

A one-dimensional ABX_3 -type coordination polymer: *catena*-poly[benzyltrimethylammonium [tri- μ -chlorido-cadmium(II)]]

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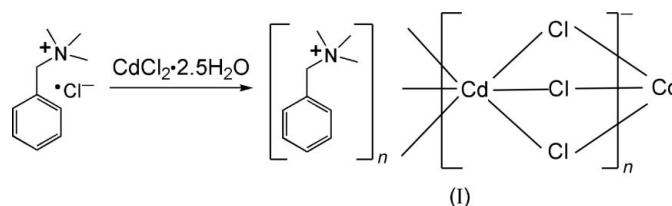
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The crystal structure of the title novel one-dimensional ABX_3 -type organic–inorganic hybrid complex $\{(\text{C}_{10}\text{H}_{16}\text{N})[\text{CdCl}_3]\}_n$, (I), consists of benzyltrimethylammonium (Me_3BzN^+) cations and one-dimensional anionic $\{[\text{Cd}(\mu\text{-Cl})_3]^- \}_\infty$ chains. Each Cd^{II} centre is hexacoordinated by bridging chloride ligands, giving a slightly distorted octahedral $\text{Cd}(\mu\text{-Cl})_6$ arrangement. The octahedra are linked by two opposite shared faces, giving rise to an almost perfectly linear anionic $\{[\text{Cd}(\mu\text{-Cl})_3]^- \}_\infty$ chain in the a -axis direction. Me_3BzN^+ cations located in the inter-chain spaces balance the charge. Noncovalent static attracting forces (Coulombic and van der Waals forces) and nonclassical $\text{C}\cdots\text{H}\cdots\text{Cl}$ hydrogen-bond interactions stabilize the crystal structure.

Comment

The understanding of ABX_3 -type perovskites remains one of the most challenging topics at the boundary between solid-state physics and solid-state chemistry. Perovskite materials exhibit many interesting and intriguing properties, from both the theoretical and application points of view. These compounds are used as sensors and catalyst electrodes in certain types of fuel cells and are candidates for memory devices and spintronics applications (Coey *et al.*, 1999). It should be noted that a columnar arrangement is found frequently in ABX_3 -type compounds, which have been extensively studied because numerous crystal structures containing the methylammonium cation exhibit phase transitions related to the dynamics of the organic cations and inorganic anions (Doudin & Chapuis, 1992; Morosin, 1972; Puget *et al.*, 1991; Wařkowska *et al.*, 1990). Layered A_2MX_4 perovskites have attracted sustained interest because of their magnetic, electronic and other physical properties and the possibility of tuning both geometries and properties by variation of the organic cations (Gillon *et al.*, 1999). Although perovskites have been known for a long time, new and intri-

guing physical effects are periodically discovered and their understanding remains an internationally highly competitive area. With these considerations in mind, we have used the benzyltrimethylammonium (Me_3BzN^+) cation to replace the $\text{N}(\text{CH}_3)_4^+$ cation and have synthesized the title new one-dimensional ABX_3 -type organic–inorganic coordination polymer, (I).



The asymmetric unit of (I) consists of a trichlorido-cadmium(II) anion and a Me_3BzN^+ cation, as shown in Fig. 1. The other three chloride ligands (Cl1^i , Cl2^i and Cl3^i) are produced by the corresponding chloride ligands through the $(x + \frac{1}{2}, -y + \frac{1}{2}, z)$ a -glide plane operation (Fig. 2). The Cd^{II} centres are hexacoordinated by chloride ligands, giving a slightly distorted octahedral $\text{Cd}(\mu\text{-Cl})_6$ arrangement. The $\text{Cd}\text{--Cl}$ bond lengths are in the range 2.6271 (12)–2.6685 (13) Å and the $\text{Cl}\text{--Cd}\text{--Cl}$ angles are in the ranges 82.72 (4)–100.45 (4) and 174.25 (5)–175.25 (7)°, deviating slightly from ideal octahedral angle values (90 and 180°). The octahedra are linked by two opposite shared faces, giving rise to infinite $\{[\text{Cd}(\mu\text{-Cl})_3]^- \}_\infty$ chains parallel to the a axis, with a $\text{Cd1}\cdots\text{Cd1}^i$ distance of 3.3769 (7) Å and a $\text{Cd1}^i\cdots\text{Cd1}\cdots\text{Cd1}^{\text{ii}}$ angle of 179.436 (13)° [symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, z$], indicating that the polymer chain is perfectly linear (Fig. 2). Thus, all chloride ligands act as bridges between two consecutive Cd atoms, and each pair of consecutive Cd atoms is linked by three corner-shared bridging chloride ligands. It should be noted that this columnar arrangement is found frequently in ABX_3 compounds (Corradi *et al.*, 1997; Costin-Hogan *et al.*, 2008; Jian *et al.*, 2006; López-Garzón *et al.*,

