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A one-dimensional coordination polymer: *catena*-poly[[diaqua(2,4-dihydroxybenzoato)cadmium(II)]-μ-2,4-dihydroxybenzoato]

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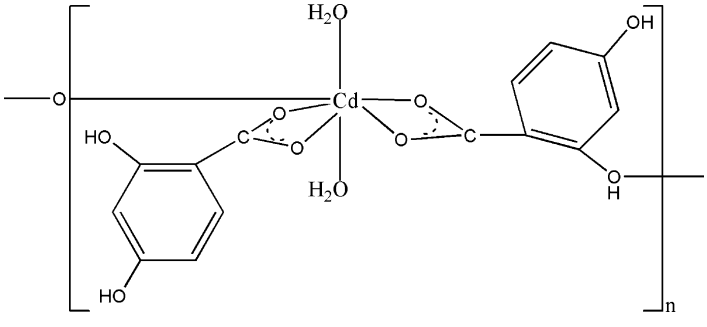
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.029; wR factor = 0.068; data-to-parameter ratio = 12.4.

The title compound, $[Cd(C_7H_5O_4)_2(H_2O)_2]_n$, consists of a one-dimensional chain, in which the Cd^{2+} centre is coordinated by four O atoms from two bidentate carboxylate groups of two 2,4-dihydroxybenzoate anions, two water molecules, and one hydroxyl O atom of another 2,4-dihydroxybenzoate anion. This results in a distorted pentagonal–bipyramidal CdO_7 polyhedron.

Related literature

For related literature, see: Tao *et al.* (2000), Thirumurugan & Natarajan (2004) and Zhang *et al.* (2005).



Experimental

Crystal data

$[Cd(C_7H_5O_4)_2(H_2O)_2]$
M_r = 454.65
Orthorhombic, *Pbca*
a = 11.964 (2) Å
b = 7.7882 (16) Å
c = 33.893 (7) Å
V = 3158.1 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.44 mm^{-1}
T = 292 (2) K
0.35 × 0.20 × 0.04 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.633, T_{max} = 0.945
19791 measured reflections
3063 independent reflections
2847 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.069
S = 1.05
3063 reflections
248 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O9	2.196 (2)	Cd1—O3^{i}	2.397 (2)
Cd1—O10	2.268 (3)	Cd1—O5	2.428 (2)
Cd1—O6	2.327 (2)	Cd1—O1	2.459 (2)
Cd1—O2	2.364 (2)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···O1	0.80 (5)	1.80 (5)	2.536 (3)	154 (5)
O4—H4A···O8^{ii}	0.82	1.96	2.775 (3)	173
O7—H7···O6	0.82	1.81	2.535 (3)	147
O8—H8···O7^{iii}	0.82	1.99	2.732 (3)	151
O9—H91···O2^{iv}	0.813 (10)	1.928 (11)	2.738 (3)	175 (3)
O9—H92···O5^{v}	0.812 (10)	1.896 (10)	2.706 (3)	175 (3)
O10—H101···O2^{vi}	0.809 (10)	2.074 (15)	2.855 (3)	162 (3)

Symmetry codes: (ii) $-x+\frac{3}{2}, -y+1, z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (iv) $-x+2, -y, -z+1$; (v) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (vi) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2367).

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supplementary materials

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A one-dimensional coordination polymer: *catena*-poly[[diaqua(2,4-dihydroxybenzoato)cadmium(II)]-μ-2,4-dihydroxybenzoato]

Z.-L. Wang and Y.-P. Niu

Comment

Design and synthesis of metal coordination polymers based on benzene carboxylates have been attracting chemist's interests and constitutes an important area of research (Thirumurugan & Natarajan, 2004). During the past years, lots of novel benzene multicarboxylates base compounds have been reported (Tao *et al.*, 2000; Zhang *et al.*, 2005). However, in those reported literatures, the common features tried to construct predictable one-, two, three-dimensional coordination networks by changing the numbers or relative position of carboxylates. In contrast, benzene carboxylates containing the hydroxyl can be utilized to coordinate to metal ions and generate unusual structures have never been reported. Herein, we report the title compound (I).

