

Poly[di- μ_2 -chlorido- μ_4 -hexamethylene-tetramine-bis[chlorido(methanol- κ O)-cadmium(II)]]

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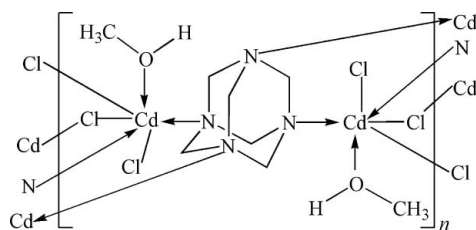
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Key indicators: single-crystal X-ray study; $T = 130$ K; mean $\sigma(\text{N}-\text{C}) = 0.008$ Å; R factor = 0.052; wR factor = 0.097; data-to-parameter ratio = 18.0.

In the title complex, $[\text{Cd}_2\text{Cl}_4(\text{C}_6\text{H}_{12}\text{N}_4)(\text{CH}_3\text{OH})_2]_n$, the hexamethylenetetramine (hmta) ligand is located on a twofold rotation axis and bridges four Cd^{II} ions through its four N atoms. Each Cd^{II} atom is coordinated, with a distorted octahedral geometry, by two N atoms from hmta ligands, two μ_2 -chloride anions, one terminal chloride anion and one methanol molecule. The μ_2 -chloride anions and hmta molecules link the Cd^{II} cations to form the three-dimensional polymeric structure. $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonding between the methanol ligands and the terminal chloride anions is observed in the three-dimensional polymeric structure.

Related literature

For general background, see: Cheng *et al.* (2005); Tong *et al.* (2000); Wang *et al.* (2006). For a related structure, see: Batten *et al.* (1998). For related literature, see: Fang *et al.* (2004).



Experimental

Crystal data

$[\text{Cd}_2\text{Cl}_4(\text{C}_6\text{H}_{12}\text{N}_4)(\text{CH}_3\text{O})_2]$ $Z = 8$
 $M_r = 568.86$ Mo $K\alpha$ radiation
 Tetragonal, $I4_1/a$ $\mu = 3.36 \text{ mm}^{-1}$
 $a = 12.7307(7) \text{ \AA}$ $T = 130 \text{ K}$
 $c = 19.5433(18) \text{ \AA}$ $0.11 \times 0.10 \times 0.10 \text{ mm}$
 $V = 3167.4(4) \text{ \AA}^3$

Data collection

Rigaku Mercury70 diffractometer 5447 measured reflections
 Absorption correction: multi-scan 1816 independent reflections
 (*CrystalClear*; Rigaku, 2000) 1552 reflections with $I > 2\sigma(I)$
 $T_{\text{min}} = 0.712$, $T_{\text{max}} = 0.722$ $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$ H atoms treated by a mixture of
 $wR(F^2) = 0.097$ independent and constrained
 $S = 1.10$ refinement
 1816 reflections $\Delta\rho_{\text{max}} = 1.25 \text{ e \AA}^{-3}$
 101 parameters $\Delta\rho_{\text{min}} = -0.68 \text{ e \AA}^{-3}$
 1 restraint

Table 1

Selected geometric parameters (Å, °).

Cd1—Cl1	2.6041 (16)	Cd1—O1	2.308 (5)
Cd1—Cl1 ⁱ	2.6526 (16)	Cd1—N1	2.531 (5)
Cd1—Cl2	2.4825 (17)	Cd1—N2 ⁱⁱ	2.498 (5)
O1—Cd1—Cl2	89.46 (13)	N2 ⁱⁱ —Cd1—Cl1	87.50 (12)
O1—Cd1—N2 ⁱⁱ	90.87 (18)	N1—Cd1—Cl1	90.87 (12)
Cl2—Cd1—N2 ⁱⁱ	91.50 (13)	O1—Cd1—Cl1 ⁱ	179.70 (14)
O1—Cd1—N1	85.60 (17)	Cl2—Cd1—Cl1 ⁱ	90.84 (5)
Cl2—Cd1—N1	89.58 (12)	N2 ⁱⁱ —Cd1—Cl1 ⁱ	89.13 (12)
N2 ⁱⁱ —Cd1—N1	176.29 (17)	N1—Cd1—Cl1 ⁱ	94.41 (12)
O1—Cd1—Cl1	81.44 (13)	Cl1—Cd1—Cl1 ⁱ	98.26 (6)
Cl2—Cd1—Cl1	170.82 (6)	Cd1—Cl1—Cd1 ⁱⁱⁱ	154.11 (7)