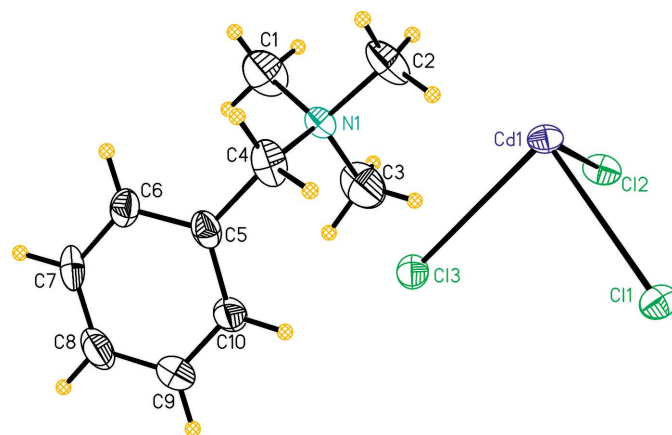


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

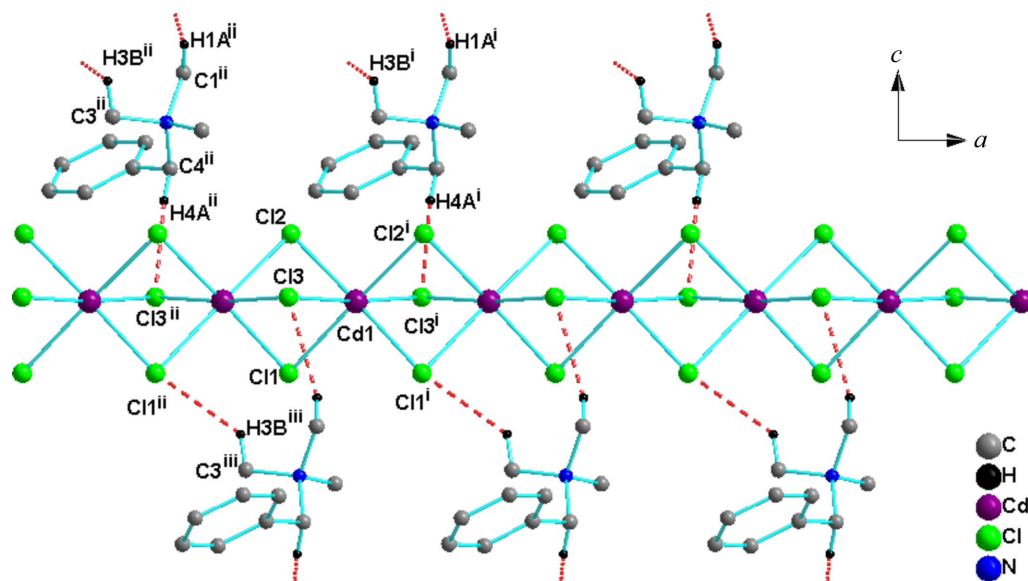


Figure 2

The one-dimensional triple-stranded $[\text{Cd}(\mu\text{-Cl})_3]_\infty$ chain, viewed along the a axis, showing the hydrogen-bond interactions with the cations as dashed lines. [Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, z$; (iii) $x, y, z - 1$.]

1995; Ma *et al.*, 2006; Maldonado *et al.*, 2008). For example, the $[\text{Cd}_3\text{Cl}_9]^{3-}$ anion reported by Jian *et al.* (2006) was also a one-dimensional inorganic chain, in which each Cd^{II} cation is octahedrally surrounded by six bridging Cl atoms, giving rise to polymeric chains. In the $[\text{NH}(\text{CH}_3)_3]\text{CdCl}_3$ (TrMCD) compound reported by Chapuis & Zuniga (1980), the Cd atoms are located at the centres of face-sharing CdCl_6 octahedra, forming infinite one-dimensional chains perpendicular to a hexagonal or nearly hexagonal net. The interchain distances are determined by the size of the organic cation which occupies the space between the octahedra, with a hydrogen bond between the alkylammonium cation and a chloride ligand.