The title compound (I) present a one-dimensional chain $[Cd(C_7O_4H_5)_2(H_2O)_2]_n$, in which Cd^{2+} is coordinated by four oxygen atoms from two 2,4-dihydroxybenzoate anion, two water molecules, and one oxygen from the hydroxyl of another 2,4-dihydroxybenzoate anion. The environment of Cd ion is in a distorted pentagonal bipyramid (Fig. 1). In the equatorial plane, Cd1 ion is coordinated by four carboxylates oxygen (O1, O2, O5, O6) and one oxygen (O3b) of the hydroxyl. The Cd1—O distances range from 2.327 (2) to 2.459 (2)Å (Table 1). The mean deviation from the equatorial plane is 0.129 Å. The axial sites are occupied by two water oxygen atoms (O9 and O10) with Cd1—O lengths ranging from 2.196 (2) to 2.268 (3)Å (Table 1). The obvious differences of Cd1—O length show that the water more greatly interact with the Cd^{2+} ion than that of the carboxylate. The axial O9—Cd1—O10 bond angle is 177.80 (9) Å.

In addition, the intra-molecular hydrogen bonds exhibit in the compound, O7—H7 and O3—H31 acting as hydrogen bond donor, and O6 and O1 as hydrogen bond acceptor, constructing two S(6) rings (Fig. 1, Table 2). These units are linked into a one-dimensional chain-like structure by the hydroxyl oxygen atom O3 (Fig. 2).

Experimental

Solid $CdCO_3$ (1 mmol, 0.172 g) was added to an aqueous solution (25 ml) of 2,4-dihydroxybenzoic acid (2.0 mmol, 0.308 g). The mixture was stirred for 10 minutes under the temperature of 373 K. The solution was filtered, and the filtrate was kept at the room temperature. After ten days weeks, colorless crystals of (I) were obtained.

Refinement

The H atoms bonded to water were located in a difference synthesis and refined with distance restraints O—H = 0.82 (1) Å and H···H = 1.34 (2) Å and U_{iso}(H) = U_{eq}(O). The remaining H atoms were positioned geometrically, with C—H = 0.93 Å and O—H = 0.82 Å, and were refined as riding with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(O).

Figures

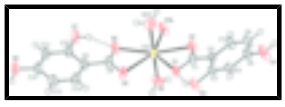

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. For clarity, H atoms not involved in hydrogen bonds are omitted. [Symmetry code: (*b*) 1/2 + *x*, 1/2 − *y*, 1 − *z*]

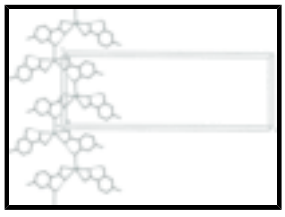

Fig. 2. One-dimensional structure of (I), For clarity, H atoms not involved in hydrogen bonds are omitted.

catena-poly[[diaqua(2,4-dihydroxybenzoato)cadmium(II)]-μ-2,4-dihydroxybenzoato]

Crystal data

$[Cd(C_7H_5O_4)_2(H_2O)_2]$	F_{000} = 1808
M_r = 454.65	D_x = 1.912 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5177 reflections
a = 11.964 (2) Å	θ = 3.0–28.2º
b = 7.7882 (16) Å	μ = 1.44 mm^{-1}
c = 33.893 (7) Å	*T* = 292 (2) K
V = 3158.1 (11) Å^3	Plate, colourless
Z = 8	0.35 × 0.20 × 0.04 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3063 independent reflections
Radiation source: fine-focus sealed tube	2847 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 292(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	*h* = −14→14
T_{min} = 0.633, T_{max} = 0.945	*k* = −9→9
19791 measured reflections	*l* = −41→41

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H atoms treated by a mixture of independent and constrained refinement

