

Poly[[bis(μ -1,2-bis(4-pyridyl)ethene)-bis(trichloroacetato)cadmium(II)] monohydrate]

Jin Hoon Kim,^a Cheal Kim^{a*} and Youngmee Kim^{b*}

^aDepartment of Fine Chemistry, and Eco-Product and Materials Education Center, Seoul National University of Science and Technology, Seoul 139-743, Republic of Korea, and ^bDepartment of Chemistry and Nano Science, Ewha Womans University, Seoul 120-750, Republic of Korea

Correspondence e-mail: chealkim@seoultech.ac.kr, ymeekim@ewha.ac.kr

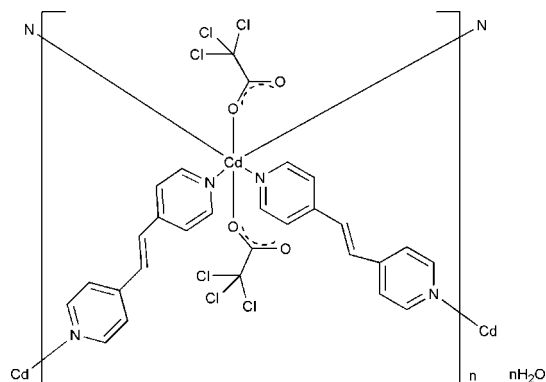
Received 19 November 2010; accepted 26 November 2010

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.032; wR factor = 0.085; data-to-parameter ratio = 15.3.

In the crystal structure of the title compound, $\{[\text{Cd}(\text{C}_2\text{Cl}_3\text{O}_2)_2(\text{C}_{12}\text{H}_{10}\text{N}_2)_2] \cdot \text{H}_2\text{O}\}_n$, the Cd^{II} ion lies on a twofold rotation axis and 1,2-bis(4-pyridyl)ethene ligands bridge symmetry-related Cd^{II} ions, forming a two-dimensional structure. Two trichloroacetate ligands complete the coordination around the Cd^{II} ion, forming a distorted octahedral environment. In the crystal, solvent water molecules, which also lie on twofold rotation axes, form intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, which connect the two-dimensional structure into a three-dimensional network. The crystal studied was an inversion twin, the refined ratio of twin components being 0.75 (4):0.25 (4).

Related literature

For background to self-assembly processes, see: Batten & Robson (1998); Moler *et al.* (2001); Moulton & Zaworotko (2001); Kim (2002); Evans & Lin (2002). For supramolecular assemblies, see: Sauvage & Hosseini (1995); Fujita *et al.* (2001); Aromí *et al.* (2006). For optical sensors and heterogeneous catalysts, see: Yoo *et al.* (2003); Takizawa *et al.* (2003); Hong *et al.* (2004); Kitagawa *et al.* (2004); Hong *et al.* (2005); Han *et al.* (2006).



Experimental

Crystal data

$[\text{Cd}(\text{C}_2\text{Cl}_3\text{O}_2)_2(\text{C}_{12}\text{H}_{10}\text{N}_2)_2] \cdot \text{H}_2\text{O}$
 $M_r = 819.60$
 Orthorhombic, *Iba2*
 $a = 19.618$ (4) Å
 $b = 9.5760$ (19) Å
 $c = 17.517$ (4) Å

$V = 3290.8$ (11) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.19$ mm⁻¹
 $T = 293$ K
 $0.25 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.751$, $T_{\text{max}} = 0.788$

8746 measured reflections
 3146 independent reflections
 2738 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.085$
 $S = 1.07$
 3146 reflections
 205 parameters
 1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.69$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³
 Absolute structure: Flack (1983), 1477 Friedel pairs
 Flack parameter: 0.25 (4)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1S}-\text{H1S} \cdots \text{O3}^i$	0.97 (6)	1.97 (6)	2.924 (6)	167 (5)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; 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*.

Financial support from the Korea Ministry of the Environment "ET-Human resource development Project", the Korean Science Technology Development (S121010L080120) is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5170).