Symmetry codes: (i) $-y + \frac{1}{4}, x + \frac{1}{4}, -z + \frac{1}{4}$; (ii) $y - \frac{1}{4}, -x + \frac{3}{4}, z - \frac{1}{4}$; (iii) $y - \frac{1}{4}, -x + \frac{1}{4}, -z + \frac{1}{4}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1—H6 ^{iv} ···Cl2 ^{iv}	0.897 (10)	2.124 (13)	3.020 (5)	176 (8)

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2326).

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supplementary materials

Acta Cryst. (2007). E63, m2751 [doi:10.1107/S1600536807046715]

Poly[di- μ_2 -chlorido- μ_4 -hexamethylenetetramine-bis[chlorido(methanol- κ O)cadmium(II)]]

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Comment

Hexamethylenetetramine (hmta) as a potential polydentate ligand has been of interest in recent years. The combination of the hmta ligand with metal ions has produced several complexes with diverse structural topologies (Cheng *et al.*, 2005; Tong *et al.*, 2000; Wang *et al.*, 2006). The compounds of hmta are easier to exhibit high-dimensional structure because of the abundant coordination atoms. The methanol solution of hmta diffuse into the aqua solution of CdCl₂ producing the title compound. We present its structure here.

The asymmetric unit consists of one Cd ion, two Cl anions, one methanol molecule, and a half of hmta molecule. The hmta ligand is located on a twofold rotation axis, which passes through atom C2 and C3, and bridges four cadmium ions through its four N atoms. As depicted in Fig. 1, the Cd atom is coordinated by two μ_2 Cl atoms, one terminal Cl atom, one oxygen atom from methanol ligand and two N atoms from hmta ligands with a distorted octahedral geometry; the CdCl₃N₂O octahedron is seriously distorted (Table 1). The bond lengths involving the Cd atom are normal and are comparable to the values found in a related Cd^{II} complex (Batten *et al.*, 1998). Two types of Cl anions occur in the structure; one is the bridging and the other is the terminal. Four μ_2 Cl atoms bridge four Cd atoms to form a 8-membered ring, as shown in Fig. 2. Each hmta ligand bridges four Cd atoms through its four N atoms (Fig. 1). The 8-membered rings are further bridge by the hmta ligands through Cd—N bonds to generate a three-dimensional framework, as shown in Fig. 3. The O—H...Cl hydrogen bond between the methanol molecule and the terminal Cl anion is observed within the three-dimensional structure (Table 2).

Experimental

Orange block-shaped crystals of the title compound were obtained from a diffusion reaction in a U-tube with H₂O as diffusion mediate. A methanol solution (6 ml) of hmta (0.014 g, 0.10 mmol) was carefully added to one side of the diffusion tube, and a aqua solution (7 ml) of CdCl₂·2.5H₂O (0.0456 g, 0.20 mmol) was added to the other side. The tube was located at room temperature for about two weeks, and well shaped crystals were obtained.

Refinement

The H atoms bonded to C atoms were placed in calculated positions and treated using a riding-model approximation (C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl group; C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methylene group). H atoms bonded to O atoms were located in a difference map and were refined with a restraint of O—H = 0.90 (1) Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The highest peak in the final difference Fourier map is 1.78 Å apart from H4B atom.

