

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# Di- $\mu_3$ -chlorido-tetra- $\mu_2$ -chlorido-dichloridobis(dimethylformamide- $\kappa$ O)-hexakis(1*H*-imidazole- $\kappa$ N<sup>3</sup>)tetracadmium

Run-Qiang Zhu

Ordered Matter Science Research Center, College of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, People's Republic of China  
Correspondence e-mail: zhurunqiang@163.com

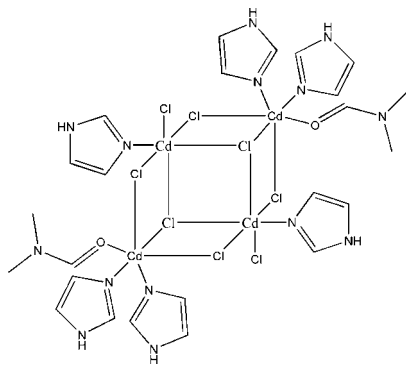
Received 21 August 2011; accepted 16 September 2011

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.028;  $wR$  factor = 0.069; data-to-parameter ratio = 20.4.

The centrosymmetric molecule of the title complex,  $[\text{Cd}_4\text{Cl}_8(\text{C}_3\text{H}_4\text{N}_2)_6(\text{C}_3\text{H}_7\text{NO})_2]$ , contains four  $\text{Cd}^{\text{II}}$  atoms, six imidazole, two dimethylformamide and eight chloride ligands. The structure shows a novel chloride-bridged tetranuclear cadmium quasi-cubane cluster. The coordination geometry of all  $\text{Cd}^{\text{II}}$  atoms is distorted octahedral, with the two metal atoms in the asymmetric unit in different coordination environments. One of the  $\text{Cd}^{2+}$  ions is coordinated by five  $\text{Cl}^-$  ions and by one N atom from an imidazole ligand, while the second is coordinated by three chloride ligands, two N atoms from two imidazole ligands and one O atom from a dimethylformamide molecule. Intermolecular  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds link the molecules into a two-dimensional polymeric structure parallel to the  $ab$  plane.

## Related literature

For general background to ferroelectric compounds with metal-organic frameworks, see: Ye *et al.* (2009); Zhang *et al.* (2009).



## Experimental

### Crystal data

$[\text{Cd}_4\text{Cl}_8(\text{C}_3\text{H}_4\text{N}_2)_6(\text{C}_3\text{H}_7\text{NO})_2]$   
 $M_r = 1287.92$   
 Monoclinic,  $P2_1/c$   
 $a = 8.2540$  (17) Å  
 $b = 12.290$  (3) Å  
 $c = 21.119$  (4) Å  
 $\beta = 99.23$  (3)°  
 $V = 2114.6$  (8) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 2.53$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.30 \times 0.25 \times 0.20$  mm

### Data collection

Rigaku SCXmini diffractometer  
 Absorption correction: multi-scan  
 (*CrystalClear*; Rigaku, 2005)  
 $T_{\text{min}} = 0.472$ ,  $T_{\text{max}} = 0.603$   
 21502 measured reflections  
 4833 independent reflections  
 4241 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.069$   
 $S = 1.05$   
 4833 reflections  
 237 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.34$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.66$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N}2-\text{H}2A\cdots\text{Cl}2^{\text{i}}$	0.86	2.44	3.226 (3)	152
$\text{N}4-\text{H}4A\cdots\text{Cl}1^{\text{ii}}$	0.86	2.45	3.212 (3)	148
$\text{N}6-\text{H}6A\cdots\text{Cl}2^{\text{iii}}$	0.86	2.63	3.314 (3)	137

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

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: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97*.

The author is grateful to the starter fund of Southeast University for financial support to buy the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2402).

## References

- Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.  
 Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Ye, H. Y., Fu, D. W., Zhang, Y., Zhang, W., Xiong, R. G. & Huang, S. P. (2009). *J. Am. Chem. Soc.* **131**, 42–43.  
 Zhang, W., Cheng, L. Z., Xiong, R. G., Nakamura, T. & Huang, S. P. (2009). *J. Am. Chem. Soc.* **131**, 12544–12545.