References

- Aromí, G., Stoeckli-Evans, H., Teat, S. J., Cano, J. & Ribas, J. (2006). *J. Mater. Chem.* **16**, 2635–2644.
- Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.
- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Evans, O. R. & Lin, W. (2002). *Acc. Chem. Res.* **35**, 511–522.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Fujita, M., Umemoto, K., Yoshizawa, M., Fujita, N., Kusakawa, T. & Biradha, K. (2001). *Chem. Commun.* pp. 509–518.
- Han, H., Zhang, S., Hou, H., Fan, Y. & Zhu, Y. (2006). *Eur. J. Inorg. Chem.* pp. 1594–1600.
- Hong, S. J., Ryu, J. Y., Lee, J. Y., Kim, C., Kim, S.-J. & Kim, Y. (2004). *Dalton Trans.* pp. 2697–2701.
- Hong, S. J., Seo, J. S., Ryu, J. Y., Lee, J. H., Kim, C., Kim, S.-J., Kim, Y. & Lough, A. J. (2005). *J. Mol. Struct.* **751**, 22–28.
- Kim, K. (2002). *Chem. Soc. Rev.* **31**, 96–107.
- Kitagawa, S., Kitaura, R. & Noro, S.-I. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.
- Moler, D. B., Li, H., Chen, B., Reineke, T. M., O’Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.
- Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.
- Sauvage, J.-P. & Hosseini, M. W. (1995). *Comprehensive Supramolecular Chemistry*, Vol. 9, edited by J.-M. Lehn. Oxford: Pergamon Press.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Takizawa, S., Somei, H., Jayaprakash, D. & Sasai, H. (2003). *Angew. Chem. Int. Ed.* **42**, 5711–5714.
- Yoo, S.-K., Ryu, J. Y., Lee, J. Y., Kim, C., Kim, S.-J. & Kim, Y. (2003). *Dalton Trans.* pp. 1454–1456.

supporting information

Acta Cryst. (2011). E67, m3–m4 [https://doi.org/10.1107/S1600536810049457]

Poly[[bis[μ -1,2-bis(4-pyridyl)ethene]bis(trichloroacetato)cadmium(II)] monohydrate]

Jin Hoon Kim, Cheal Kim and Youngmee Kim

S1. Comment

Self-assembly processes involving metal ions and organic ligands directed by either metal coordination or hydrogen bonds have attracted much attention in the field of supramolecular chemistry and current coordination chemistry (Batten, *et al.*, 1998; Moler, *et al.*, 2001; Moulton, *et al.*, 2001; Kim, *et al.*, 2002; Evans, *et al.*, 2002). The use of rigid or flexible spacer ligands is of considerable interests in recent years owing to their potential as building blocks for supramolecular assemblies (Sauvage, *et al.*, 1995; Fujita, *et al.*, 2001; Aromí, *et al.*, 2006) and their ability to act as optical sensors and heterogeneous catalysts (Yoo, *et al.*, 2003; Takizawa, *et al.*, 2003; Hong, *et al.*, 2004; Kitagawa, *et al.*, 2004; Hong, *et al.*, 2005; Han, *et al.*, 2006). In our attempt to investigate the design and control of the self-assembly of coordination polymers with the rigid bridging ligands, we have employed Cd^{II} to develop a new polymeric complex with the ligand 1,2-bis(4-pyridyl)ethene. We report herein the crystal structure of the title compound [Cd(O₂C₂Cl₃)₂(C₁₂H₁₀N₂)₂]_n (C₁₂H₁₀N₂ = 1,2-bis(4-pyridyl)ethene).

The asymmetric unit of the title compound is shown in Fig. 1. The unique Cd^{II} ion lies on a twofold roation axis and 1,2-bis(4-pyridyl)ethene ligands bridge symmetry related Cd^{II} ions to form a two-dimensional structure (Fig. 2). Two trichloroacetato ligands complete the coordination around the Cd^{II} ion to form a distorted octahedral environment. In the crystal structure solvent water molecules, which also lie on twofold roation axes, form intermolecular O–H...O hydrogen bonds which connect the two-dimensional structure into a three-dimensional network.

S2. Experimental

39.3 mg (0.125 mmol) of Cd(NO₃)₂·4H₂O and 41.3 mg (0.25 mmol) of CCl₃COOH and 15.8 mg (0.125 mmol) of NH₄OH were dissolved in 4 ml water and carefully layered by 4 ml ethanol of 1,2-bis(4-pyridyl)ethene ligand (47.0 mg, 0.25 mmol). Suitable crystals of the title compound for X-ray analysis were obtained in a month.

