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Diaquabis{4-[(6-chloropyridin-3-yl)-methoxy]benzoato}cadmium(II)

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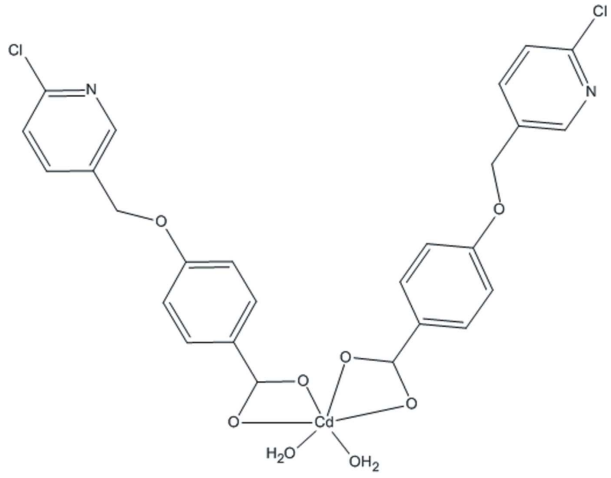
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.107; data-to-parameter ratio = 17.2.

The title compound, $[Cd(C_{13}H_9ClNO_3)_2(H_2O)_2]$, is a mononuclear complex in which the Cd^{II} atom, located on a twofold axis, shows an octahedral coordination geometry. It is surrounded by four carboxylate O atoms from two 4-[(6-chloropyridin-3-yl)methoxy]benzoate acid ligands and two water molecules. O—H···O hydrogen bonds link these complexes to generate a two-dimensional supramolecular network.

Related literature

For related literature, see: Fujita *et al.* (1994); Inoue *et al.* (1996); Kitazawa *et al.* (1994); Ermer (1991).



Experimental

Crystal data

$[Cd(C_{13}H_9ClNO_3)_2(H_2O)_2]$
M_r = 673.76
Monoclinic, $C2/c$
a = 42.179 (8) Å
b = 5.355 (1) Å
c = 12.068 (2) Å
β = 105.688 (3)°
V = 2624.2 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.09 mm^{-1}
T = 293 (2) K
0.35 × 0.32 × 0.28 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.668, T_{max} = 0.742
7350 measured reflections
3053 independent reflections
2705 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.107
S = 1.09
3053 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −1.32 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1B···O2^{i}	0.84	1.88	2.708 (3)	169
O1W—H1A···O3^{ii}	0.85	1.95	2.799 (3)	175

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Putz, 2004); software used to prepare material for publication: *SHELXL97*.

We thank the Analysis and Testing Foundation of Northeast Normal University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2258).

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supplementary materials

Acta Cryst. (2007). E**63**, m2956 [**doi:10.1107/S1600536807055341**]

Diaquabis{4-[(6-chloropyridin-3-yl)methoxy]benzoato}cadmium(II)

S.-L. Li, J. Liu and Y.-Y. Liu

Comment

The synthesis and characterization of coordination compounds with infinite two- and three-dimensional networks have been an area of rapid growth in recent years because of the potential of these polymers in various applications, such as catalysis, electrical conductivity, host–guest chemistry and magnetism (Ermer, 1991; Fujita *et al.*,1994; Inoue *et al.*,1996; Kitazawa *et al.*,1994). In this paper, we report a new coordination compound, (I).

The asymmetric part of the unit cell contains one 4-((6-chloropyridin-3-yl)methoxy)benzoic acid (hereafter *L*) molecule, one water molecule and half Cd (II) atom located on a two fold axis (Fig. 1). Cd(II) atom is octahedrally surrounded by four carboxylate O atoms from *L* ligands and two water molecules. Each complex is linked to four adjacent molecules through O—H···O hydrogen bonds building a two-dimensional supramolecular structure (Table 1, Fig. 2).

