Mo $K\alpha$ radiation

 $\mu = 3.61 \text{ mm}^{-1}$

T = 296 (2) K $0.56 \times 0.20 \times 0.10 \text{ mm}$

Z = 2

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Poly[1-carboxymethyl-3-methylimidazolium [aquadi- μ_3 -chlorido-di- μ_2 chlorido-chloridodicadmate(II)11

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.004 Å; R factor = 0.021; wR factor = 0.056; data-to-parameter ratio = 21.1.

The title compound, $\{(C_6H_9N_2O_2)[Cd_2Cl_5(H_2O)]\}_n$, consists of 1-methyl-3-carboxymethylimidazole cations and infinite onedimensional polymeric inorganic chains of $\{[Cd_2Cl_5(H_2O)]^-\}_n$ running along the *a* axis. The imidazole-ring cations form onedimensional chains adjacent to the inorganic chains via $\pi - \pi$ stacking interactions (π - π distance = 3.736 Å).

Related literature

For related literature, see: Corradi et al. (1993); Jian et al. (2006).



Experimental

Crystal data $(C_6H_9N_2O_2)[Cd_2Cl_5(H_2O)]$ $M_r = 561.24$

Triclinic, P1 a = 7.580 (2) Å

b = 10.339(3) Å	
c = 10.371 (3) Å	
$\alpha = 74.593 \ (15)^{\circ}$	
$\beta = 81.568 \ (17)^{\circ}$	
$\gamma = 83.781 \ (16)^{\circ}$	
V = 773.0 (4) Å ³	

Data collection

Bruker SMART CCD area-detector	9462 measured reflections
diffractometer	3446 independent reflections
Absorption correction: multi-scan	3191 reflections with $I > 2\sigma(I)$
(SADABS; Sheldrick, 1996)	$R_{\rm int} = 0.022$
$T_{\min} = 0.424, \ T_{\max} = 0.697$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$	163 parameters
$wR(F^2) = 0.056$	H-atom parameters constrained
S = 1.01	$\Delta \rho_{\rm max} = 0.52 \text{ e } \text{\AA}^{-3}$
3446 reflections	$\Delta \rho_{\rm min} = -0.90 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$O1-H1\cdots O2^i$	0.83	1.84	2.673 (3)	176
$O1W - H1WA \cdots Cl5^{ii}$	0.85	2.54	3.375 (2)	165
$O1W-H1WB\cdots Cl5^{iii}$	0.84	2.40	3.171 (2)	152

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

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); 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, 2002); 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: RK2025).

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supplementary materials

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Poly[1-carboxymethyl-3-methylimidazolium chloridodicadmate(II)]]

[aquadi- μ_3 -chlorido-di- μ_2 -chlorido-

X. Shi, J. Zhang, T.-K. Ying and G.-L. Zhao

Comment

In recent years, there has been an increasing interest in the coordination chemistry of cadmium due to the increased recognition of it's role in biological organisms and molecular-based materials (Jian *et al.*, 2006). Here, we report a novel one-dimensional Cd string complex (I), which contains one $[Cd_2Cl_5(H_2O)]^-$ anion and one 1-methyl-3-carboxymethylimidazole cation in the asymmetric unit, (Fig.1).

The inorganic chain is formed by two paralleled chains of corner-sharing $[Cd_2Cl_2]$ quadrangular, which are displaced by half distance of Cd1—Cd2 and connected by tridentate bridging chlorine atoms. In the crystal structure, two independent cadmium atoms are present, which are connected by a bidentate and a tridentate bridging chlorine atom. The six-coordination is completed on the Cd(1) atom by a tridentate bridging chlorine atom and a coordinated water molecule, while on the Cd(2) atom by a tridentate bridging and a terminal chlorine atom. In each one of paralled chains, the terminal atoms (chlorine atom and water molecule) are in *cis*-position to each other, but in *trans*-position to the terminal atoms in the other paralled chain.

Each Cd atom shows a distorted octahedral geometry, gives rise to a polymeric linear chain of edge-sharing octahedra running along the *a* axis. Cd—C1 distances vary according to the different bonding mode of the C1 atoms; their values normally increasing in the order terminal < dibridged < tribridged, which are in agreement with the compound repoted by Corradi (Corradi *et al.*, 1993).

Imidazole cations form one-dimensional chains next to the inorganic chain *via* π - π stacking interactions. Furthermore, there are O–H···Cl and O–H···O intermolecule hydrogen bond involving coordinated water O1w atom and terminate Cl atom, as well as carboxyl O1 atom and carboxyl O2 atom (see table), which stabilize the three-dimensional network.