S3. Refinement

H atoms were placed incalculated positions with C—H distances of 0.93 Å (phenyl). They were included in the refinement in riding-motion approximation with U_{iso}(H) = 1.2U_{eq}(C). The unique H atom bonded to the water molecule was refined independently with an isotropic displacement parameter.

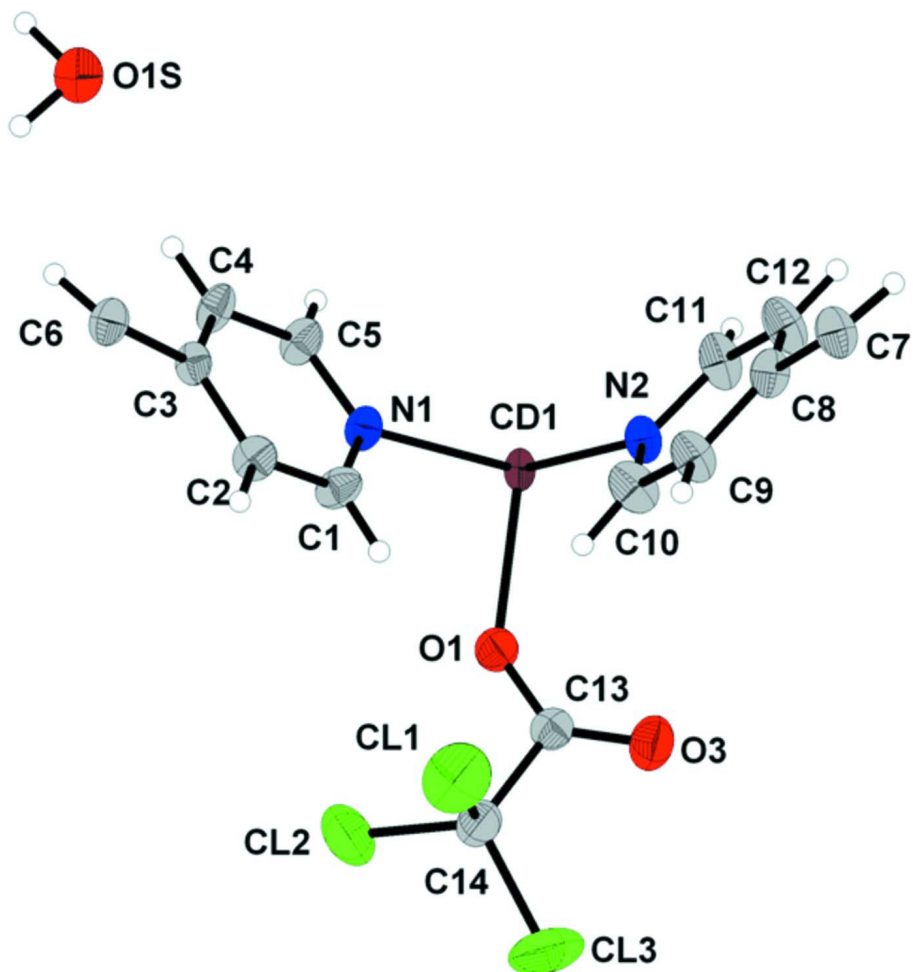


Figure 1

The asymmetric unit of the title compound with labeling scheme. Displacement ellipsoids are shown at the 50% probability level. The water molecule in the asymmetric unit is half occupancy.