$wR(F^2) = 0.069$	$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 3.765P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.002$
3063 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
248 parameters	$\Delta\rho_{min} = -0.47$ e Å^{-3}
18 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.903474 (16)	0.23166 (3)	0.448614 (5)	0.02615 (9)
O1	0.75857 (17)	0.2302 (3)	0.50006 (5)	0.0358 (5)
O2	0.93525 (17)	0.2420 (3)	0.51741 (6)	0.0370 (5)
O3	0.60334 (16)	0.2867 (4)	0.54931 (6)	0.0423 (6)
H31	0.635 (4)	0.265 (5)	0.5293 (14)	0.063*
O4	0.69862 (19)	0.4547 (4)	0.67789 (7)	0.0659 (8)
H4A	0.7529	0.4701	0.6922	0.099*
O5	0.74055 (18)	0.2508 (3)	0.40614 (6)	0.0383 (5)
O6	0.90716 (16)	0.2860 (3)	0.38111 (6)	0.0411 (5)
O7	0.93668 (17)	0.3721 (4)	0.30975 (6)	0.0560 (7)
H7	0.9543	0.3431	0.3322	0.084*
O8	0.62706 (19)	0.4682 (4)	0.22892 (7)	0.0636 (8)
H8	0.5632	0.4326	0.2256	0.095*
O9	0.91561 (19)	−0.0476 (3)	0.44064 (8)	0.0487 (6)
H91	0.9608 (19)	−0.100 (3)	0.4540 (8)	0.033 (9)*
H92	0.871 (2)	−0.113 (3)	0.4305 (9)	0.039 (9)*
O10	0.8982 (2)	0.5205 (3)	0.45687 (8)	0.0489 (6)
H101	0.949 (2)	0.571 (4)	0.4677 (8)	0.049*
H102	0.886 (3)	0.551 (4)	0.4348 (4)	0.049*
C1	0.8319 (2)	0.2536 (3)	0.52658 (8)	0.0288 (6)
C2	0.7975 (2)	0.3003 (4)	0.56677 (7)	0.0260 (5)
C3	0.6847 (2)	0.3185 (4)	0.57667 (7)	0.0274 (6)
C4	0.6530 (2)	0.3707 (4)	0.61387 (8)	0.0373 (7)
H4	0.5778	0.3843	0.6200	0.045*

C5	0.7336 (2)	0.4025 (4)	0.64192 (8)	0.0374 (7)
C6	0.8462 (2)	0.3834 (5)	0.63318 (8)	0.0412 (8)
H6	0.9002	0.4036	0.6524	0.049*
C7	0.8769 (2)	0.3343 (5)	0.59590 (9)	0.0383 (7)
H7A	0.9524	0.3234	0.5899	0.046*
C8	0.8016 (2)	0.2865 (4)	0.37699 (8)	0.0310 (6)
C9	0.7541 (2)	0.3296 (4)	0.33825 (8)	0.0312 (6)
C10	0.8238 (2)	0.3718 (4)	0.30639 (8)	0.0357 (7)
C11	0.7786 (2)	0.4173 (5)	0.27043 (8)	0.0448 (8)
H11	0.8254	0.4477	0.2497	0.054*
C12	0.6648 (3)	0.4178 (5)	0.26516 (9)	0.0432 (8)
C13	0.5936 (2)	0.3759 (6)	0.29596 (10)	0.0500 (10)
H13	0.5165	0.3771	0.2924	0.060*
C14	0.6393 (2)	0.3325 (5)	0.33174 (9)	0.0411 (8)
H14	0.5917	0.3038	0.3524	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02635 (12)	0.03452 (14)	0.01758 (12)	0.00370 (8)	−0.00053 (7)	−0.00107 (8)
O1	0.0321 (10)	0.0571 (14)	0.0182 (9)	0.0013 (9)	−0.0009 (8)	−0.0076 (9)
O2	0.0271 (10)	0.0589 (14)	0.0249 (11)	0.0110 (9)	0.0036 (8)	−0.0027 (9)
O3	0.0221 (11)	0.0808 (18)	0.0240 (12)	−0.0032 (10)	−0.0025 (8)	−0.0144 (11)
O4	0.0374 (12)	0.135 (3)	0.0259 (12)	−0.0068 (15)	0.0072 (10)	−0.0328 (14)
O5	0.0383 (11)	0.0570 (14)	0.0196 (10)	0.0076 (10)	0.0051 (9)	0.0051 (9)
O6	0.0298 (11)	0.0700 (16)	0.0234 (11)	0.0086 (10)	−0.0049 (8)	0.0051 (10)
O7	0.0200 (10)	0.120 (2)	0.0282 (11)	−0.0045 (12)	−0.0004 (9)	0.0217 (14)
O8	0.0331 (12)	0.129 (3)	0.0284 (12)	−0.0190 (14)	−0.0113 (9)	0.0305 (14)
O9	0.0404 (13)	0.0364 (13)	0.0692 (17)	0.0016 (10)	−0.0271 (12)	−0.0001 (12)
O10	0.0490 (8)	0.0467 (8)	0.0511 (8)	0.0002 (6)	0.0005 (6)	0.0001 (6)
C1	0.0294 (14)	0.0336 (15)	0.0234 (14)	0.0049 (11)	0.0006 (11)	−0.0010 (11)
C2	0.0279 (13)	0.0346 (15)	0.0153 (12)	0.0014 (11)	0.0011 (10)	−0.0032 (11)
C3	0.0222 (12)	0.0388 (15)	0.0213 (13)	−0.0018 (11)	−0.0021 (10)	−0.0026 (11)
C4	0.0235 (14)	0.063 (2)	0.0249 (14)	−0.0066 (13)	0.0042 (11)	−0.0097 (14)
C5	0.0331 (15)	0.059 (2)	0.0197 (13)	−0.0068 (14)	0.0023 (11)	−0.0089 (13)
C6	0.0288 (15)	0.071 (2)	0.0233 (15)	−0.0037 (14)	−0.0057 (12)	−0.0128 (14)
C7	0.0222 (13)	0.065 (2)	0.0281 (15)	0.0025 (14)	−0.0004 (11)	−0.0082 (15)
C8	0.0316 (14)	0.0402 (16)	0.0212 (13)	0.0064 (12)	0.0003 (11)	−0.0006 (11)
C9	0.0274 (13)	0.0453 (17)	0.0211 (13)	0.0005 (12)	0.0003 (11)	0.0032 (12)
C10	0.0210 (13)	0.061 (2)	0.0251 (14)	−0.0028 (13)	−0.0016 (11)	0.0046 (13)
C11	0.0273 (15)	0.086 (3)	0.0211 (14)	−0.0115 (16)	−0.0002 (11)	0.0129 (15)
C12	0.0337 (16)	0.074 (2)	0.0219 (15)	−0.0074 (15)	−0.0075 (12)	0.0116 (15)
C13	0.0219 (15)	0.094 (3)	0.0345 (18)	−0.0077 (16)	−0.0028 (12)	0.0161 (18)
C14	0.0253 (14)	0.073 (2)	0.0253 (15)	−0.0031 (15)	0.0042 (11)	0.0111 (15)