Figures

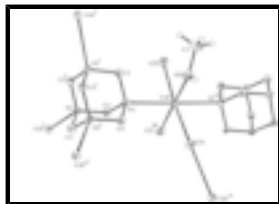


Fig. 1. The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 60% probability level and H atoms are shown as small spheres of arbitrary radii. H atoms of hmta ligands are omitted for clarity. [Symmetry codes: (i) $-x + 1, -y + 1/2, z$; (ii) $-x + 3/4, y - 1/4, z - 1/4$; (iii) $x + 1/4, -y + 1/4, -z + 1/4$; (iv) $-x + 1/4, y - 1/4, -z + 1/4$; (v) $x + 1/4, -y + 3/4, z + 1/4$; (vi) $-x + 1/4, y + 1/4, z + 1/4$]

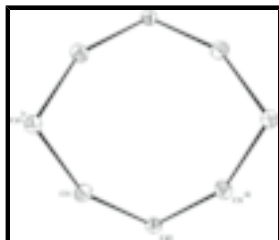


Fig. 2. A view of the Cd_4Cl_4 8-membered ring. [Symmetry codes: (iii) $x + 1/4, -y + 1/4, -z + 1/4$; (iv) $-x + 1/4, y - 1/4, -z + 1/4$.]

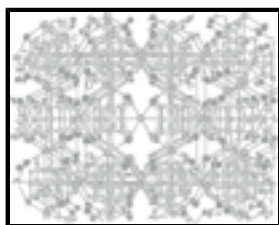


Fig. 3. A view of the three-dimensional framework of (I) (viewed down the c axis)

Poly[di- μ_2 -chlorido- μ_4 -hexamethylenetetramine- λ bis[chlorido(methanol- κ O)cadmium(II)]]

Crystal data

$[\text{Cd}_2\text{Cl}_4(\text{C}_6\text{H}_{12}\text{N}_4)(\text{CH}_4\text{O})_2]$

$M_r = 568.86$

Tetragonal, $I4_1/a$

Hall symbol: $-I\ 4ad$

$a = 12.7307(7)\ \text{\AA}$

$b = 12.7307(7)\ \text{\AA}$

$c = 19.5433(18)\ \text{\AA}$

$\alpha = 90^\circ$

$\beta = 90^\circ$

$\gamma = 90^\circ$

$V = 3167.4(4)\ \text{\AA}^3$

$Z = 8$

$F_{000} = 2192$

$D_x = 2.386\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3283 reflections

$\theta = 3.1\text{--}27.5^\circ$

$\mu = 3.36\ \text{mm}^{-1}$

$T = 130\ \text{K}$

Block, orange

$0.11 \times 0.10 \times 0.10\ \text{mm}$

Data collection

Rigaku Mercury70 (2x2 bin mode) diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 130\ \text{K}$

1816 independent reflections

1552 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\text{max}} = 27.5^\circ$

ω scans	$\theta_{\min} = 3.1^\circ$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2000)	$h = -15 \rightarrow 15$
$T_{\min} = 0.712$, $T_{\max} = 0.722$	$k = -6 \rightarrow 16$
5447 measured reflections	$l = -22 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.097$	$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 61.3128P]$
$S = 1.10$	where $P = (F_o^2 + 2F_c^2)/3$
1816 reflections	$(\Delta/\sigma)_{\max} < 0.001$
101 parameters	$\Delta\rho_{\max} = 1.26 \text{ e } \text{\AA}^{-3}$
1 restraint	$\Delta\rho_{\min} = -0.67 \text{ e } \text{\AA}^{-3}$
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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cd1	0.24683 (4)	0.25555 (4)	0.05984 (2)	0.01140 (14)	
O1	0.3287 (4)	0.1206 (4)	0.0017 (3)	0.0194 (10)	
H6	0.329 (7)	0.0504 (11)	0.006 (4)	0.029*	
Cl1	0.15990 (12)	0.09779 (12)	0.12298 (8)	0.0147 (3)	
Cl2	0.34179 (13)	0.38436 (13)	-0.01275 (9)	0.0183 (3)	
N1	0.4031 (4)	0.2487 (4)	0.1398 (3)	0.0104 (11)	
N2	0.4993 (4)	0.3459 (4)	0.2283 (3)	0.0098 (10)	
C1	0.3784 (6)	0.1214 (6)	-0.0629 (4)	0.0255 (17)	
H1A	0.4051	0.0525	-0.0729	0.038*	
H1B	0.4353	0.1708	-0.0624	0.038*	
H1C	0.3285	0.1413	-0.0974	0.038*	