Experimental

A mixture of *L* (0.39 g, 1.50 mmol), $Cd(OAc)_2{\cdot}2H_2O$ (0.20 g, 0.75 mmol), NaOH (0.08 g, 2.00 mmol) and H_2O (10 ml) was stirred for 1 h and then sealed in a 25 ml Teflonlined stainless steel container. The container was heated to 150 °C and held at that temperature for 72 h, then cooled to 100 °C at a rate of 5 °C.h^{-1}, and held for 8 h, followed by further cooling to 30 °C at a rate of 3 °C.h^{-1}. Colorless crystals of I were collected in 72.9% yield based on $Cd(OAc)_2{\cdot}2H_2O$.

Refinement

All H atoms attached to C atom were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.97 Å (methylene) with U_{iso}(H) = 1.2U_{eq}(C). H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H= 0.85 (1)Å and H···H= 1.39 (2) Å) with U_{iso}(H) = 1.5U_{eq}(O).

Figures

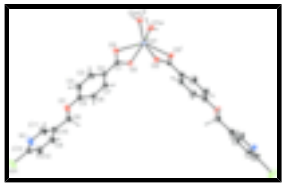

Fig. 1. Molecular view of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. [Symmetry code: (i) −*x*, *y*, −*z* + 1/2]

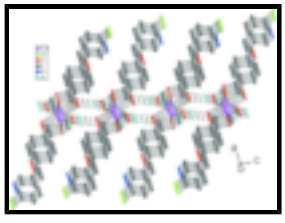

Fig. 2. Ball-stick representation of the two-dimensional supramolecular structure of (I). H atoms not involved in hydrogen bondings have been omitted for clarity.

diaquabis{4-[(6-chloropyridin-3-yl)methoxy]benzoato}cadmium(II)

Crystal data

$[Cd(C_{13}H_9ClNO_3)_2(H_2O)_2]$	$Z = 4$
$M_r = 673.76$	$F_{000} = 1352$
Monoclinic, $C2/c$	$D_x = 1.705$ Mg m^{-3}
Hall symbol: -C2yc	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 42.179$ (8) Å	$\theta = 1.0$–28.5º
$b = 5.3550$ (10) Å	$\mu = 1.09$ mm^{-1}
$c = 12.068$ (2) Å	$T = 293$ (2) K
$\beta = 105.688$ (3)º	Block, colorless
$V = 2624.2$ (8) Å^3	0.35 × 0.32 × 0.28 mm