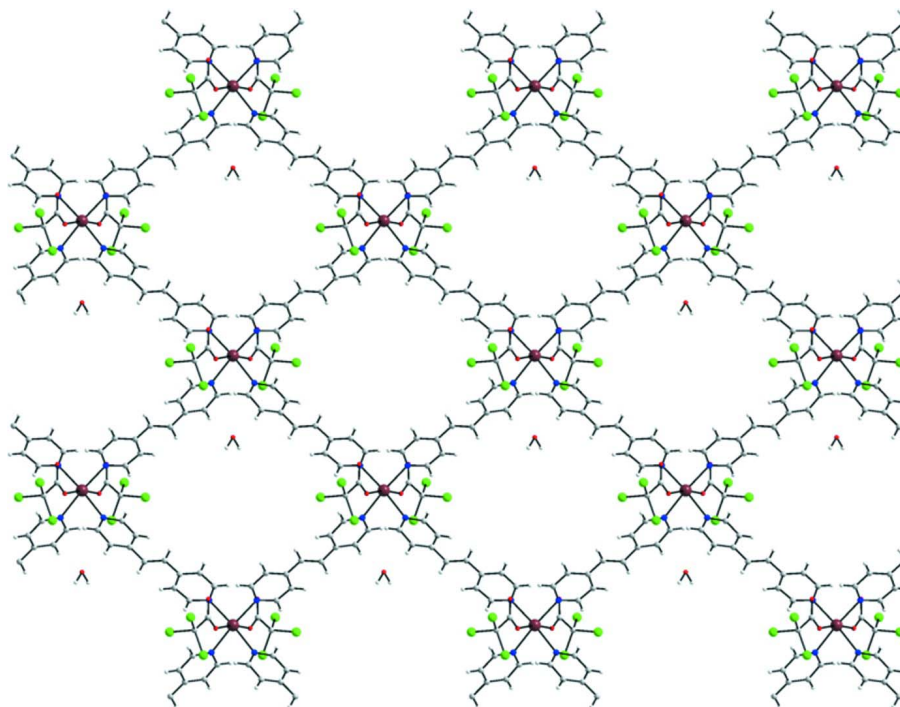


Figure 2

Part of a two-dimensional sheet of the title compound.

Poly[[bis(μ -1,2-bis(4-pyridyl)ethene)bis(trichloroacetato)cadmium(II)] monohydrate]

Crystal data

$[\text{Cd}(\text{C}_2\text{Cl}_3\text{O}_2)_2(\text{C}_{12}\text{H}_{10}\text{N}_2)_2] \cdot \text{H}_2\text{O}$

$M_r = 819.60$

Orthorhombic, *Iba*2

Hall symbol: I 2 -2c

$a = 19.618(4) \text{ \AA}$

$b = 9.5760(19) \text{ \AA}$

$c = 17.517(4) \text{ \AA}$

$V = 3290.8(11) \text{ \AA}^3$

$Z = 4$

$F(000) = 1632$

$D_x = 1.654 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3648 reflections

$\theta = 2.4\text{--}26.3^\circ$

$\mu = 1.19 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colorless

$0.25 \times 0.20 \times 0.20 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.751$, $T_{\max} = 0.788$

8746 measured reflections

3146 independent reflections

2738 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -23 \rightarrow 24$

$k = -11 \rightarrow 8$

$l = -21 \rightarrow 21$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.032$ $wR(F^2) = 0.085$ $S = 1.07$

3146 reflections

205 parameters

1 restraint

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 0.189P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.69 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.49 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack (1983), 1477 Friedel
pairs

Absolute structure parameter: 0.25 (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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1330 (3)	0.5206 (5)	0.3412 (4)	0.0483 (15)
H1	0.1462	0.4440	0.3121	0.058*
C2	0.1778 (2)	0.5728 (5)	0.3947 (3)	0.0452 (10)
H2	0.2203	0.5317	0.4013	0.054*
C3	0.15908 (19)	0.6871 (4)	0.4386 (2)	0.0370 (9)
C4	0.0939 (2)	0.7358 (6)	0.4289 (2)	0.0483 (11)
H4	0.0779	0.8075	0.4598	0.058*
C5	0.0521 (2)	0.6800 (5)	0.3739 (2)	0.0474 (11)
H5	0.0086	0.7171	0.3678	0.057*
C6	0.20672 (19)	0.7556 (5)	0.4922 (2)	0.0454 (12)
H6	0.1884	0.8097	0.5312	0.055*
C7	0.2262 (2)	0.7553 (5)	-0.0119 (3)	0.0496 (12)
H7	0.2086	0.8121	-0.0503	0.060*
C8	0.17672 (19)	0.6860 (5)	0.0386 (2)	0.0437 (10)
C9	0.1933 (2)	0.5842 (5)	0.0904 (2)	0.0509 (12)
H9	0.2381	0.5534	0.0942	0.061*
C10	0.1447 (3)	0.5281 (7)	0.1361 (4)	0.0547 (16)
H10	0.1578	0.4583	0.1700	0.066*
C11	0.0618 (2)	0.6619 (6)	0.0834 (2)	0.0530 (13)
H11	0.0163	0.6882	0.0794	0.064*
C12	0.1090 (2)	0.7238 (7)	0.0345 (3)	0.0576 (14)
H12	0.0949	0.7904	-0.0007	0.069*
C13	0.0825 (2)	0.1977 (4)	0.1993 (3)	0.0433 (9)