There are thus three features in the structure of (I). Firstly, all the Cd^{II} cations are collinear. Secondly, the $\text{Cd1} \cdots \text{Cd1}$ distance is much shorter than those reported in other one-dimensional cadmium polymers bridged by Cl atoms (average *ca.* 4.14 Å) (Huang *et al.*, 1998; Hu *et al.*, 2003; Laskar *et al.*, 2002). Although the $\text{Cd} \cdots \text{Cd}$ distance in complex (I) is larger than the interatomic distance in bulk Cd (2.98 Å; Stuhlmann *et al.*, 1998), it is still shorter than 115% of the total sum of two Cd metal radii (3.427 Å; Bender *et al.*, 1985). There seems to be no good theoretically supported argument for the existence of a Cd–Cd metal bond in (I) (Bender *et al.*, 1985). Finally, the Me_3BzN^+ cations on each side of the inorganic chain are arranged in a zigzag configuration. The charges of the cations are balanced by the anionic $[\text{Cd}(\mu\text{-Cl})_3]_\infty$ polymer chain. The Me_3BzN^+ cations are located in the inter-chain space, with noncovalent static attracting forces (Coulombic and van der Waals forces) and nonclassical C–H \cdots Cl hydrogen-bond interactions with the anionic chains to stabilize the crystal structure (Table 1 and Fig. 2). The bond lengths and angles of the Me_3BzN^+ cations are in agreement with those reported in the literature (Müller *et al.*, 1994; Hauge & Maroy, 1996).

Our interest in one-dimensional ABX_3 -type organic–inorganic hybrid complexes is based mainly on their potential uses in molecular dielectrics and ferroelectrics. The variable-temperature dielectric response, especially in the relatively high-frequency range, is very useful in the search for phase transitions (Wu *et al.*, 2011; Wu & Jin, 2012). However, we were unable to detect any dielectric anomalies within the temperature range 93–460 K when we measured the variation of the dielectric properties of (I) with temperature, implying that there are no structural phase transitions within that temperature range and that (I) may not have ferroelectric properties (Ye *et al.*, 2009; Fu *et al.*, 2007). Further ABX_3 -type ferroelectrics still need to be sought and studied.

Experimental

Benzyltrimethylammonium chloride (97%, Alfa Aesar) and $\text{CdCl}_2 \cdot 2.5\text{H}_2\text{O}$ (Sinopharm) were used as commercial products without further purification. ^1H NMR and ^{13}C NMR spectra were measured on a Bruker Biospin AG Magnet System 300 MHz NMR instrument in D_2O solution with trimethylsulfoxane as internal standard. IR spectra ($4000\text{--}400\text{ cm}^{-1}$) were recorded on a Shimadzu IR Prestige-21 spectrophotometer with KBr pellets. The melting point was determined using an uncorrected X-4 melting-point apparatus (Beijing Kaifu Company).

Compound (I) was prepared by dissolving equimolar amounts of benzyltrimethylammonium chloride and $\text{CdCl}_2 \cdot 2.5\text{H}_2\text{O}$ in a mixture of water and methanol (1:1 *v/v*) to afford a colourless solution. This solution was left to evaporate at room temperature in air for two weeks to afford colourless plate-like crystals of (I) suitable for single-crystal X-ray diffraction (yield 90%; m.p. 471–472 K with decomposition). ^1H NMR (D_2O): δ 2.91 (s, 9H, CH_3), 4.30 (s, 2H, CH_2), 7.20–7.37 (5H in phenyl ring); ^{13}C NMR (D_2O): δ 52.43 (CH_3), 69.57 (CH_2), 127.38, 129.21, 130.85, 132.85 (C in phenyl ring); IR (KBr pellet, ν , cm^{-1}): 3022, 2986, 2955, 1498, 1471, 1450, 973.

Crystal data

(C ₁₀ H ₁₆ N)[CdCl ₃]	$V = 1382.7 (5) \text{ \AA}^3$
$M_r = 368.99$	$Z = 4$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 6.7538 (14) \text{ \AA}$	$\mu = 2.13 \text{ mm}^{-1}$
$b = 22.852 (5) \text{ \AA}$	$T = 291 \text{ K}$
$c = 8.9590 (18) \text{ \AA}$	$0.24 \times 0.22 \times 0.20 \text{ mm}$

