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μ -Pyrazine-bis[tetraaquacadmium(II)] μ -pyrazine-bis[tetraacetatocadmium(II)]

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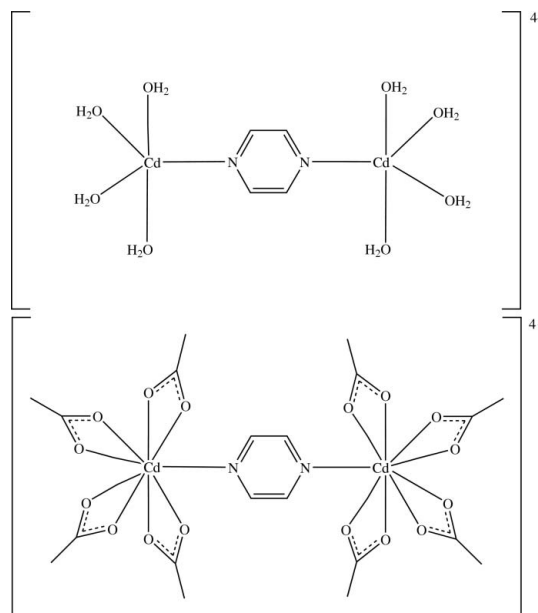
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; disorder in main residue; R factor = 0.016; wR factor = 0.034; data-to-parameter ratio = 17.1.

In the title dinuclear ionic complex, $[\text{Cd}_2(\text{C}_4\text{H}_4\text{N}_2)(\text{H}_2\text{O})_8]^-$ [$\text{Cd}_2(\text{CH}_3\text{CO}_2)_8(\text{C}_4\text{H}_4\text{N}_2)$], the cation and anion are disordered equally over a site with symmetry mmm . The Cd^{II} ions and the N atoms of the bridging pyrazine ligand lie on the intersection of two crystallographic mirror planes. The C atoms of the bridging pyrazine ligand lie on one of these mirror planes, and the acetate groups and water molecules lie across the intersecting mirror planes. Each Cd^{II} atom in the cation is five-coordinated by four O atoms from four water molecules and one N atom from the bridging pyrazine ligand, whereas each Cd^{II} in the anion is nine-coordinated by four pairs of O atoms from the bidentate acetate ligands and one N atom from the bridging pyrazine ligand. In the crystal structure, each anion is surrounded by eight nearest-neighbour cations and *vice versa*. The crystal structure is stabilized by ionic interactions as well as by $\text{C}-\text{H}\cdots\text{O}$ interactions.

Related literature

For bond-length data, see: Allen *et al.* (1987). For Cd^{II} coordination chemistry, applications and related structures, see: Filipović *et al.* (2008); Inoue *et al.* (2000); Pons *et al.* (2007); Xia *et al.* (2004).



Experimental

Crystal data

$[\text{Cd}_2(\text{C}_4\text{H}_4\text{N}_2)(\text{H}_2\text{O})_8]^-$
 $[\text{Cd}_2(\text{C}_2\text{H}_3\text{O}_2)_8(\text{C}_4\text{H}_4\text{N}_2)]$
 $M_r = 1226.26$
 Tetragonal, $I4/mcm$
 $a = 16.7103$ (4) Å
 $c = 7.3533$ (2) Å

$V = 2053.29$ (9) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.13$ mm⁻¹
 $T = 100.0$ (1) K
 $0.58 \times 0.08 \times 0.05$ mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
 $T_{\text{min}} = 0.371$, $T_{\text{max}} = 0.895$

12617 measured reflections
 1246 independent reflections
 1145 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.016$
 $wR(F^2) = 0.034$
 $S = 1.06$
 1246 reflections
 73 parameters
 2 restraints

H atoms treated by a mixture of
 independent and constrained
 refinement
 $\Delta\rho_{\text{max}} = 0.59$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.44$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}1-\text{H}1\text{A}\cdots\text{O}2$	0.96	2.47	3.0405 (18)	118
$\text{C}1-\text{H}1\text{A}\cdots\text{O}1\text{W}^{\text{i}}$	0.96	2.56	3.2700 (17)	131
$\text{C}1-\text{H}1\text{A}\cdots\text{O}2^{\text{ii}}$	0.96	2.47	3.0405 (18)	118
$\text{C}1-\text{H}1\text{A}\cdots\text{O}1\text{W}^{\text{iii}}$	0.96	2.56	3.2700 (17)	131

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

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: SAINT (Bruker, 2005); program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2576).