## supporting information

*Acta Cryst.* (2011). E67, m1416 [https://doi.org/10.1107/S1600536811037834]

## Di- $\mu_3$ -chlorido-tetra- $\mu_2$ -chlorido-dichloridobis(dimethylformamide- $\kappa O$ )hexakis-(1*H*-imidazole- $\kappa N^3$ )tetracadmium

Run-Qiang Zhu

### S1. Comment

The title compound (I) was prepared from imidazole and cadmium(II) chloride in DMF. The solid state structure of (I) at 298 K shows a novel centrosymmetric tetranuclear cadmium quasi-cubane cluster with a  $\text{Cd}_4(\text{Cl})_2(\mu\text{-Cl})_4(\mu_3\text{-Cl})_2$  core structure surrounded by six imidazole and two DMF molecules (Fig. 1). There are two different coordination environments about the Cd centers: Cd(1) is coordinated by one imidazole ligand, four bridging and one terminal Cl ions, and Cd(2) is coordinated by one O atom from DMF, two N atoms from two imidazole ligands and three bridging Cl ions. The shortest intra-molecular Cd(1)—Cd(1 A) separation is 4.103 (5) Å.

In the tetranuclear cluster, the cadmium atoms are connected by six Cl atoms among which the Cl1 and Cl3 atoms act as bridges between Cd(1) and Cd(2) centers, and the Cl(4) atom is a node to connect two Cd1 and one Cd2 together. The bond length Cd1—Cl2 to the terminal Cl ligand of 2.5475 (10) Å is shorter than the mean values of Cd—Cl( $\mu$ ) [2.654 (2) Å] and Cd—Cl( $\mu_3$ ) [2.729 (2) Å] bond lengths.

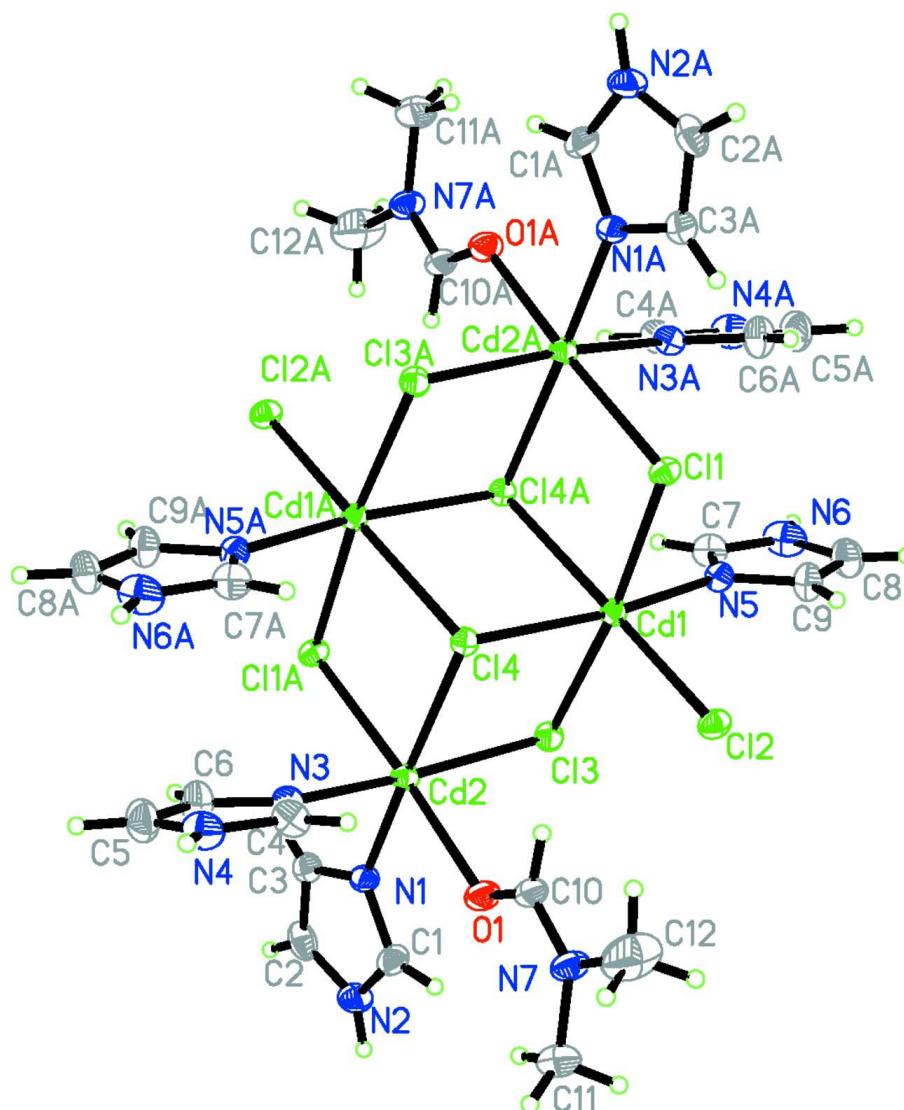
In order to check a possibility of a structural phase transitions in compound (I), we measured its temperature-dependent dielectric constant. Large dielectric anomalies usually indicate structural changes such as paraelectric-to-ferroelectric phase transitions. Unfortunately, the dielectric constant of compound (I) goes smoothly in the temperature range 93–273 K, suggesting no distinct phase transitions occurring in this temperature range (Ye *et al.*, 2009; Zhang *et al.*, 2009).