C14	0.1275 (2)	0.0920 (5)	0.2461 (3)	0.0567 (12)
Cd1	0.0000	0.5000	0.22812 (5)	0.03111 (11)
Cl1	0.20978 (7)	0.1774 (2)	0.25364 (11)	0.1014 (6)
Cl2	0.09814 (9)	0.0658 (2)	0.33949 (9)	0.0954 (5)
Cl3	0.14021 (12)	-0.06656 (19)	0.19892 (14)	0.1285 (9)
N1	0.07119 (15)	0.5758 (4)	0.32947 (19)	0.0398 (8)
N2	0.07875 (16)	0.5669 (5)	0.13543 (19)	0.0403 (8)
O1	0.05695 (13)	0.2898 (3)	0.23965 (17)	0.0488 (7)
O3	0.08109 (18)	0.1802 (4)	0.13081 (19)	0.0680 (9)
O1S	0.0000	1.0000	0.5313 (4)	0.0764 (17)
H1S	0.021 (3)	0.941 (6)	0.570 (3)	0.059 (14)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.044 (3)	0.044 (3)	0.057 (3)	-0.0035 (19)	-0.009 (3)	-0.013 (2)
C2	0.0299 (19)	0.054 (3)	0.052 (2)	0.0011 (19)	-0.0088 (17)	-0.005 (2)
C3	0.0309 (19)	0.045 (2)	0.0349 (19)	-0.0118 (17)	-0.0088 (15)	-0.0007 (16)
C4	0.042 (2)	0.063 (3)	0.040 (2)	-0.001 (2)	-0.0068 (17)	-0.018 (2)
C5	0.034 (2)	0.060 (3)	0.049 (2)	0.005 (2)	-0.0116 (18)	-0.014 (2)
C6	0.039 (2)	0.056 (2)	0.042 (3)	-0.0081 (18)	-0.0075 (17)	-0.0070 (18)
C7	0.0405 (18)	0.065 (3)	0.044 (3)	-0.0112 (19)	0.010 (2)	0.012 (2)
C8	0.0314 (19)	0.061 (3)	0.039 (2)	-0.0055 (18)	0.0066 (17)	-0.002 (2)
C9	0.033 (2)	0.069 (3)	0.050 (3)	-0.001 (2)	0.0095 (18)	0.017 (2)
C10	0.034 (3)	0.069 (3)	0.062 (4)	-0.004 (2)	0.014 (3)	0.018 (3)
C11	0.029 (2)	0.085 (4)	0.045 (2)	-0.003 (2)	0.0042 (17)	0.015 (2)
C12	0.039 (2)	0.083 (4)	0.051 (3)	-0.003 (2)	0.008 (2)	0.026 (3)
C13	0.040 (2)	0.042 (2)	0.048 (2)	-0.0078 (17)	0.0007 (17)	-0.0015 (17)
C14	0.058 (2)	0.059 (3)	0.054 (3)	0.009 (2)	-0.007 (2)	-0.010 (2)
Cd1	0.02345 (16)	0.04508 (18)	0.02480 (16)	-0.01014 (13)	0.000	0.000
Cl1	0.0462 (6)	0.1336 (14)	0.1242 (14)	0.0178 (7)	-0.0158 (8)	-0.0198 (11)
Cl2	0.1164 (13)	0.0992 (12)	0.0706 (9)	0.0192 (10)	0.0012 (9)	0.0275 (9)
Cl3	0.173 (2)	0.0646 (10)	0.148 (2)	0.0378 (12)	-0.0147 (15)	-0.0328 (11)
N1	0.0336 (18)	0.049 (2)	0.0363 (19)	-0.0101 (16)	-0.0033 (14)	-0.0055 (17)
N2	0.0304 (18)	0.057 (2)	0.0334 (18)	-0.0074 (17)	0.0056 (13)	0.0067 (17)
O1	0.0489 (14)	0.0503 (15)	0.0471 (18)	0.0042 (12)	0.0031 (13)	-0.0007 (14)
O3	0.074 (2)	0.078 (2)	0.051 (2)	0.0024 (18)	-0.0073 (16)	-0.0095 (17)
O1S	0.091 (5)	0.078 (4)	0.060 (4)	0.001 (3)	0.000	0.000