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supplementary materials

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μ -Pyrazine-bis[tetraaquacadmium(II)] μ -pyrazine-bis[tetraacetatocadmium(II)]

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Comment

The investigations of coordination compounds between cadmium(II) and O and N donors atoms have attracted much attention due to their potential application in a number of areas (Inoue *et al.*, 2000; Pons *et al.*, 2007; Xia *et al.*, 2004), including cytotoxic activities (Filipović *et al.*, 2008). We report herein, the synthesis and crystal structure of the title compound which exhibits a mixed coordination for Cd^{II} atom i.e nine- and five-coordination mode for Cd^{II}, which is a rare case.

In the title compound, both [Cd₂(H₂O)₈(C₄H₄N₂)]⁴⁺ cations and [Cd₂(CH₃CO₂)₈(C₄H₄N₂)]⁴⁻ anions lie on the site symmetry *mmm*. The Cd^{II} and the N atoms of the bridging pyrazine ligand lie on the intersection of two crystallographic mirror planes, one perpendicular to the *c* axis (*z* = 0) and the other parallel to the *c* axis and passing through the mid points of the *a* and *b* axis. The C atoms of the bridging pyrazine ligand lie on the *z* = 0 mirror plane, and the acetate groups and water molecules lie across the intersecting mirror planes. There are two molecules of the title complex in the unit cell.

In the structure, the cation contains two Cd^{II} ions, eight water molecules and one bridging pyrazine ligand whereas the anion contains two Cd^{II} ions, eight acetate and one bridging pyrazine ligands. Each of the Cd^{II} in the cation is five-coordinated with four O atoms from four water molecules and one N atom from a bridging pyrazine ligand, whereas each Cd^{II} in the anion is nine-coordinated with four pairs of chelate O atoms from the bidentate acetate ligands and one N atom from the bridging pyrazine ligand. The Cd—O(acetate) bond distances are 2.3458 (14) and 2.5200 (14) Å, and the Cd—O(water) and Cd—N distances are 2.2783 (15) Å and 2.3470 (15) Å, respectively. The O(water)—Cd—O(water) bond angles lie in the range 64.15 (8)°-174.10 (7)°, whereas, the O(acetate)—Cd—O(acetate) bond angles are in the range 53.57 (7)°-158.87 (6)°. The N—Cd—O(water) angle is 92.95 (3)° and N—Cd—O(acetate) angles are 132.77 (3)° and 79.43 (3)°, respectively. The geometric parameters are comparable to those reported for other Cd—O and Cd—N donor complexes (Inoue *et al.*, 2000; Pons *et al.*, 2007; Xia *et al.*, 2004).

In the crystal packing (Fig. 2 and Fig.3), each anion is surrounded by eight nearest neighbour cations and *vice-versa*. The crystal structure is stabilized by ionic interactions as well as by weak C—H...O interactions (Table 1).

Experimental

The title compound was synthesized by mixing Cd(CH₃COO)₂ and pyrazine with a 2:1 molar ratio in a hot methanol-water (2:1 *v/v*) solution and stirred for 10 min at room temperature. The solution was then left at ambient temperature to allow the solvent to slowly evaporate. Colourless crystals of the title compound suitable for X-ray structure determination were obtained after a few weeks.

Refinement

Water H atoms were located in a difference map and refined isotropically, with a O—H distance restraint of 0.800 (1) Å. C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.96 Å. The U_{iso} value of H1A was constrained to $1.2U_{\text{eq}}(\text{C1})$ and for other H atoms the U_{iso} values were refined. A rotating group model was used for the methyl group.

