 (7)
C1	0.0462 (11)	0.0358 (10)	0.0389 (11)	−0.0145 (8)	0.0051 (8)	−0.0158 (9)
C2	0.0583 (13)	0.0353 (10)	0.0387 (11)	−0.0171 (9)	0.0089 (9)	−0.0151 (8)
C3	0.0692 (15)	0.0313 (10)	0.0334 (11)	−0.0084 (10)	0.0050 (10)	−0.0011 (8)
C4	0.0710 (15)	0.0336 (11)	0.0300 (11)	−0.0079 (10)	0.0097 (10)	−0.0033 (8)
C5	0.0350 (9)	0.0318 (9)	0.0268 (9)	−0.0094 (7)	−0.0010 (7)	−0.0003 (8)
C6	0.0656 (14)	0.0310 (10)	0.0317 (10)	−0.0099 (9)	0.0056 (9)	−0.0043 (8)
C7	0.0636 (14)	0.0370 (11)	0.0297 (10)	−0.0091 (10)	0.0065 (9)	−0.0035 (8)

Geometric parameters (Å, °)

Cd1—O2W^{i}	2.259 (2)	O2—C1	1.257 (3)
Cd1—O2W	2.259 (2)	N1—C3	1.331 (3)
Cd1—N1^{i}	2.295 (2)	N1—C7	1.338 (3)
Cd1—N1	2.295 (2)	C1—C2	1.495 (3)
Cd1—O1W	2.348 (2)	C2—C2^{ii}	1.293 (5)
Cd1—O1W^{i}	2.348 (2)	C2—H2	0.9300
O1W—H1WA	0.76 (5)	C3—C4	1.373 (3)
O1W—H1WB	0.71 (4)	C3—H3	0.9300
O2W—H2WA	0.73 (3)	C4—C5	1.394 (3)
O2W—H2WB	0.72 (4)	C4—H4	0.9300
O3W—H3WA	0.85 (4)	C5—C6	1.390 (3)
O3W—H3WB	0.74 (4)	C5—C5^{iii}	1.476 (4)
O4W—H4WA	0.70 (4)	C6—C7	1.373 (3)
O4W—H4WB	0.77 (4)	C6—H6	0.9300
O1—C1	1.246 (3)	C7—H7	0.9300
O2W^{i}—Cd1—O2W	180.0	C3—N1—Cd1	120.40 (15)
O2W^{i}—Cd1—N1^{i}	89.00 (8)	C7—N1—Cd1	121.73 (15)
O2W—Cd1—N1^{i}	91.00 (8)	O1—C1—O2	124.9 (2)
O2W^{i}—Cd1—N1	91.00 (8)	O1—C1—C2	120.0 (2)
O2W—Cd1—N1	89.00 (8)	O2—C1—C2	115.1 (2)
N1^{i}—Cd1—N1	180.0	C2^{ii}—C2—C1	124.4 (3)
O2W^{i}—Cd1—O1W	86.81 (9)	C2^{ii}—C2—H2	117.8
O2W—Cd1—O1W	93.19 (9)	C1—C2—H2	117.8
N1^{i}—Cd1—O1W	89.40 (8)	N1—C3—C4	123.1 (2)