Geometric parameters (Å, °)

C1—N1	1.338 (7)	C10—N2	1.347 (7)
C1—C2	1.379 (8)	C10—H10	0.9300
C1—H1	0.9300	C11—N2	1.330 (6)
C2—C3	1.387 (6)	C11—C12	1.393 (6)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.371 (6)	C12—H12	0.9300
C3—C6	1.479 (5)	C13—O3	1.212 (5)

C4—C5	1.374 (6)	C13—O1	1.236 (5)
C4—H4	0.9300	C13—C14	1.573 (6)
C5—N1	1.320 (6)	C14—C13	1.746 (5)
C5—H5	0.9300	C14—C12	1.753 (5)
C6—C7 ⁱ	1.323 (6)	C14—C11	1.815 (5)
C6—H6	0.9300	Cd1—O1 ⁱⁱⁱ	2.311 (3)
C7—C6 ⁱⁱ	1.322 (6)	Cd1—O1	2.311 (3)
C7—C8	1.471 (6)	Cd1—N2	2.331 (3)
C7—H7	0.9300	Cd1—N2 ⁱⁱⁱ	2.331 (3)
C8—C9	1.371 (6)	Cd1—N1	2.373 (3)
C8—C12	1.379 (6)	Cd1—N1 ⁱⁱⁱ	2.373 (3)
C9—C10	1.356 (7)	O1S—H1S	0.97 (6)
C9—H9	0.9300		
N1—C1—C2	122.6 (5)	C8—C12—H12	120.1
N1—C1—H1	118.7	C11—C12—H12	120.1
C2—C1—H1	118.7	O3—C13—O1	131.0 (4)
C1—C2—C3	119.6 (4)	O3—C13—C14	116.0 (4)
C1—C2—H2	120.2	O1—C13—C14	112.9 (4)
C3—C2—H2	120.2	C13—C14—C13	113.2 (3)
C4—C3—C2	116.5 (4)	C13—C14—C12	113.2 (3)
C4—C3—C6	121.1 (4)	C13—C14—C12	111.4 (3)
C2—C3—C6	122.3 (4)	C13—C14—C11	104.3 (3)
C3—C4—C5	120.8 (4)	C13—C14—C11	107.4 (3)
C3—C4—H4	119.6	C12—C14—C11	106.8 (3)
C5—C4—H4	119.6	O1 ⁱⁱⁱ —Cd1—O1	169.98 (15)
N1—C5—C4	122.5 (4)	O1 ⁱⁱⁱ —Cd1—N2	98.16 (13)
N1—C5—H5	118.8	O1—Cd1—N2	88.84 (13)
C4—C5—H5	118.8	O1 ⁱⁱⁱ —Cd1—N2 ⁱⁱⁱ	88.85 (13)
C7 ⁱ —C6—C3	124.0 (4)	O1—Cd1—N2 ⁱⁱⁱ	98.16 (13)
C7 ⁱ —C6—H6	118.0	N2—Cd1—N2 ⁱⁱⁱ	91.69 (17)
C3—C6—H6	118.0	O1 ⁱⁱⁱ —Cd1—N1	87.28 (12)
C6 ⁱⁱ —C7—C8	126.0 (4)	O1—Cd1—N1	85.22 (12)
C6 ⁱⁱ —C7—H7	117.0	N2—Cd1—N1	92.69 (10)
C8—C7—H7	117.0	N2 ⁱⁱⁱ —Cd1—N1	174.52 (14)
C9—C8—C12	116.7 (4)	O1 ⁱⁱⁱ —Cd1—N1 ⁱⁱⁱ	85.22 (12)
C9—C8—C7	124.2 (4)	O1—Cd1—N1 ⁱⁱⁱ	87.29 (12)
C12—C8—C7	119.1 (4)	N2—Cd1—N1 ⁱⁱⁱ	174.52 (14)
C10—C9—C8	120.4 (4)	N2 ⁱⁱⁱ —Cd1—N1 ⁱⁱⁱ	92.69 (10)
C10—C9—H9	119.8	N1—Cd1—N1 ⁱⁱⁱ	83.13 (16)
C8—C9—H9	119.8	C5—N1—C1	117.7 (4)
N2—C10—C9	124.1 (5)	C5—N1—Cd1	120.3 (3)
N2—C10—H10	117.9	C1—N1—Cd1	121.8 (3)
C9—C10—H10	117.9	C11—N2—C10	115.8 (4)
N2—C11—C12	123.1 (4)	C11—N2—Cd1	120.0 (3)
N2—C11—H11	118.5	C10—N2—Cd1	123.7 (3)
C12—C11—H11	118.5	C13—O1—Cd1	140.1 (3)
C8—C12—C11	119.8 (5)		