Data collection

Rigaku Mercury2 diffractometer	13516 measured reflections
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku, 2005)	3167 independent reflections
$T_{\min} = 0.590$, $T_{\max} = 0.650$	2743 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$	H-atom parameters constrained
$wR(F^2) = 0.056$	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
$S = 1.06$	$\Delta\rho_{\text{min}} = -0.41 \text{ e \AA}^{-3}$
3167 reflections	Absolute structure: Flack (1983),
140 parameters	with 1482 Bijvoet pairs
1 restraint	Flack parameter: $-0.07 (4)$

H atoms were placed in calculated positions, with C—H = 0.93 (aromatic), 0.96 (methyl) or 0.97 Å (methylene), and treated as riding, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl groups and $1.2U_{\text{eq}}(\text{C})$ otherwise. The refinement of the Flack (1983) parameter to $-0.07 (4)$ clearly indicates that the model corresponds with the true absolute structure.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK3472). Services for accessing these data are described at the back of the journal.

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Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C1—H1A \cdots Cl3 ⁱⁱⁱ	0.96	2.74	3.600 (6)	149
C3—H3B \cdots Cl1 ^{iv}	0.96	2.83	3.586 (7)	137
C4—H4A \cdots Cl3	0.97	2.68	3.645 (5)	171

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

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supplementary materials

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A one-dimensional ABX_3 -type coordination polymer: *catena*-poly[benzyltrimethylammonium [tri- μ -chlorido-cadmium(II)]]

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catena-Poly[benzyltrimethylammonium [tri- μ -chlorido-cadmium(II)]]

Crystal data

(C₁₀H₁₆N)[CdCl₃]

$M_r = 368.99$

Orthorhombic, *Pna*2₁

Hall symbol: P 2c -2n

$a = 6.7538$ (14) Å

$b = 22.852$ (5) Å

$c = 8.9590$ (18) Å

$V = 1382.7$ (5) Å³

$Z = 4$

$F(000) = 728$

$D_x = 1.773$ Mg m⁻³

Melting point = 471–472 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 12682 reflections

$\theta = 3.0$ – 27.5°

$\mu = 2.13$ mm⁻¹

$T = 291$ K

Plate, colourless

$0.24 \times 0.22 \times 0.20$ mm

Data collection

Rigaku Mercury2

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 13.6612 pixels mm⁻¹

CCD profile fitting scans

Absorption correction: multi-scan

(*CrystalClear*; Rigaku, 2005)

$T_{\min} = 0.590$, $T_{\max} = 0.650$

13516 measured reflections

3167 independent reflections

2743 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.2^\circ$

$h = -8 \rightarrow 8$

$k = -29 \rightarrow 29$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.056$

$S = 1.06$

3167 reflections

140 parameters

1 restraint

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from

neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0132P)^2 + 0.2094P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.26$ e Å⁻³

$\Delta\rho_{\min} = -0.41$ e Å⁻³

Extinction correction: *SHELXL97* (Sheldrick,

2008), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0246 (5)

Absolute structure: Flack (1983), with 1482

Bijvoet Pairs

Flack parameter: -0.07 (4)

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.4914 (11)	0.1034 (3)	0.8740 (5)	0.092 (2)
H1A	0.4935	0.1313	0.9540	0.137*
H1B	0.6216	0.0874	0.8606	0.137*
H1C	0.4005	0.0725	0.8979	0.137*
C2	0.5601 (6)	0.18467 (17)	0.7107 (7)	0.0743 (13)
H2A	0.5121	0.2076	0.6285	0.111*
H2B	0.6919	0.1713	0.6893	0.111*
H2C	0.5615	0.2081	0.7995	0.111*
C3	0.2256 (5)	0.1557 (2)	0.7500 (12)	0.116 (3)
H3A	0.2067	0.1879	0.6828	0.174*
H3B	0.2062	0.1688	0.8508	0.174*
H3C	0.1320	0.1254	0.7274	0.174*
C4	0.4414 (8)	0.0915 (2)	0.6028 (5)	0.0588 (13)
H4A	0.4182	0.1135	0.5119	0.071*
H4B	0.5756	0.0764	0.5983	0.071*
C5	0.3023 (7)	0.04091 (17)	0.6056 (4)	0.0487 (10)
C6	0.3486 (5)	−0.01128 (18)	0.6770 (4)	0.0517 (11)
H6	0.4710	−0.0155	0.7233	0.062*
C7	0.2155 (6)	−0.05671 (16)	0.6798 (5)	0.0625 (13)
H7	0.2488	−0.0916	0.7272	0.075*
C8	0.0355 (7)	−0.0510 (2)	0.6138 (6)	0.0732 (14)
H8	−0.0556	−0.0815	0.6183	0.088*
C9	−0.0116 (10)	−0.0001 (3)	0.5405 (7)	0.100 (2)
H9	−0.1341	0.0036	0.4941	0.120*
C10	0.1216 (7)	0.0453 (2)	0.5354 (5)	0.0750 (16)
H10	0.0893	0.0794	0.4841	0.090*
Cd1	0.63883 (2)	0.249637 (8)	0.22732 (13)	0.03124 (8)
Cl1	0.38657 (14)	0.28920 (5)	0.02411 (8)	0.0366 (3)
Cl2	0.39437 (15)	0.29886 (5)	0.41788 (9)	0.0390 (3)
Cl3	0.38566 (8)	0.16118 (3)	0.23929 (13)	0.0364 (2)
N1	0.4268 (3)	0.13288 (10)	0.7335 (5)	0.0368 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.146 (6)	0.087 (4)	0.042 (3)	−0.036 (4)	−0.024 (3)	0.016 (3)
C2	0.096 (3)	0.067 (3)	0.060 (3)	−0.043 (2)	0.012 (3)	−0.008 (3)