Geometric parameters (Å, °)

Cd1—O9	2.196 (2)	O10—H101	0.809 (10)
Cd1—O10	2.268 (3)	O10—H102	0.798 (10)

Cd1—O6	2.327 (2)	C1—C2	1.469 (4)
Cd1—O2	2.364 (2)	C2—C7	1.396 (4)
Cd1—O3^{i}	2.397 (2)	C2—C3	1.398 (4)
Cd1—O5	2.428 (2)	C3—C4	1.378 (4)
Cd1—O1	2.459 (2)	C4—C5	1.377 (4)
O1—C1	1.270 (3)	C4—H4	0.9300
O2—C1	1.278 (4)	C5—C6	1.387 (4)
O3—C3	1.367 (3)	C6—C7	1.370 (4)
O3—Cd1^{ii}	2.397 (2)	C6—H6	0.9300
O3—H31	0.80 (5)	C7—H7A	0.9300
O4—C5	1.352 (3)	C8—C9	1.470 (4)
O4—H4A	0.8200	C9—C14	1.391 (4)
O5—C8	1.260 (3)	C9—C10	1.403 (4)
O6—C8	1.270 (3)	C10—C11	1.379 (4)
O7—C10	1.356 (3)	C11—C12	1.373 (4)
O7—H7	0.8200	C11—H11	0.9300
O8—C12	1.366 (3)	C12—C13	1.386 (4)
O8—H8	0.8200	C13—C14	1.372 (4)
O9—H91	0.813 (10)	C13—H13	0.9300
O9—H92	0.812 (10)	C14—H14	0.9300
O9—Cd1—O10	177.80 (9)	C7—C2—C1	120.8 (2)
O9—Cd1—O6	93.31 (9)	C3—C2—C1	121.3 (2)
O10—Cd1—O6	86.65 (9)	O3—C3—C4	118.6 (2)
O9—Cd1—O2	98.31 (9)	O3—C3—C2	120.4 (2)
O10—Cd1—O2	81.31 (8)	C4—C3—C2	121.0 (2)
O6—Cd1—O2	163.85 (8)	C5—C4—C3	119.5 (3)
O9—Cd1—O3^{i}	83.02 (9)	C5—C4—H4	120.3
O10—Cd1—O3^{i}	94.78 (9)	C3—C4—H4	120.3
O6—Cd1—O3^{i}	91.19 (7)	O4—C5—C4	117.4 (3)
O2—Cd1—O3^{i}	79.20 (7)	O4—C5—C6	121.7 (3)
O9—Cd1—O5	92.35 (8)	C4—C5—C6	120.9 (3)
O10—Cd1—O5	89.42 (8)	C7—C6—C5	119.2 (3)
O6—Cd1—O5	54.63 (7)	C7—C6—H6	120.4
O2—Cd1—O5	135.39 (7)	C5—C6—H6	120.4
O3^{i}—Cd1—O5	145.31 (7)	C6—C7—C2	121.5 (3)
O9—Cd1—O1	97.43 (9)	C6—C7—H7A	119.2
O10—Cd1—O1	84.11 (8)	C2—C7—H7A	119.2
O6—Cd1—O1	135.35 (7)	O5—C8—O6	119.3 (3)
O2—Cd1—O1	54.13 (7)	O5—C8—C9	121.8 (3)
O3^{i}—Cd1—O1	133.03 (7)	O6—C8—C9	118.9 (2)
O5—Cd1—O1	81.64 (7)	O5—C8—Cd1	61.99 (15)
C1—O1—Cd1	90.81 (17)	O6—C8—Cd1	57.45 (14)
C1—O2—Cd1	94.99 (17)	C9—C8—Cd1	174.7 (2)
C3—O3—Cd1^{ii}	134.54 (17)	C14—C9—C10	117.4 (2)
C3—O3—H31	106 (3)	C14—C9—C8	121.8 (2)
Cd1^{ii}—O3—H31	120 (3)	C10—C9—C8	120.7 (3)
C5—O4—H4A	109.5	O7—C10—C11	117.6 (2)