N1—C1—C2—C3	0.0 (8)	O1—Cd1—N1—C5	-156.1 (3)
C1—C2—C3—C4	4.1 (6)	N2—Cd1—N1—C5	115.2 (4)
C1—C2—C3—C6	-174.7 (5)	N1 ⁱⁱⁱ —Cd1—N1—C5	-68.3 (3)
C2—C3—C4—C5	-5.0 (7)	O1 ⁱⁱⁱ —Cd1—N1—C1	-159.2 (4)
C6—C3—C4—C5	173.9 (4)	O1—Cd1—N1—C1	27.4 (4)
C3—C4—C5—N1	1.8 (8)	N2—Cd1—N1—C1	-61.2 (4)
C4—C3—C6—C7 ⁱ	-158.2 (5)	N1 ⁱⁱⁱ —Cd1—N1—C1	115.3 (4)
C2—C3—C6—C7 ⁱ	20.6 (7)	C12—C11—N2—C10	-3.0 (8)
C6 ⁱⁱ —C7—C8—C9	-9.8 (8)	C12—C11—N2—Cd1	169.0 (4)
C6 ⁱⁱ —C7—C8—C12	170.4 (5)	C9—C10—N2—C11	3.2 (9)
C12—C8—C9—C10	-1.8 (8)	C9—C10—N2—Cd1	-168.5 (5)
C7—C8—C9—C10	178.4 (5)	O1 ⁱⁱⁱ —Cd1—N2—C11	-31.9 (4)
C8—C9—C10—N2	-0.8 (10)	O1—Cd1—N2—C11	155.3 (4)
C9—C8—C12—C11	1.9 (8)	N2 ⁱⁱⁱ —Cd1—N2—C11	57.1 (3)
C7—C8—C12—C11	-178.3 (5)	N1—Cd1—N2—C11	-119.6 (4)
N2—C11—C12—C8	0.5 (9)	O1 ⁱⁱⁱ —Cd1—N2—C10	139.4 (4)
O3—C13—C14—C13	-23.4 (5)	O1—Cd1—N2—C10	-33.4 (4)
O1—C13—C14—C13	159.9 (3)	N2 ⁱⁱⁱ —Cd1—N2—C10	-131.5 (5)
O3—C13—C14—C12	-151.3 (4)	N1—Cd1—N2—C10	51.8 (4)
O1—C13—C14—C12	32.1 (4)	O3—C13—O1—Cd1	-7.5 (7)
O3—C13—C14—C11	93.0 (4)	C14—C13—O1—Cd1	168.5 (3)
O1—C13—C14—C11	-83.6 (4)	O1 ⁱⁱⁱ —Cd1—O1—C13	-179.3 (4)
C4—C5—N1—C1	2.5 (7)	N2—Cd1—O1—C13	-44.8 (4)
C4—C5—N1—Cd1	-174.1 (4)	N2 ⁱⁱⁱ —Cd1—O1—C13	46.8 (4)
C2—C1—N1—C5	-3.3 (7)	N1—Cd1—O1—C13	-137.6 (4)
C2—C1—N1—Cd1	173.2 (4)	N1 ⁱⁱⁱ —Cd1—O1—C13	139.1 (4)
O1 ⁱⁱⁱ —Cd1—N1—C5	17.2 (3)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1S-H1S\cdots O3^{iv}$	0.97 (6)	1.97 (6)	2.924 (6)	167 (5)

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