C3	0.051 (2)	0.077 (3)	0.220 (8)	0.013 (2)	0.018 (5)	−0.058 (6)
C4	0.097 (4)	0.048 (3)	0.031 (2)	−0.007 (3)	0.015 (2)	−0.001 (2)
C5	0.073 (3)	0.035 (2)	0.037 (2)	−0.003 (2)	−0.002 (2)	−0.0065 (17)
C6	0.061 (2)	0.040 (2)	0.054 (3)	0.0121 (19)	0.0014 (17)	−0.0043 (18)
C7	0.080 (3)	0.027 (2)	0.080 (4)	0.008 (2)	0.011 (2)	0.0008 (19)
C8	0.077 (3)	0.043 (3)	0.099 (4)	−0.013 (2)	0.002 (3)	−0.015 (3)
C9	0.094 (4)	0.059 (3)	0.148 (6)	−0.012 (3)	−0.059 (5)	−0.009 (5)
C10	0.107 (4)	0.045 (3)	0.074 (3)	−0.010 (3)	−0.050 (3)	0.007 (2)
Cd1	0.01888 (11)	0.04055 (14)	0.03429 (13)	−0.00048 (8)	0.0028 (3)	−0.00021 (14)
Cl1	0.0284 (5)	0.0486 (7)	0.0328 (5)	0.0003 (4)	0.0029 (5)	0.0073 (5)
Cl2	0.0300 (6)	0.0498 (7)	0.0372 (6)	−0.0024 (4)	0.0063 (5)	−0.0122 (5)
Cl3	0.0291 (3)	0.0340 (4)	0.0461 (5)	0.0009 (3)	0.0050 (6)	0.0031 (6)
N1	0.0426 (12)	0.0387 (14)	0.0291 (13)	−0.0064 (11)	0.007 (2)	−0.006 (2)

Geometric parameters (Å, °)

C1—N1	1.493 (6)	C6—H6	0.9300
C1—H1A	0.9600	C7—C8	1.358 (6)
C1—H1B	0.9600	C7—H7	0.9300
C1—H1C	0.9600	C8—C9	1.373 (7)
C2—N1	1.501 (4)	C8—H8	0.9300
C2—H2A	0.9600	C9—C10	1.374 (7)
C2—H2B	0.9600	C9—H9	0.9300
C2—H2C	0.9600	C10—H10	0.9300
C3—N1	1.463 (4)	Cd1—Cl1 ⁱ	2.6271 (12)
C3—H3A	0.9600	Cd1—Cl2	2.6279 (13)
C3—H3B	0.9600	Cd1—Cl3 ⁱ	2.6351 (8)
C3—H3C	0.9600	Cd1—Cl3	2.6497 (8)
C4—C5	1.489 (6)	Cd1—Cl1	2.6523 (13)
C4—N1	1.509 (5)	Cd1—Cl2 ⁱ	2.6685 (13)
C4—H4A	0.9700	Cd1—Cd1 ⁱ	3.3769 (7)
C4—H4B	0.9700	Cl1—Cd1 ⁱⁱ	2.6271 (12)
C5—C10	1.377 (6)	Cl2—Cd1 ⁱⁱ	2.6686 (13)
C5—C6	1.389 (5)	Cl3—Cd1 ⁱⁱ	2.6351 (8)
C6—C7	1.373 (5)		
N1—C1—H1A	109.5	C9—C10—H10	119.7
N1—C1—H1B	109.5	C5—C10—H10	119.7
H1A—C1—H1B	109.5	Cl1 ⁱ —Cd1—Cl2	174.25 (5)
N1—C1—H1C	109.5	Cl1 ⁱ —Cd1—Cl3 ⁱ	83.49 (4)
H1A—C1—H1C	109.5	Cl2—Cd1—Cl3 ⁱ	92.29 (4)
H1B—C1—H1C	109.5	Cl1 ⁱ —Cd1—Cl3	100.45 (4)
N1—C2—H2A	109.5	Cl2—Cd1—Cl3	83.96 (4)
N1—C2—H2B	109.5	Cl3 ⁱ —Cd1—Cl3	175.25 (7)
H2A—C2—H2B	109.5	Cl1 ⁱ —Cd1—Cl1	92.79 (5)
N1—C2—H2C	109.5	Cl2—Cd1—Cl1	84.05 (3)
H2A—C2—H2C	109.5	Cl3 ⁱ —Cd1—Cl1	99.83 (4)
H2B—C2—H2C	109.5	Cl3—Cd1—Cl1	82.72 (4)
N1—C3—H3A	109.5	Cl1 ⁱ —Cd1—Cl2 ⁱ	83.75 (3)
N1—C3—H3B	109.5	Cl2—Cd1—Cl2 ⁱ	99.70 (6)