Figures

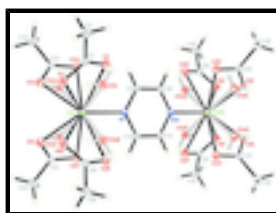


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering. The cations and anions occupy the same site with equal occupancy. Symmetry codes for the Cd1A ion: (A) $-x, 1 - y, -z$. Symmetry codes for aqua and acetate atoms: (A) $x, y, -z$; (B) $1/2 - y, 1/2 - x, z$; (C) $1/2 - y, 1/2 - x, -z$; (D) $y - 1/2, 1/2 + x, -z$; (E) $y - 1/2, 1/2 + x, z$; (F) $-x, 1 - y, -z$; (G) $-x, 1 - y, z$. Symmetry codes for ring C atoms: (A) $1/2 - y, 1/2 - x, z$; (B) $y - 1/2, 1/2 + x, -z$; (C) $-x, 1 - y, -z$. Symmetry code for the N1 atom: (A) $-x, 1 - y, -z$.

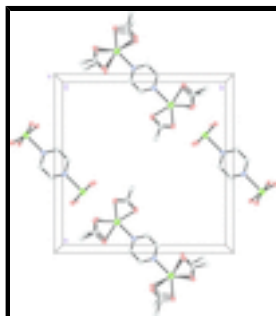


Fig. 2. The crystal packing of the title compound, viewed along the c axis, showing a layer of the cations and anions.

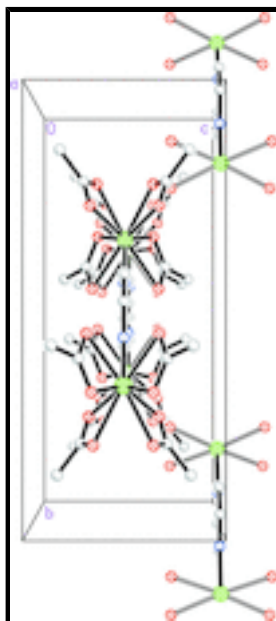


Fig. 3. The crystal packing of the title compound, viewed along the a axis, showing the same layer of cations and anions in Fig. 2.

μ -Pyrazine-bis[tetraaquacadmium(II)] μ -pyrazine-bis[tetraacetatocadmium(II)]

Crystal data

$[\text{Cd}_2(\text{C}_4\text{H}_4\text{N}_2)(\text{H}_2\text{O})_8][\text{Cd}_2(\text{C}_2\text{H}_3\text{O}_2)_8(\text{C}_4\text{H}_4\text{N}_2)]$	$D_x = 1.983 \text{ Mg m}^{-3}$
$M_r = 1226.26$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Tetragonal, $I4/mcm$	Cell parameters from 1246 reflections
Hall symbol: $-I 4 2c$	$\theta = 1.7\text{--}35.0^\circ$
$a = 16.7103 (4) \text{ \AA}$	$\mu = 2.13 \text{ mm}^{-1}$
$c = 7.3533 (2) \text{ \AA}$	$T = 100 \text{ K}$
$V = 2053.29 (9) \text{ \AA}^3$	Needle, colourless
$Z = 2$	$0.58 \times 0.08 \times 0.05 \text{ mm}$
$F(000) = 1208$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	1246 independent reflections
Radiation source: fine-focus sealed tube graphite	1145 reflections with $I > 2\sigma(I)$
Detector resolution: $8.33 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.037$
ω scans	$\theta_{\text{max}} = 35.0^\circ$, $\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -26 \rightarrow 26$
$T_{\text{min}} = 0.371$, $T_{\text{max}} = 0.895$	$k = -26 \rightarrow 26$
12617 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.016$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0089P)^2 + 1.5621P]$
1246 reflections	where $P = (F_o^2 + 2F_c^2)/3$
73 parameters	$(\Delta/\sigma)_{\text{max}} = 0.002$
2 restraints	$\Delta\rho_{\text{max}} = 0.59 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.44 \text{ e \AA}^{-3}$