Experimental

A mixture of CdCl₂ (1 mmol), 1-methyl-3-carboxymethylimidazole ion liquid (1 mmol) and water (20 ml) was sealed in a 25 ml Teflon-lined stainless steel reactor and heated at 393 K for 48 h. A colourless solution was obtained after cooling the reaction to room temperature, colourless single crystals were obtained after two weeks.

Refinement

The structure was solved by direct methods and successive Fourier difference synthesis. The H atoms bonded to C atoms were positioned geometrically and refined using a riding model [C—H = 0.97 (2) Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The H atoms bonded to O atoms were located in a difference Fourier maps and refined with O—H distance restraints of 0.85 (2) Å and $U_{iso}(H) = 1.2U_{eq}(O)$.

Figures



Fig. 1. A view of the molecule of (I) showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability.

$Poly [1-methyl-1-carboxymethyl-3-methylimidazolium\ [aqua-di-\mu_3-chlorido-di-\mu_2-chlorido-di-\mu_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di-h_3-chlorido-di$ chloridodicadmate(II)]]

Z = 2
$F_{000} = 532$
$D_{\rm x} = 2.411 {\rm ~Mg~m^{-3}}$
Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Cell parameters from 5396 reflections
$\theta = 2.5 - 27.8^{\circ}$
$\mu = 3.61 \text{ mm}^{-1}$
T = 296 (2) K
Block, colourless
$0.56 \times 0.20 \times 0.10 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	3446 independent reflections
Radiation source: fine-focus sealed tube	3191 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.022$
T = 296(2) K	$\theta_{\text{max}} = 27.8^{\circ}$
ω scans	$\theta_{\min} = 2.5^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{\min} = 0.424, \ T_{\max} = 0.697$	$k = -13 \rightarrow 13$
9462 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.021$	H-atom parameters constrained
$wR(F^2) = 0.056$	$w = 1/[\sigma^2(F_0^2) + (0.033P)^2 + 0.3014P]$

	where $P = (F_0^2 + 2F_c^2)/3$
<i>S</i> = 1.01	$(\Delta/\sigma)_{max} = 0.002$
3446 reflections	$\Delta \rho_{max} = 0.52 \text{ e} \text{ Å}^{-3}$
163 parameters	$\Delta \rho_{min} = -0.90 \text{ e } \text{\AA}^{-3}$

Primary atom site location: structure-invariant direct 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 $F^2 > 2\sigma(F^2)$ 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 (A^2)

	x	У	Ζ	$U_{\rm iso}$ */ $U_{\rm eq}$
Cd1	-0.65421 (2)	1.144477 (16)	0.049066 (16)	0.02828 (6)
Cd2	-0.84758 (2)	0.825988 (16)	-0.030118 (16)	0.02783 (6)
C1	-0.8088 (3)	1.0934 (2)	0.5265 (2)	0.0318 (5)
C2	-0.6479 (3)	1.1611 (2)	0.5415 (2)	0.0322 (5)
H2A	-0.6095	1.1199	0.6293	0.039*
H2B	-0.5503	1.1475	0.4736	0.039*
C3	-0.7179 (4)	1.3985 (2)	0.4081 (3)	0.0441 (6)
НЗА	-0.7117	1.3816	0.3238	0.053*
C4	-0.7576 (4)	1.5190 (3)	0.4378 (3)	0.0440 (6)
H4A	-0.7835	1.6008	0.3774	0.053*
C5	-0.7114 (3)	1.3677 (2)	0.6260 (2)	0.0331 (5)
H5A	-0.7005	1.3272	0.7162	0.040*
C6	-0.7922 (5)	1.5991 (3)	0.6535 (3)	0.0551 (8)
H6A	-0.7777	1.5570	0.7460	0.083*
H6B	-0.9130	1.6369	0.6472	0.083*
H6C	-0.7115	1.6692	0.6188	0.083*
N1	-0.7525 (3)	1.49781 (19)	0.5738 (2)	0.0362 (5)
N2	-0.6886 (3)	1.30571 (17)	0.52722 (18)	0.0308 (4)
01	-0.7649 (2)	0.97628 (16)	0.50150 (18)	0.0440 (5)
H1	-0.8520	0.9380	0.4935	0.053*
O1W	-0.6345 (3)	1.37162 (17)	-0.07118 (18)	0.0430 (4)
H1WA	-0.5308	1.3949	-0.0691	0.052*
H1WB	-0.7130	1.4161	-0.0313	0.052*
O2	-0.9607 (2)	1.14584 (16)	0.53634 (17)	0.0381 (4)
Cl1	-0.43258 (8)	1.17746 (6)	0.20317 (6)	0.03400 (13)
Cl2	-0.62407 (8)	0.87957 (5)	0.13734 (5)	0.02852 (11)