H3A—C3—H3B	109.5	Cl3 ⁱ —Cd1—Cl2 ⁱ	83.45 (4)
N1—C3—H3C	109.5	Cl3—Cd1—Cl2 ⁱ	94.28 (4)
H3A—C3—H3C	109.5	Cl1—Cd1—Cl2 ⁱ	174.96 (5)
H3B—C3—H3C	109.5	Cl1 ⁱ —Cd1—Cd1 ⁱ	50.56 (3)
C5—C4—N1	115.6 (3)	Cl2—Cd1—Cd1 ⁱ	128.77 (3)
C5—C4—H4A	108.4	Cl3 ⁱ —Cd1—Cd1 ⁱ	50.474 (17)
N1—C4—H4A	108.4	Cl3—Cd1—Cd1 ⁱ	130.470 (19)
C5—C4—H4B	108.4	Cl1—Cd1—Cd1 ⁱ	129.84 (3)
N1—C4—H4B	108.4	Cl2 ⁱ —Cd1—Cd1 ⁱ	49.86 (3)
H4A—C4—H4B	107.4	Cl1 ⁱ —Cd1—Cd1 ⁱⁱ	129.68 (3)
C10—C5—C6	118.2 (4)	Cl2—Cd1—Cd1 ⁱⁱ	50.92 (3)
C10—C5—C4	119.6 (4)	Cl3 ⁱ —Cd1—Cd1 ⁱⁱ	128.963 (19)
C6—C5—C4	122.2 (4)	Cl3—Cd1—Cd1 ⁱⁱ	50.092 (17)
C7—C6—C5	120.7 (4)	Cl1—Cd1—Cd1 ⁱⁱ	49.91 (3)
C7—C6—H6	119.6	Cl2 ⁱ —Cd1—Cd1 ⁱⁱ	130.45 (3)
C5—C6—H6	119.6	Cd1 ⁱ —Cd1—Cd1 ⁱⁱ	179.436 (13)
C8—C7—C6	120.3 (4)	Cd1 ⁱⁱ —Cl1—Cd1	79.53 (4)
C8—C7—H7	119.8	Cd1—Cl2—Cd1 ⁱⁱ	79.22 (4)
C6—C7—H7	119.8	Cd1 ⁱⁱ —Cl3—Cd1	79.43 (3)
C7—C8—C9	119.8 (5)	C3—N1—C1	110.3 (5)
C7—C8—H8	120.1	C3—N1—C2	106.8 (3)
C9—C8—H8	120.1	C1—N1—C2	107.2 (4)
C8—C9—C10	120.2 (5)	C3—N1—C4	111.3 (5)
C8—C9—H9	119.9	C1—N1—C4	110.6 (3)
C10—C9—H9	119.9	C2—N1—C4	110.5 (4)
C9—C10—C5	120.7 (5)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1A \cdots Cl3 ⁱⁱⁱ	0.96	2.74	3.600 (6)	149
C3—H3B \cdots Cl1 ^{iv}	0.96	2.83	3.586 (7)	137
C4—H4A \cdots Cl3	0.97	2.68	3.645 (5)	171

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