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C2	0.5000	0.2500	0.0967 (5)	0.0111 (17)	
H2	0.5008	0.1884	0.0678	0.013*	0.50
C3	0.5000	0.2500	0.2704 (5)	0.0109 (17)	
H3	0.4384	0.2495	0.2993	0.013*	0.50
C4	0.4035 (5)	0.3443 (5)	0.1837 (3)	0.0114 (12)	
H4A	0.3410	0.3451	0.2121	0.014*	
H4B	0.4025	0.4066	0.1551	0.014*	
C5	0.4069 (5)	0.1547 (5)	0.1839 (3)	0.0126 (12)	
H5A	0.4073	0.0924	0.1554	0.015*	
H5B	0.3444	0.1525	0.2121	0.015*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0110 (2)	0.0118 (2)	0.0114 (2)	-0.00013 (17)	0.00009 (17)	0.00014 (17)
O1	0.025 (3)	0.014 (2)	0.019 (3)	-0.001 (2)	0.004 (2)	-0.001 (2)
Cl1	0.0126 (7)	0.0143 (7)	0.0173 (8)	-0.0015 (6)	0.0020 (6)	0.0028 (6)
Cl2	0.0172 (8)	0.0166 (8)	0.0210 (8)	-0.0009 (6)	-0.0007 (7)	0.0061 (6)
N1	0.011 (3)	0.008 (2)	0.012 (3)	0.0010 (19)	0.003 (2)	-0.001 (2)
N2	0.010 (3)	0.008 (2)	0.011 (3)	-0.0018 (19)	-0.001 (2)	-0.003 (2)
C1	0.031 (4)	0.029 (4)	0.017 (4)	0.004 (3)	0.007 (3)	-0.003 (3)
C2	0.009 (4)	0.012 (4)	0.012 (4)	-0.004 (3)	0.000	0.000
C3	0.016 (4)	0.004 (4)	0.013 (4)	0.001 (3)	0.000	0.000
C4	0.011 (3)	0.010 (3)	0.014 (3)	0.000 (2)	0.000 (2)	-0.002 (2)
C5	0.012 (3)	0.013 (3)	0.013 (3)	-0.003 (2)	0.000 (3)	0.000 (3)

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

Cd1—Cl1	2.6041 (16)	N2—Cd1 ^{iv}	2.498 (5)
Cd1—Cl1 ⁱ	2.6526 (16)	C1—H1A	0.9600
Cd1—Cl2	2.4825 (17)	C1—H1B	0.9600
Cd1—O1	2.308 (5)	C1—H1C	0.9600
Cd1—N1	2.531 (5)	C2—N1 ⁱⁱⁱ	1.493 (7)
Cd1—N2 ⁱⁱ	2.498 (5)	C2—H2	0.9700
O1—C1	1.413 (8)	C3—N2 ⁱⁱⁱ	1.473 (7)
O1—H6	0.897 (10)	C3—H3	0.9700
N1—C5	1.475 (8)	C4—H4A	0.9700
N1—C4	1.490 (8)	C4—H4B	0.9700
N1—C2	1.493 (7)	C5—N2 ⁱⁱⁱ	1.476 (8)
N2—C3	1.473 (7)	C5—H5A	0.9700
N2—C5 ⁱⁱⁱ	1.476 (8)	C5—H5B	0.9700
N2—C4	1.498 (8)		
O1—Cd1—Cl2	89.46 (13)	C3—N2—Cd1 ^{iv}	106.3 (4)
O1—Cd1—N2 ⁱⁱ	90.87 (18)	C5 ⁱⁱⁱ —N2—Cd1 ^{iv}	113.5 (3)
Cl2—Cd1—N2 ⁱⁱ	91.50 (13)	C4—N2—Cd1 ^{iv}	111.2 (4)
O1—Cd1—N1	85.60 (17)	O1—C1—H1A	109.5
Cl2—Cd1—N1	89.58 (12)	O1—C1—H1B	109.5