Data collection

Bruker APEX CCD area-detector diffractometer	3053 independent reflections
Radiation source: fine-focus sealed tube	2705 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 293(2)$ K	$\theta_{max} = 28.5$º
ω scans	$\theta_{min} = 1.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -47\rightarrow56$
$T_{min} = 0.668$, $T_{max} = 0.742$	$k = -5\rightarrow7$
7350 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
3053 reflections	$\Delta\rho_{max} = 1.11$ e Å^{-3}
177 parameters	$\Delta\rho_{min} = -1.32$ 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.10193 (5)	0.2500	0.03122 (12)
Cl1	0.22388 (3)	2.0232 (2)	0.93684 (10)	0.0703 (3)
O3	0.02898 (5)	0.2671 (4)	0.43946 (15)	0.0407 (5)
O1	0.13219 (6)	1.1274 (4)	0.64750 (19)	0.0482 (6)
O2	0.04099 (5)	0.3902 (3)	0.28184 (16)	0.0338 (4)
O1W	0.01884 (6)	−0.1942 (4)	0.15699 (17)	0.0491 (6)
H1A	0.0218	−0.2068	0.0906	0.074*
H1B	0.0231	−0.3320	0.1916	0.074*
C1	0.04501 (7)	0.4065 (5)	0.3902 (2)	0.0305 (6)
C2	0.06863 (7)	0.5953 (5)	0.4555 (2)	0.0331 (6)
C5	0.11184 (7)	0.9573 (6)	0.5787 (2)	0.0377 (7)
N1	0.18116 (8)	1.6700 (7)	0.8646 (3)	0.0625 (9)
C4	0.09167 (9)	0.8246 (7)	0.6313 (3)	0.0514 (9)
H4	0.0925	0.8554	0.7078	0.062*
C10	0.17138 (7)	1.4579 (6)	0.6830 (3)	0.0380 (6)
C6	0.11068 (8)	0.9102 (5)	0.4640 (3)	0.0395 (7)
H6	0.1243	0.9969	0.4283	0.047*
C13	0.20380 (8)	1.7999 (7)	0.8364 (3)	0.0453 (7)
C7	0.08877 (7)	0.7310 (6)	0.4039 (2)	0.0362 (6)
H7	0.0876	0.7014	0.3270	0.043*
C3	0.07039 (9)	0.6467 (7)	0.5699 (3)	0.0503 (9)
H3	0.0569	0.5592	0.6058	0.060*
C12	0.21300 (9)	1.7701 (8)	0.7365 (3)	0.0567 (9)
H12	0.2300	1.8642	0.7218	0.068*
C8	0.15233 (7)	1.2737 (6)	0.5960 (3)	0.0420 (7)
H8A	0.1388	1.3619	0.5298	0.050*
H8B	0.1674	1.1667	0.5699	0.050*
C11	0.16489 (9)	1.5008 (9)	0.7877 (3)	0.0593 (10)
H11	0.1484	1.4076	0.8059	0.071*
C9	0.19618 (9)	1.5959 (6)	0.6588 (3)	0.0522 (9)
H9	0.2016	1.5715	0.5898	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0474 (2)	0.02401 (17)	0.02261 (16)	0.000	0.01016 (12)	0.000
Cl1	0.0774 (6)	0.0702 (7)	0.0622 (6)	−0.0228 (5)	0.0169 (5)	−0.0343 (6)

O3	0.0606 (13)	0.0427 (12)	0.0210 (9)	−0.0154 (9)	0.0149 (8)	−0.0019 (9)
O1	0.0626 (14)	0.0560 (15)	0.0288 (11)	−0.0288 (10)	0.0171 (10)	−0.0100 (9)
O2	0.0513 (12)	0.0329 (11)	0.0198 (9)	−0.0038 (8)	0.0139 (8)	−0.0023 (7)
O1W	0.0920 (17)	0.0349 (11)	0.0275 (10)	0.0200 (11)	0.0284 (10)	0.0051 (9)
C1	0.0443 (15)	0.0275 (13)	0.0211 (12)	0.0015 (10)	0.0115 (11)	0.0002 (10)
C2	0.0458 (16)	0.0332 (15)	0.0223 (13)	−0.0051 (10)	0.0124 (12)	−0.0037 (10)
C5	0.0494 (17)	0.0384 (16)	0.0257 (14)	−0.0108 (12)	0.0106 (12)	−0.0059 (12)
N1	0.076 (2)	0.077 (2)	0.0399 (15)	−0.0291 (17)	0.0250 (15)	−0.0222 (16)
C4	0.076 (2)	0.060 (2)	0.0243 (14)	−0.0297 (18)	0.0239 (15)	−0.0139 (15)
C10	0.0435 (15)	0.0398 (16)	0.0303 (14)	−0.0042 (12)	0.0093 (12)	−0.0014 (12)
C6	0.0505 (17)	0.0443 (18)	0.0273 (14)	−0.0112 (12)	0.0168 (13)	0.0001 (12)
C13	0.0524 (18)	0.0437 (18)	0.0391 (16)	−0.0091 (14)	0.0109 (14)	−0.0116 (15)
C7	0.0473 (15)	0.0453 (17)	0.0185 (11)	−0.0047 (12)	0.0131 (11)	−0.0014 (12)
C3	0.073 (2)	0.059 (2)	0.0262 (15)	−0.0309 (16)	0.0254 (15)	−0.0115 (14)
C12	0.059 (2)	0.065 (2)	0.052 (2)	−0.0275 (17)	0.0250 (16)	−0.0152 (19)
C8	0.0496 (17)	0.0472 (18)	0.0304 (14)	−0.0138 (13)	0.0129 (12)	−0.0020 (13)
C11	0.071 (2)	0.072 (2)	0.0427 (19)	−0.032 (2)	0.0281 (18)	−0.0167 (19)
C9	0.062 (2)	0.065 (2)	0.0365 (17)	−0.0242 (16)	0.0244 (15)	−0.0140 (15)