supplementary materials

C13	-1.13417 (7)	0.89355 (5)	0.12270 (5)	0.02748 (11)
Cl4	-1.06544 (8)	0.81267 (6)	-0.19757 (6)	0.03600 (13)
C15	-0.80425 (10)	0.58296 (6)	0.09300 (7)	0.04500 (16)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02405 (10)	0.03030 (9)	0.03304 (10)	-0.00022 (6)	-0.00257 (7)	-0.01366 (7)
Cd2	0.02290 (10)	0.02877 (9)	0.03250 (10)	0.00080 (6)	-0.00173 (7)	-0.01092 (7)
C1	0.0441 (14)	0.0252 (10)	0.0267 (11)	0.0008 (9)	-0.0075 (10)	-0.0073 (8)
C2	0.0343 (13)	0.0279 (10)	0.0343 (12)	0.0020 (9)	-0.0016 (10)	-0.0109 (9)
C3	0.0650 (18)	0.0354 (12)	0.0289 (12)	-0.0021 (12)	-0.0034 (12)	-0.0048 (10)
C4	0.0580 (18)	0.0327 (12)	0.0378 (13)	-0.0015 (11)	-0.0099 (12)	-0.0013 (10)
C5	0.0410 (14)	0.0289 (10)	0.0299 (11)	-0.0022 (9)	-0.0038 (10)	-0.0087 (9)
C6	0.075 (2)	0.0373 (14)	0.0616 (18)	0.0083 (13)	-0.0160 (16)	-0.0276 (13)
N1	0.0445 (13)	0.0269 (9)	0.0393 (11)	0.0003 (8)	-0.0078 (9)	-0.0118 (8)
N2	0.0376 (11)	0.0258 (9)	0.0286 (9)	-0.0020 (7)	-0.0010 (8)	-0.0082 (7)
01	0.0427 (11)	0.0308 (8)	0.0657 (13)	0.0035 (7)	-0.0139 (10)	-0.0231 (8)
O1W	0.0531 (12)	0.0322 (8)	0.0447 (10)	0.0042 (8)	-0.0075 (9)	-0.0140 (7)
O2	0.0369 (10)	0.0319 (8)	0.0479 (10)	0.0032 (7)	-0.0071 (8)	-0.0153 (7)
Cl1	0.0270 (3)	0.0497 (3)	0.0301 (3)	-0.0041 (2)	-0.0004 (2)	-0.0195 (2)
Cl2	0.0282 (3)	0.0285 (2)	0.0297 (3)	-0.00082 (19)	-0.0014 (2)	-0.0105 (2)
C13	0.0262 (3)	0.0310 (2)	0.0255 (2)	-0.00225 (19)	-0.0002 (2)	-0.00919 (19)
Cl4	0.0278 (3)	0.0518 (3)	0.0336 (3)	0.0035 (2)	-0.0023 (2)	-0.0231 (3)
C15	0.0624 (4)	0.0270 (3)	0.0432 (3)	-0.0011 (3)	-0.0051 (3)	-0.0063 (2)

Geometric parameters (Å, °)

Cd1—O1W	2.3575 (18)	C3—N2	1.379 (3)
Cd1—Cl4 ⁱ	2.5066 (9)	С3—НЗА	0.9300
Cd1—Cl1	2.5873 (8)	C4—N1	1.374 (4)
Cd1—Cl2	2.6430 (9)	C4—H4A	0.9300
Cd1—Cl2 ⁱⁱ	2.6822 (9)	C5—N2	1.328 (3)
Cd1—Cl3 ⁱ	2.6922 (8)	C5—N1	1.331 (3)
Cd2—C15	2.5082 (9)	С5—Н5А	0.9300
Cd2—Cl1 ⁱⁱ	2.5753 (9)	C6—N1	1.479 (3)
Cd2—Cl4	2.6037 (9)	С6—Н6А	0.9600
Cd2—Cl3	2.6398 (9)	С6—Н6В	0.9600
Cd2—Cl2	2.7876 (8)	С6—Н6С	0.9600
Cd2—Cl3 ⁱ	2.7968 (10)	O1—H1	0.8303
C1—O2	1.221 (3)	O1W—H1WA	0.8511
C1—O1	1.303 (2)	O1W—H1WB	0.8405
C1—C2	1.517 (3)	Cl1—Cd2 ⁱⁱ	2.5753 (9)
C2—N2	1.465 (3)	Cl2—Cd1 ⁱⁱ	2.6822 (9)
C2—H2A	0.9700	Cl3—Cd1 ⁱ	2.6922 (8)
C2—H2B	0.9700	Cl3—Cd2 ⁱ	2.7968 (10)
C3—C4	1.353 (3)	Cl4—Cd1 ⁱ	2.5066 (9)