N2 ⁱⁱ —Cd1—N1	176.29 (17)	H1A—C1—H1B	109.5
O1—Cd1—Cl1	81.44 (13)	O1—C1—H1C	109.5
Cl2—Cd1—Cl1	170.82 (6)	H1A—C1—H1C	109.5
N2 ⁱⁱ —Cd1—Cl1	87.50 (12)	H1B—C1—H1C	109.5
N1—Cd1—Cl1	90.87 (12)	N1 ⁱⁱⁱ —C2—N1	111.4 (7)
O1—Cd1—Cl1 ⁱ	179.70 (14)	N1 ⁱⁱⁱ —C2—H2	109.2
Cl2—Cd1—Cl1 ⁱ	90.84 (5)	N1—C2—H2	109.2
N2 ⁱⁱ —Cd1—Cl1 ⁱ	89.13 (12)	N2—C3—N2 ⁱⁱⁱ	112.0 (7)
N1—Cd1—Cl1 ⁱ	94.41 (12)	N2—C3—H3	109.1
Cl1—Cd1—Cl1 ⁱ	98.26 (6)	N2 ⁱⁱⁱ —C3—H3	109.1
C1—O1—Cd1	129.6 (4)	N1—C4—N2	110.4 (5)
C1—O1—H6	95 (6)	N1—C4—H4A	109.6
Cd1—O1—H6	134 (6)	N2—C4—H4A	109.6
Cd1—Cl1—Cd1 ^v	154.11 (7)	N1—C4—H4B	109.6
C5—N1—C4	109.0 (5)	N2—C4—H4B	109.6
C5—N1—C2	108.1 (4)	H4A—C4—H4B	108.1
C4—N1—C2	108.2 (4)	N1—C5—N2 ⁱⁱⁱ	112.0 (5)
C5—N1—Cd1	114.5 (4)	N1—C5—H5A	109.2
C4—N1—Cd1	109.3 (3)	N2 ⁱⁱⁱ —C5—H5A	109.2
C2—N1—Cd1	107.5 (4)	N1—C5—H5B	109.2
C3—N2—C5 ⁱⁱⁱ	108.6 (4)	N2 ⁱⁱⁱ —C5—H5B	109.2
C3—N2—C4	108.6 (4)	H5A—C5—H5B	107.9
C5 ⁱⁱⁱ —N2—C4	108.4 (5)		
Cl2—Cd1—O1—C1	-19.3 (6)	Cl1—Cd1—N1—C2	130.7 (2)
N2 ⁱⁱ —Cd1—O1—C1	72.2 (6)	Cl1 ⁱ —Cd1—N1—C2	-130.9 (2)
N1—Cd1—O1—C1	-108.9 (6)	C5—N1—C2—N1 ⁱⁱⁱ	-58.6 (4)
Cl1—Cd1—O1—C1	159.5 (6)	C4—N1—C2—N1 ⁱⁱⁱ	59.3 (4)
O1—Cd1—Cl1—Cd1 ^v	-150.0 (2)	Cd1—N1—C2—N1 ⁱⁱⁱ	177.3 (3)
N2 ⁱⁱ —Cd1—Cl1—Cd1 ^v	-58.79 (19)	C5 ⁱⁱⁱ —N2—C3—N2 ⁱⁱⁱ	-58.6 (4)
N1—Cd1—Cl1—Cd1 ^v	124.54 (19)	C4—N2—C3—N2 ⁱⁱⁱ	59.2 (4)
Cl1 ⁱ —Cd1—Cl1—Cd1 ^v	29.97 (13)	Cd1 ^{iv} —N2—C3—N2 ⁱⁱⁱ	178.9 (3)
O1—Cd1—N1—C5	-70.7 (4)	C5—N1—C4—N2	58.0 (6)
Cl2—Cd1—N1—C5	-160.2 (4)	C2—N1—C4—N2	-59.3 (6)
Cl1—Cd1—N1—C5	10.6 (4)	Cd1—N1—C4—N2	-176.2 (4)
Cl1 ⁱ —Cd1—N1—C5	109.0 (4)	C3—N2—C4—N1	-58.4 (6)
O1—Cd1—N1—C4	166.7 (4)	C5 ⁱⁱⁱ —N2—C4—N1	59.5 (6)
Cl2—Cd1—N1—C4	77.2 (4)	Cd1 ^{iv} —N2—C4—N1	-175.0 (4)
Cl1—Cd1—N1—C4	-112.0 (4)	C4—N1—C5—N2 ⁱⁱⁱ	-58.4 (6)
Cl1 ⁱ —Cd1—N1—C4	-13.6 (4)	C2—N1—C5—N2 ⁱⁱⁱ	59.1 (6)
O1—Cd1—N1—C2	49.4 (3)	Cd1—N1—C5—N2 ⁱⁱⁱ	178.9 (4)
Cl2—Cd1—N1—C2	-40.1 (2)		