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

supplementary materials

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cd1	0.158218 (5)	0.341782 (5)	0.0000	0.01214 (4)	
O1	0.16811 (7)	0.21686 (8)	0.1438 (2)	0.0156 (2)	0.50
O2	0.04830 (8)	0.27097 (9)	0.1708 (2)	0.0183 (3)	0.50
C2	0.09773 (11)	0.21621 (11)	0.2069 (3)	0.0144 (3)	0.50
C3	0.07138 (12)	0.14714 (12)	0.3238 (3)	0.0212 (4)	0.50
H3A	0.0344	0.1659	0.4142	0.036 (9)*	0.50
H3B	0.1172	0.1240	0.3825	0.038 (8)*	0.50
H3C	0.0458	0.1075	0.2493	0.031 (8)*	0.50
O1W	0.11198 (8)	0.28563 (8)	0.2621 (2)	0.0170 (3)	0.50
H1W1	0.0654 (4)	0.2746 (17)	0.262 (4)	0.020 (7)*	0.50
H2W1	0.1447 (16)	0.2523 (16)	0.287 (5)	0.055 (11)*	0.50
N1	0.05890 (6)	0.44110 (6)	0.0000	0.0131 (3)	
C1	-0.01905 (7)	0.42237 (7)	0.0000	0.0144 (2)	
H1A	-0.0354	0.3673	0.0000	0.017*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.00955 (4)	0.00955 (4)	0.01731 (7)	0.00080 (4)	0.000	0.000
O1	0.0119 (5)	0.0133 (5)	0.0216 (7)	0.0003 (4)	0.0008 (5)	0.0015 (5)
O2	0.0137 (6)	0.0151 (6)	0.0260 (8)	0.0028 (5)	0.0007 (6)	0.0037 (5)
C2	0.0131 (7)	0.0118 (7)	0.0181 (8)	-0.0016 (5)	-0.0025 (6)	0.0004 (6)
C3	0.0189 (9)	0.0195 (9)	0.0251 (10)	-0.0014 (7)	0.0006 (7)	0.0074 (8)
O1W	0.0121 (5)	0.0156 (6)	0.0233 (7)	0.0022 (5)	0.0023 (5)	0.0030 (5)
N1	0.0119 (4)	0.0119 (4)	0.0155 (7)	0.0010 (5)	0.000	0.000
C1	0.0122 (5)	0.0113 (5)	0.0196 (6)	0.0004 (4)	0.000	0.000

Geometric parameters (\AA , $^\circ$)

Cd1—O1W	2.2782 (15)	O1—C2	1.264 (2)
Cd1—O1W ⁱ	2.2783 (15)	O2—C2	1.261 (2)
Cd1—O1W ⁱⁱ	2.2783 (15)	C2—C3	1.505 (3)
Cd1—O1W ⁱⁱⁱ	2.2783 (15)	C3—H3A	0.96
Cd1—O1	2.3458 (14)	C3—H3B	0.96
Cd1—O1 ⁱ	2.3458 (14)	C3—H3C	0.96