O1W—Cd1—Cl4 ⁱ	94.81 (5)	N2—C2—H2B	109.3
O1W—Cd1—Cl1	89.02 (5)	C1—C2—H2B	109.3
Cl4 ⁱ —Cd1—Cl1	96.61 (3)	H2A—C2—H2B	107.9
O1W—Cd1—Cl2	166.91 (5)	C4—C3—N2	106.7 (2)
Cl4 ⁱ —Cd1—Cl2	97.76 (3)	С4—С3—НЗА	126.7
Cl1—Cd1—Cl2	93.17 (3)	N2—C3—H3A	126.7
O1W—Cd1—Cl2 ⁱⁱ	79.77 (5)	C3—C4—N1	107.2 (2)
Cl4 ⁱ —Cd1—Cl2 ⁱⁱ	172.27 (2)	C3—C4—H4A	126.4
Cl1—Cd1—Cl2 ⁱⁱ	88.85 (3)	N1—C4—H4A	126.4
Cl2—Cd1—Cl2 ⁱⁱ	87.37 (3)	N2	108.3 (2)
O1W—Cd1—Cl3 ⁱ	90.75 (5)	N2—C5—H5A	125.8
Cl4 ⁱ —Cd1—Cl3 ⁱ	87.22 (3)	N1—C5—H5A	125.8
Cl1—Cd1—Cl3 ⁱ	176.167 (17)	N1—C6—H6A	109.5
Cl2—Cd1—Cl3 ⁱ	86.20 (2)	N1—C6—H6B	109.5
Cl2 ⁱⁱ —Cd1—Cl3 ⁱ	87.34 (3)	Н6А—С6—Н6В	109.5
Cl5—Cd2—Cl1 ⁱⁱ	95.21 (3)	N1—C6—H6C	109.5
Cl5—Cd2—Cl4	101.03 (3)	Н6А—С6—Н6С	109.5
Cl1 ⁱⁱ —Cd2—Cl4	93.72 (3)	Н6В—С6—Н6С	109.5
Cl5—Cd2—Cl3	98.51 (3)	C5—N1—C4	108.8 (2)
Cl1 ⁱⁱ —Cd2—Cl3	166.00 (2)	C5—N1—C6	124.2 (2)
Cl4—Cd2—Cl3	86.37 (3)	C4—N1—C6	127.0 (2)
C15—Cd2—Cl2	86.97 (3)	C5—N2—C3	109.01 (19)
Cl1 ⁱⁱ —Cd2—Cl2	86.83 (3)	C5—N2—C2	126.23 (19)
Cl4—Cd2—Cl2	171.891 (18)	C3—N2—C2	124.70 (19)
Cl3—Cd2—Cl2	91.15 (3)	C1—O1—H1	113.3
Cl5—Cd2—Cl3 ⁱ	168.10 (2)	Cd1—O1W—H1WA	108.9
Cl1 ⁱⁱ —Cd2—Cl3 ⁱ	87.15 (3)	Cd1—O1W—H1WB	106.3
Cl4—Cd2—Cl3 ⁱ	90.43 (3)	H1WA—O1W—H1WB	110.4
Cl3—Cd2—Cl3 ⁱ	78.85 (3)	Cd2 ⁱⁱ —Cl1—Cd1	95.48 (3)
Cl2—Cd2—Cl3 ⁱ	81.51 (2)	Cd1—Cl2—Cd1 ⁱⁱ	92.63 (3)
O2—C1—O1	125.2 (2)	Cd1—Cl2—Cd2	96.80 (2)
O2—C1—C2	122.34 (19)	Cd1 ⁱⁱ —Cl2—Cd2	88.60 (3)
01—C1—C2	112.4 (2)	Cd2—Cl3—Cd1 ⁱ	90.45 (3)
N2-C2-C1	111.75 (18)	Cd2—Cl3—Cd2 ⁱ	101.15 (3)
N2—C2—H2A	109.3	Cd1 ⁱ —Cl3—Cd2 ⁱ	95.46 (2)
C1—C2—H2A	109.3	Cd1 ⁱ —Cl4—Cd2	95.57 (3)
O2-C1-C2-N2	-17.3 (3)	Cl2 ⁱⁱ —Cd1—Cl2—Cd2	-88.90 (3)
01—C1—C2—N2	162.16 (18)	Cl3 ⁱ —Cd1—Cl2—Cd2	-1.392 (15)
N2-C3-C4-N1	-0.2 (3)	Cl5—Cd2—Cl2—Cd1	-175.66 (2)
N2	0.5 (3)	Cl1 ⁱⁱ —Cd2—Cl2—Cd1	88.94 (3)
N2C5N1C6	178.5 (2)	Cl3—Cd2—Cl2—Cd1	-77.20 (3)
C3—C4—N1—C5	-0.2 (4)	Cl3 ⁱ —Cd2—Cl2—Cd1	1.352 (14)