N1—Cd1—O1W	90.60 (8)	N1—C3—H3	118.4
O2W^{i}—Cd1—O1W^{i}	93.19 (9)	C4—C3—H3	118.4
O2W—Cd1—O1W^{i}	86.81 (9)	C3—C4—C5	120.1 (2)
N1^{i}—Cd1—O1W^{i}	90.60 (8)	C3—C4—H4	120.0
N1—Cd1—O1W^{i}	89.40 (8)	C5—C4—H4	120.0
O1W—Cd1—O1W^{i}	180.0	C6—C5—C4	116.28 (18)
Cd1—O1W—H1WA	112 (3)	C6—C5—C5^{iii}	121.9 (2)
Cd1—O1W—H1WB	117 (3)	C4—C5—C5^{iii}	121.8 (2)
H1WA—O1W—H1WB	103 (4)	C7—C6—C5	120.1 (2)
Cd1—O2W—H2WA	115 (2)	C7—C6—H6	119.9
Cd1—O2W—H2WB	124 (3)	C5—C6—H6	119.9
H2WA—O2W—H2WB	117 (4)	N1—C7—C6	123.0 (2)
H3WA—O3W—H3WB	106 (4)	N1—C7—H7	118.5
H4WA—O4W—H4WB	111 (4)	C6—C7—H7	118.5
C3—N1—C7	117.36 (19)		
O2W^{i}—Cd1—N1—C3	−144.1 (2)	C7—N1—C3—C4	0.3 (4)
O2W—Cd1—N1—C3	35.9 (2)	Cd1—N1—C3—C4	−171.6 (2)
O1W—Cd1—N1—C3	−57.3 (2)	N1—C3—C4—C5	0.0 (4)
O1W^{i}—Cd1—N1—C3	122.7 (2)	C3—C4—C5—C6	0.2 (4)
O2W^{i}—Cd1—N1—C7	44.3 (2)	C3—C4—C5—C5^{iii}	−179.8 (3)
O2W—Cd1—N1—C7	−135.7 (2)	C4—C5—C6—C7	−0.7 (3)
O1W—Cd1—N1—C7	131.1 (2)	C5^{iii}—C5—C6—C7	179.3 (3)
O1W^{i}—Cd1—N1—C7	−48.9 (2)	C3—N1—C7—C6	−0.8 (4)
O1—C1—C2—C2^{ii}	−10.8 (5)	Cd1—N1—C7—C6	171.0 (2)
O2—C1—C2—C2^{ii}	169.3 (3)	C5—C6—C7—N1	1.0 (4)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WB···O3W^{iii}	0.71 (4)	2.10 (4)	2.811 (3)	175 (4)
O1W—H1WA···O4W^{iv}	0.76 (5)	2.04 (5)	2.790 (3)	168 (5)
O4W—H4WB···O3W	0.77 (4)	2.16 (4)	2.929 (3)	173 (4)
O3W—H3WB···O1^{v}	0.74 (4)	2.06 (4)	2.759 (3)	157 (4)
O4W—H4WA···O2	0.70 (4)	2.02 (4)	2.714 (3)	170 (4)
O3W—H3WA···O1^{ii}	0.85 (4)	1.98 (4)	2.833 (3)	172 (3)
O2W—H2WB···O2^{vi}	0.72 (4)	1.91 (4)	2.615 (3)	168 (4)
O2W—H2WA···O4W^{vii}	0.73 (3)	2.02 (3)	2.748 (3)	175 (3)

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

Fig. 1

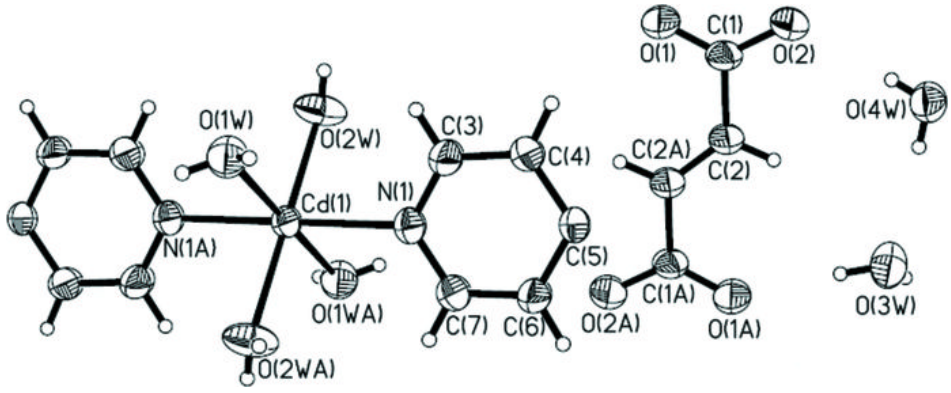
C(1)
O(1)
O(2)
O(4W)
O(1W)
O(2W)
C(3)
C(4)
C(2A)
C(2)
Cd(1)
N(1)
N(1A)
C(5)
C(1A)
O(3W)
O(1WA)
C(7)
C(6)
O(2A)
O(1A)
O(2WA)

Fig. 2