Cd1—O1 ⁱⁱ	2.3458 (14)	O1W—H1W1	0.800 (1)
Cd1—O1 ⁱⁱⁱ	2.3458 (14)	O1W—H2W1	0.800 (1)
Cd1—N1	2.3470 (15)	N1—C1 ⁱ	1.3396 (15)
Cd1—O2 ⁱ	2.5200 (14)	N1—C1	1.3397 (15)
Cd1—O2 ⁱⁱ	2.5200 (14)	C1—C1 ^{iv}	1.384 (2)
Cd1—O2	2.5200 (14)	C1—H1A	0.96
O1W—Cd1—O1W ⁱ	64.15 (8)	O1 ⁱ —Cd1—O2 ⁱⁱ	81.84 (5)
O1W—Cd1—O1W ⁱⁱ	174.10 (7)	O1 ⁱⁱ —Cd1—O2 ⁱⁱ	53.77 (4)
O1W ⁱ —Cd1—O1W ⁱⁱ	115.52 (8)	O1 ⁱⁱⁱ —Cd1—O2 ⁱⁱ	113.02 (5)
O1W—Cd1—O1W ⁱⁱⁱ	115.51 (8)	N1—Cd1—O2 ⁱⁱ	79.43 (3)
O1W ⁱ —Cd1—O1W ⁱⁱⁱ	174.10 (7)	O2 ⁱ —Cd1—O2 ⁱⁱ	59.77 (8)
O1W ⁱⁱ —Cd1—O1W ⁱⁱⁱ	64.15 (8)	O1—Cd1—O2	53.77 (4)
O1—Cd1—O1 ⁱ	70.82 (6)	O1 ⁱ —Cd1—O2	113.02 (5)
O1—Cd1—O1 ⁱⁱ	94.46 (6)	O1 ⁱⁱ —Cd1—O2	147.15 (4)
O1 ⁱ —Cd1—O1 ⁱⁱ	53.57 (7)	O1 ⁱⁱⁱ —Cd1—O2	81.84 (5)
O1—Cd1—O1 ⁱⁱⁱ	53.57 (7)	N1—Cd1—O2	79.43 (3)
O1 ⁱ —Cd1—O1 ⁱⁱⁱ	94.46 (6)	O2 ⁱ —Cd1—O2	115.86 (8)
O1 ⁱⁱ —Cd1—O1 ⁱⁱⁱ	70.82 (6)	O2 ⁱⁱ —Cd1—O2	158.87 (6)
O1W—Cd1—N1	92.95 (3)	C2—O1—Cd1	96.17 (11)
O1W ⁱ —Cd1—N1	92.95 (3)	C2—O2—Cd1	88.18 (11)
O1W ⁱⁱ —Cd1—N1	92.95 (3)	O2—C2—O1	121.73 (17)
O1W ⁱⁱⁱ —Cd1—N1	92.95 (3)	O2—C2—C3	119.02 (16)
O1—Cd1—N1	132.77 (3)	O1—C2—C3	119.23 (16)
O1 ⁱ —Cd1—N1	132.77 (3)	Cd1—O1W—H1W1	115 (2)
O1 ⁱⁱ —Cd1—N1	132.77 (3)	Cd1—O1W—H2W1	104 (3)
O1 ⁱⁱⁱ —Cd1—N1	132.77 (3)	H1W1—O1W—H2W1	120 (3)
O1—Cd1—O2 ⁱ	113.02 (5)	C1 ⁱ —N1—C1	117.01 (15)
O1 ⁱ —Cd1—O2 ⁱ	53.77 (4)	C1 ⁱ —N1—Cd1	121.49 (8)
O1 ⁱⁱ —Cd1—O2 ⁱ	81.84 (5)	C1—N1—Cd1	121.49 (8)
O1 ⁱⁱⁱ —Cd1—O2 ⁱ	147.15 (4)	N1—C1—C1 ^{iv}	121.50 (8)
N1—Cd1—O2 ⁱ	79.43 (3)	N1—C1—H1A	120.0
O1—Cd1—O2 ⁱⁱ	147.15 (4)	C1 ^{iv} —C1—H1A	118.5
O1 ⁱ —Cd1—O1—C2	137.93 (10)	O1W ⁱⁱⁱ —Cd1—N1—C1 ⁱ	-122.12 (4)
O1 ⁱⁱ —Cd1—O1—C2	-173.19 (14)	O1—Cd1—N1—C1 ⁱ	142.13 (5)
O1 ⁱⁱⁱ —Cd1—O1—C2	-111.03 (11)	O1 ⁱ —Cd1—N1—C1 ⁱ	37.87 (5)
N1—Cd1—O1—C2	6.81 (14)	O1 ⁱⁱ —Cd1—N1—C1 ⁱ	-37.87 (5)
O2 ⁱ —Cd1—O1—C2	103.79 (12)	O1 ⁱⁱⁱ —Cd1—N1—C1 ⁱ	-142.13 (5)
O2 ⁱⁱ —Cd1—O1—C2	173.28 (11)	O2 ⁱ —Cd1—N1—C1 ⁱ	30.46 (4)
O2—Cd1—O1—C2	-2.25 (11)	O2 ⁱⁱ —Cd1—N1—C1 ⁱ	-30.46 (4)
O1—Cd1—O2—C2	2.24 (11)	O2—Cd1—N1—C1 ⁱ	149.54 (4)
O1 ⁱ —Cd1—O2—C2	-38.85 (13)	O1W—Cd1—N1—C1	-57.88 (4)