Geometric parameters (Å, °)

Cd1—O1W	2.211 (2)	C5—C6	1.394 (4)
Cd1—O1W^{i}	2.211 (2)	N1—C13	1.299 (4)
Cd1—O2	2.2714 (19)	N1—C11	1.345 (5)
Cd1—O2^{i}	2.2714 (19)	C4—C3	1.379 (4)
Cd1—O3	2.4480 (19)	C4—H4	0.9300
Cd1—O3^{i}	2.4480 (19)	C10—C9	1.375 (4)
Cd1—C1	2.718 (3)	C10—C11	1.382 (4)
Cd1—C1^{i}	2.718 (3)	C10—C8	1.505 (4)
Cl1—C13	1.750 (3)	C6—C7	1.393 (4)
O3—C1	1.259 (3)	C6—H6	0.9300
O1—C5	1.368 (3)	C13—C12	1.372 (5)
O1—C8	1.417 (3)	C7—H7	0.9300
O2—C1	1.276 (3)	C3—H3	0.9300
O1W—H1A	0.8464	C12—C9	1.376 (5)
O1W—H1B	0.8432	C12—H12	0.9300
C1—C2	1.487 (4)	C8—H8A	0.9700
C2—C7	1.386 (4)	C8—H8B	0.9700
C2—C3	1.390 (4)	C11—H11	0.9300
C5—C4	1.387 (4)	C9—H9	0.9300
O1W—Cd1—O1W^{i}	88.35 (12)	C7—C2—C3	117.8 (3)
O1W—Cd1—O2	102.22 (8)	C7—C2—C1	121.5 (2)
O1W^{i}—Cd1—O2	139.74 (7)	C3—C2—C1	120.6 (2)
O1W—Cd1—O2^{i}	139.74 (7)	O1—C5—C4	115.2 (3)
O1W^{i}—Cd1—O2^{i}	102.22 (8)	O1—C5—C6	124.8 (3)
O2—Cd1—O2^{i}	94.39 (10)	C4—C5—C6	120.0 (3)
O1W—Cd1—O3	125.17 (8)	C13—N1—C11	117.0 (3)

O1W^{i}—Cd1—O3	86.69 (7)	C3—C4—C5	119.9 (3)
O2—Cd1—O3	55.35 (6)	C3—C4—H4	120.0
O2^{i}—Cd1—O3	94.44 (7)	C5—C4—H4	120.0
O1W—Cd1—O3^{i}	86.69 (7)	C9—C10—C11	117.1 (3)
O1W^{i}—Cd1—O3^{i}	125.17 (8)	C9—C10—C8	119.8 (3)
O2—Cd1—O3^{i}	94.44 (7)	C11—C10—C8	123.1 (3)
O2^{i}—Cd1—O3^{i}	55.36 (6)	C7—C6—C5	118.8 (3)
O3—Cd1—O3^{i}	137.64 (10)	C7—C6—H6	120.6
O1W—Cd1—C1	117.38 (9)	C5—C6—H6	120.6
O1W^{i}—Cd1—C1	113.62 (8)	N1—C13—C12	124.8 (3)
O2—Cd1—C1	27.82 (7)	N1—C13—Cl1	115.9 (2)
O2^{i}—Cd1—C1	93.96 (8)	C12—C13—Cl1	119.3 (3)
O3—Cd1—C1	27.57 (7)	C2—C7—C6	121.9 (2)
O3^{i}—Cd1—C1	116.93 (8)	C2—C7—H7	119.0
O1W—Cd1—C1^{i}	113.62 (8)	C6—C7—H7	119.0
O1W^{i}—Cd1—C1^{i}	117.38 (9)	C4—C3—C2	121.5 (3)
O2—Cd1—C1^{i}	93.96 (8)	C4—C3—H3	119.2
O2^{i}—Cd1—C1^{i}	27.82 (7)	C2—C3—H3	119.2
O3—Cd1—C1^{i}	116.93 (8)	C13—C12—C9	117.5 (3)
O3^{i}—Cd1—C1^{i}	27.57 (7)	C13—C12—H12	121.3
C1—Cd1—C1^{i}	106.27 (11)	C9—C12—H12	121.3
C1—O3—Cd1	88.26 (16)	O1—C8—C10	109.0 (2)
C5—O1—C8	117.0 (2)	O1—C8—H8A	109.9
C1—O2—Cd1	95.98 (16)	C10—C8—H8A	109.9
Cd1—O1W—H1A	134.7	O1—C8—H8B	109.9
Cd1—O1W—H1B	115.7	C10—C8—H8B	109.9
H1A—O1W—H1B	109.5	H8A—C8—H8B	108.3
O3—C1—O2	120.3 (3)	N1—C11—C10	123.5 (3)
O3—C1—C2	121.5 (2)	N1—C11—H11	118.2
O2—C1—C2	118.3 (2)	C10—C11—H11	118.2
O3—C1—Cd1	64.17 (14)	C10—C9—C12	120.1 (3)
O2—C1—Cd1	56.20 (14)	C10—C9—H9	120.0
C2—C1—Cd1	173.11 (19)	C12—C9—H9	120.0