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C3—C4—N1—C6	-178.0 (2)	Cl5—Cd2—Cl2—Cd1 ⁱⁱ	91.85 (3)				
N1—C5—N2—C3	-0.7 (3)	Cl1 ⁱⁱ —Cd2—Cl2—Cd1 ⁱⁱ	-3.542 (16)				
N1—C5—N2—C2	-177.8 (2)	Cl3—Cd2—Cl2—Cd1 ⁱⁱ	-169.681 (17)				
C4—C3—N2—C5	0.6 (3)	Cl3 ⁱ —Cd2—Cl2—Cd1 ⁱⁱ	-91.13 (3)				
C4—C3—N2—C2	177.7 (2)	Cl5—Cd2—Cl3—Cd1 ⁱ	-96.13 (3)				
C1—C2—N2—C5	106.3 (3)	Cl1 ⁱⁱ —Cd2—Cl3—Cd1 ⁱ	95.29 (7)				
C1—C2—N2—C3	-70.3 (3)	Cl4—Cd2—Cl3—Cd1 ⁱ	4.490 (17)				
O1W—Cd1—Cl1—Cd2 ⁱⁱ	-75.96 (5)	Cl2—Cd2—Cl3—Cd1 ⁱ	176.764 (15)				
Cl4 ⁱ —Cd1—Cl1—Cd2 ⁱⁱ	-170.68 (2)	Cl3 ⁱ —Cd2—Cl3—Cd1 ⁱ	95.65 (3)				
Cl2—Cd1—Cl1—Cd2 ⁱⁱ	91.13 (3)	Cl5—Cd2—Cl3—Cd2 ⁱ	168.22 (2)				
Cl2 ⁱⁱ —Cd1—Cl1—Cd2 ⁱⁱ	3.828 (18)	Cl1 ⁱⁱ —Cd2—Cl3—Cd2 ⁱ	-0.36 (8)				
O1W—Cd1—Cl2—Cd1 ⁱⁱ	10.7 (2)	Cl4—Cd2—Cl3—Cd2 ⁱ	-91.16 (3)				
Cl4 ⁱ —Cd1—Cl2—Cd1 ⁱⁱ	174.183 (18)	Cl2—Cd2—Cl3—Cd2 ⁱ	81.11 (3)				
Cl1—Cd1—Cl2—Cd1 ⁱⁱ	-88.70 (3)	Cl3 ⁱ —Cd2—Cl3—Cd2 ⁱ	0.0				
Cl2 ⁱⁱ —Cd1—Cl2—Cd1 ⁱⁱ	0.0	Cl5—Cd2—Cl4—Cd1 ⁱ	93.13 (3)				
Cl3 ⁱ —Cd1—Cl2—Cd1 ⁱⁱ	87.51 (3)	Cl1 ⁱⁱ —Cd2—Cl4—Cd1 ⁱ	-170.82 (2)				
O1W—Cd1—Cl2—Cd2	-78.2 (2)	Cl3—Cd2—Cl4—Cd1 ⁱ	-4.846 (18)				
Cl4 ⁱ —Cd1—Cl2—Cd2	85.28 (3)	Cl3 ⁱ —Cd2—Cl4—Cd1 ⁱ	-83.64 (3)				
Cl1—Cd1—Cl2—Cd2	-177.604 (17)						
Symmetry codes: (i) $-x-2$, $-y+2$, $-z$; (ii) $-x-1$, $-y+2$, $-z$.							

Hydrogen-bond geometry (Å, °)

D—H··· A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A
O1—H1···O2 ⁱⁱⁱ	0.83	1.84	2.673 (3)	176
O1W—H1WA…Cl5 ⁱⁱ	0.85	2.54	3.375 (2)	165
O1W—H1WB····Cl5 ^{iv}	0.84	2.40	3.171 (2)	152

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



Fig. 1