supplementary materials

O1 ⁱⁱ —Cd1—O2—C2	19.05 (17)	O1W ⁱ —Cd1—N1—C1	-122.12 (4)
O1 ⁱⁱⁱ —Cd1—O2—C2	52.55 (12)	O1W ⁱⁱ —Cd1—N1—C1	122.12 (4)
N1—Cd1—O2—C2	-171.01 (12)	O1W ⁱⁱⁱ —Cd1—N1—C1	57.88 (4)
O2 ⁱ —Cd1—O2—C2	-98.33 (12)	O1—Cd1—N1—C1	-37.87 (5)
O2 ⁱⁱ —Cd1—O2—C2	-171.01 (12)	O1 ⁱ —Cd1—N1—C1	-142.13 (5)
Cd1—O2—C2—O1	-3.94 (19)	O1 ⁱⁱ —Cd1—N1—C1	142.13 (5)
Cd1—O2—C2—C3	177.83 (17)	O1 ⁱⁱⁱ —Cd1—N1—C1	37.87 (5)
Cd1—O1—C2—O2	4.3 (2)	O2 ⁱ —Cd1—N1—C1	-149.54 (4)
Cd1—O1—C2—C3	-177.52 (16)	O2 ⁱⁱ —Cd1—N1—C1	149.54 (4)
O1W—Cd1—N1—C1 ⁱ	122.12 (4)	O2—Cd1—N1—C1	-30.46 (4)
O1W ⁱ —Cd1—N1—C1 ⁱ	57.88 (4)	C1 ⁱ —N1—C1—C1 ^{iv}	0.0
O1W ⁱⁱ —Cd1—N1—C1 ⁱ	-57.88 (4)	Cd1—N1—C1—C1 ^{iv}	180.0

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C1—H1A \cdots O2	0.96	2.47	3.0405 (18)	118
C1—H1A \cdots O1W ^v	0.96	2.56	3.2700 (17)	131
C1—H1A \cdots O2 ^{vi}	0.96	2.47	3.0405 (18)	118
C1—H1A \cdots O1W ^{vii}	0.96	2.56	3.2700 (17)	131

Symmetry codes: (v) $-x, y, -z+1/2$; (vi) $x, y, -z$; (vii) $-x, y, z-1/2$.