Symmetry codes: (i) $-x$, y, $-z+1/2$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1B···O2^{ii}	0.84	1.88	2.708 (3)	169
O1W—H1A···O3^{iii}	0.85	1.95	2.799 (3)	175

Symmetry codes: (ii) x, $y-1$, z; (iii) x, $-y$, $z-1/2$.

Fig. 1

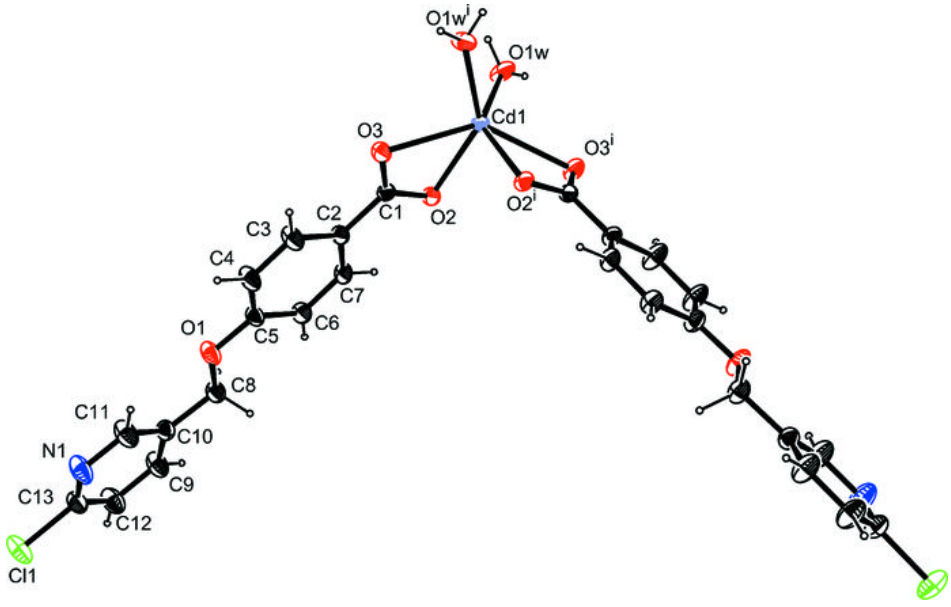
O1w^{i}
O1w
Cd1
O3
O3^{i}
O2^{i}
C1
O2
C2
C3
C4
C7
C5
C6
O1
C8
C11
C10
N1
C9
C13
C12
Cl1

Fig. 2