C8—O5—Cd1	90.73 (17)	O7—C10—C9	121.9 (2)
C8—O6—Cd1	95.15 (17)	C11—C10—C9	120.5 (3)
C10—O7—H7	109.5	C12—C11—C10	120.3 (3)
C12—O8—H8	109.5	C12—C11—H11	119.9
Cd1—O9—H91	118.1 (18)	C10—C11—H11	119.9
Cd1—O9—H92	128.9 (19)	O8—C12—C11	116.5 (3)
H91—O9—H92	110.9 (17)	O8—C12—C13	122.8 (3)
Cd1—O10—H101	121 (2)	C11—C12—C13	120.7 (3)
Cd1—O10—H102	101 (2)	C14—C13—C12	118.6 (3)
H101—O10—H102	114.2 (18)	C14—C13—H13	120.7
O1—C1—O2	119.1 (3)	C12—C13—H13	120.7
O1—C1—C2	119.9 (2)	C13—C14—C9	122.5 (3)
O2—C1—C2	121.0 (2)	C13—C14—H14	118.8
C7—C2—C3	117.9 (2)	C9—C14—H14	118.8

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H31···O1	0.80 (5)	1.80 (5)	2.536 (3)	154 (5)
O4—H4A···O8^{iii}	0.82	1.96	2.775 (3)	173
O7—H7···O6	0.82	1.81	2.535 (3)	147
O8—H8···O7^{iv}	0.82	1.99	2.732 (3)	151
O9—H91···O2^{v}	0.813 (10)	1.928 (11)	2.738 (3)	175 (3)
O9—H92···O5^{vi}	0.812 (10)	1.896 (10)	2.706 (3)	175 (3)
O10—H101···O2^{vii}	0.809 (10)	2.074 (15)	2.855 (3)	162 (3)

Symmetry codes: (iii) −*x*+3/2, −*y*+1, *z*+1/2; (iv) *x*−1/2, *y*, −*z*+1/2; (v) −*x*+2, −*y*, −*z*+1; (vi) −*x*+3/2, *y*−1/2, *z*; (vii) −*x*+2, −*y*+1, −*z*+1.

Fig. 1

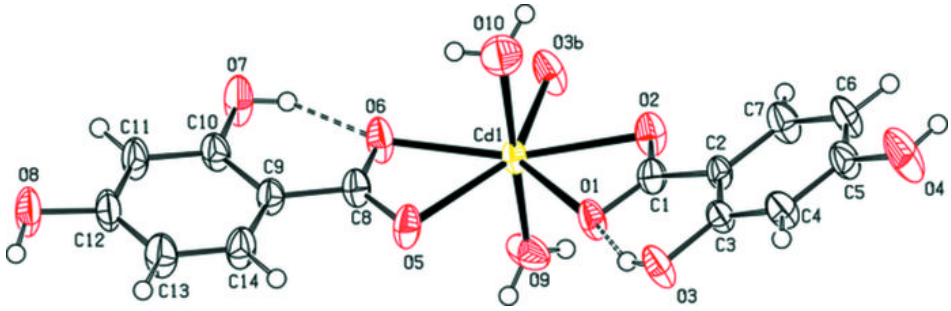
O10
O3b
O7
O6
Cd1
O2
C7
C6
C11
C10
C2
O8
C9
O1
C1
C5
O4
C12
C8
C4
C3
O5
O9
O3
C13
C14

Fig. 2