Fig. 1

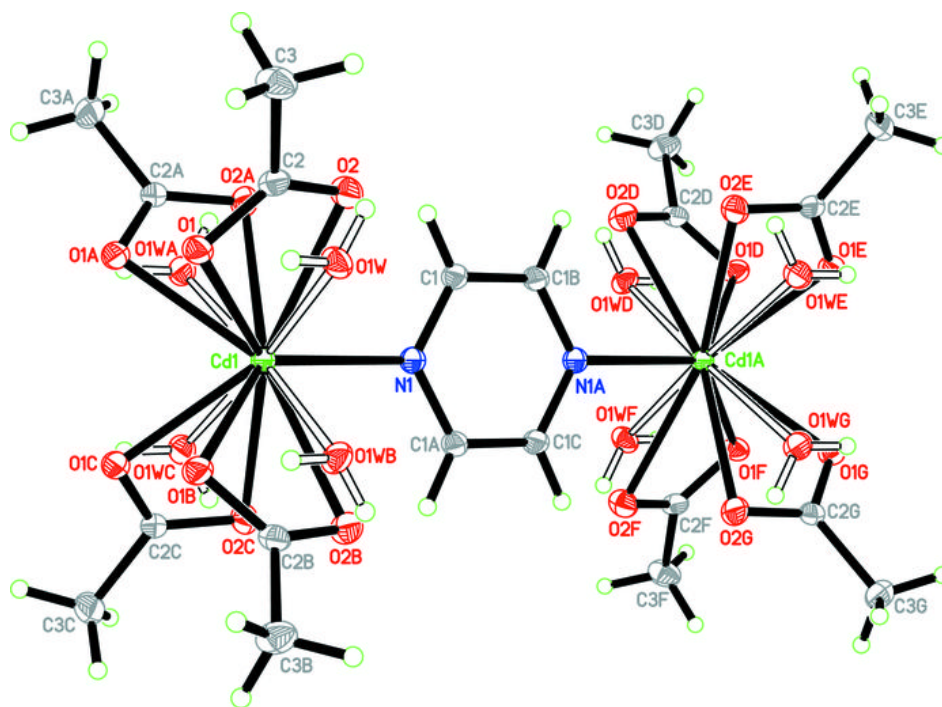


Fig. 2

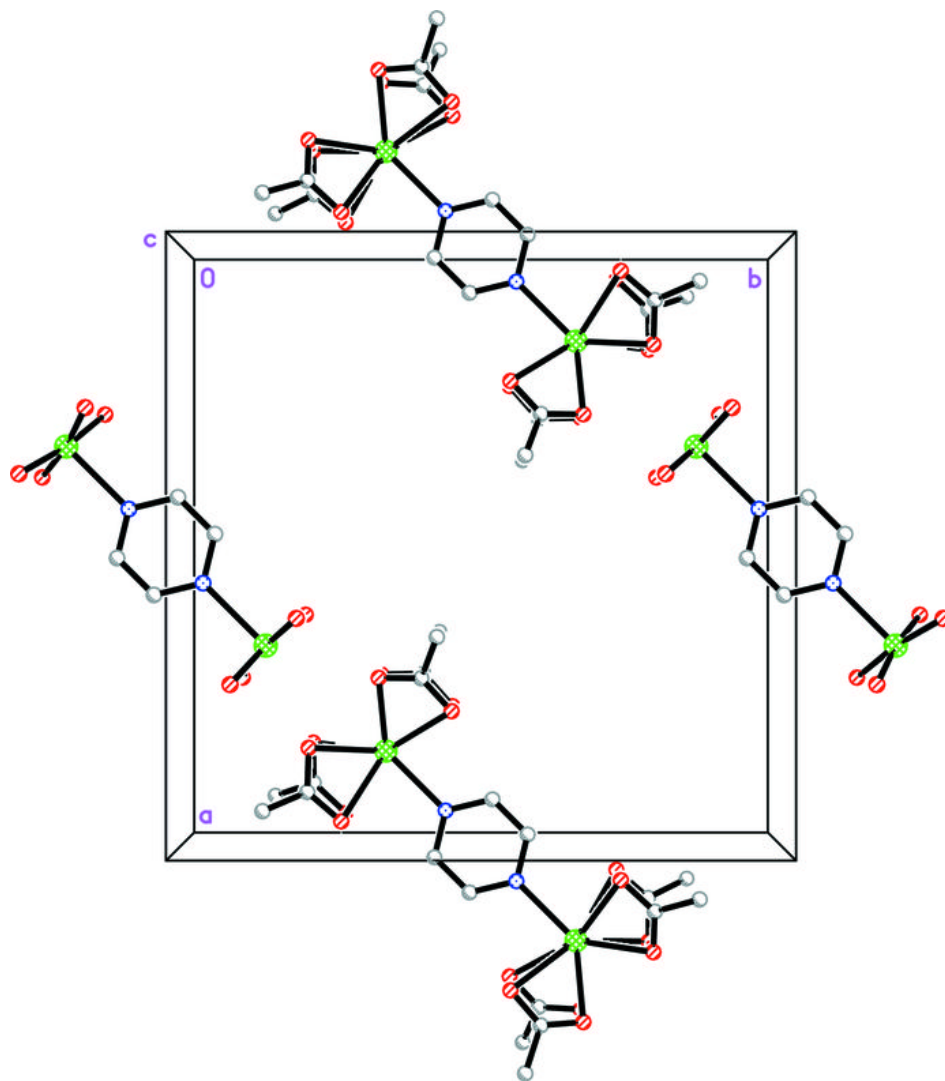


Fig. 3