Symmetry codes: (i) $-y+1/4, x+1/4, -z+1/4$; (ii) $y-1/4, -x+3/4, z-1/4$; (iii) $-x+1, -y+1/2, z$; (iv) $-y+3/4, x+1/4, z+1/4$; (v) $y-1/4, -x+1/4, -z+1/4$.

supplementary materials

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H6\cdots Cl2^{vi}$	0.897 (10)	2.124 (13)	3.020 (5)	176 (8)

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

Fig. 2

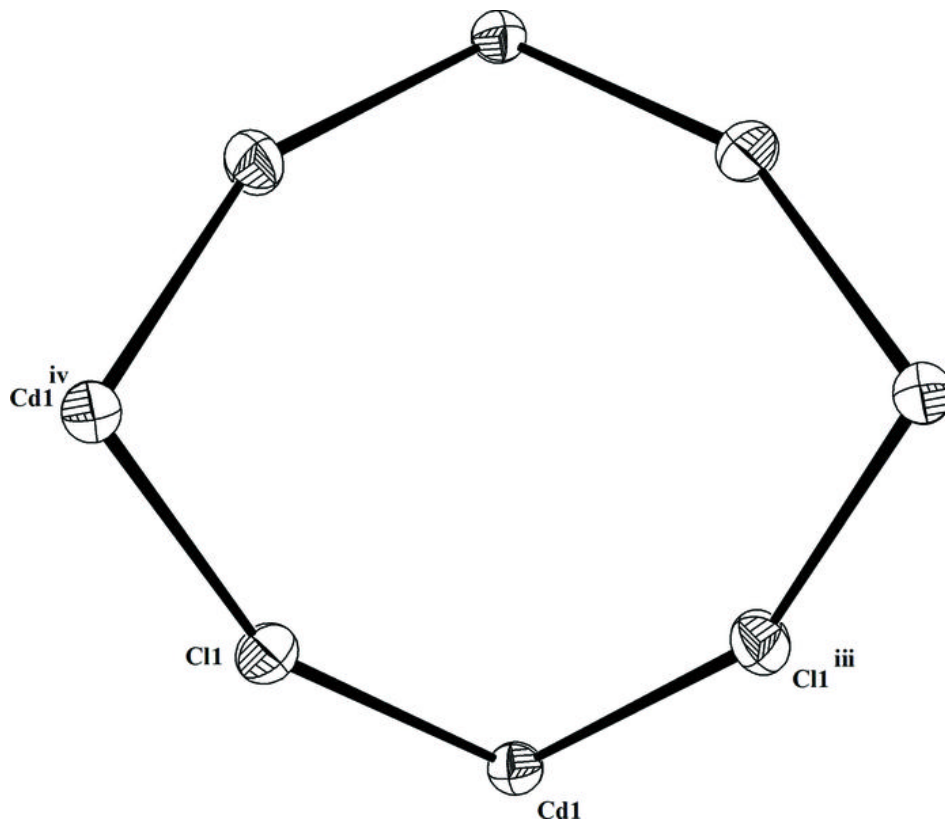


Fig. 3