### S2. Experimental

The mixture of  $\text{CdCl}_2$  (2.27 g, 10 mmol) and imidazole (2.76 g, 40 mmol) in DMF was stirred for several days at room temperature. Colourless needle-like crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the solution at room temperature over 2 weeks.

### S3. Refinement

Positional parameters of all H atoms were calculated geometrically and the H atoms were set to ride on the C atoms and N atoms to which they were bonded, with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{iso}}(\text{C}, \text{N})$  and  $1.5 U_{\text{iso}}(\text{C})$  for methyl H atoms. C—H atoms were included with bond distances ranging from 0.98 to 1.00 Å and N—H hydrogen atoms were included with the N—H distance set to 0.84 Å.



**Figure 1**

The molecular structure of the title complex with displacement ellipsoids shown at the 50% probability level. Symmetry codes for the atoms with the A label:  $-x, 1 - y, 1 - z$ .

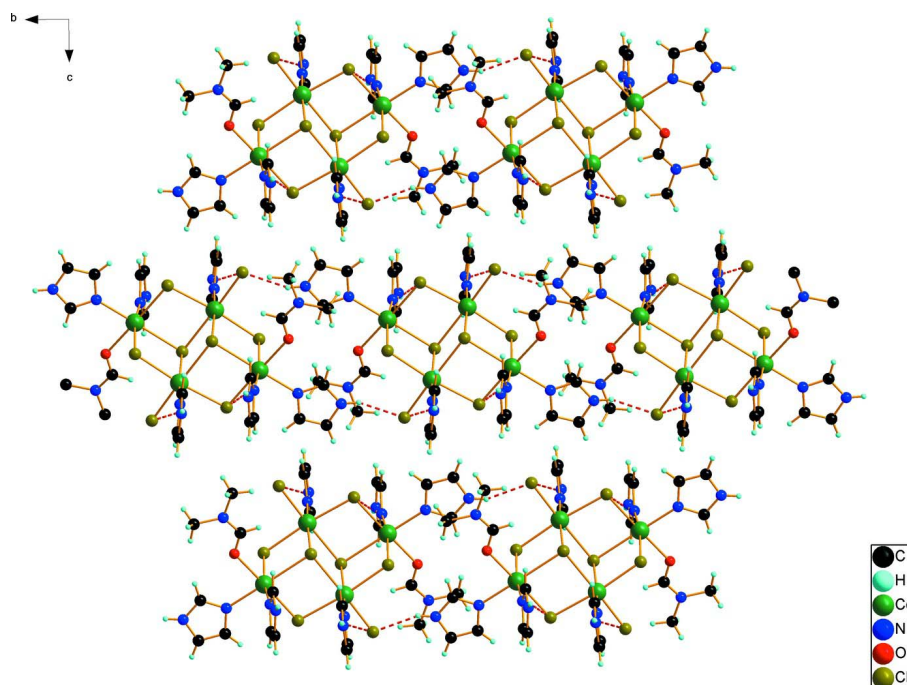


Figure 2

Packing diagram of the title compound projected along the  $a$  axis. Hydrogen bonds are shown as dashed lines.

**Di- $\mu_3$ -chlorido-tetra- $\mu_2$ -chlorido-dichloridobis(dimethylformamide- $\kappa$ O)hexakis(1*H*-imidazole- $\kappa$ N<sup>3</sup>)tetracadmium**

*Crystal data*

[Cd<sub>4</sub>Cl<sub>8</sub>(C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>)<sub>6</sub>(C<sub>3</sub>H<sub>7</sub>NO)<sub>2</sub>]

$M_r = 1287.92$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.2540$  (17) Å

$b = 12.290$  (3) Å

$c = 21.119$  (4) Å

$\beta = 99.23$  (3)°

$V = 2114.6$  (8) Å<sup>3</sup>

$Z = 2$

$F(000) = 1248$

$D_x = 2.023$  Mg m<sup>-3</sup>

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

Cell parameters from 4835 reflections

$\theta = 2.5$ – $27.5$ °

$\mu = 2.53$  mm<sup>-1</sup>

$T = 293$  K

Prism, colourless

$0.30 \times 0.25 \times 0.20$  mm

*Data collection*

Rigaku SCXmini  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

CCD\_Profile\_fitting scans

Absorption correction: multi-scan  
(*CrystalClear*; Rigaku, 2005)

$T_{\min} = 0.472$ ,  $T_{\max} = 0.603$

21502 measured reflections

4833 independent reflections

4241 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 3.0$ °

$h = -10$ → $10$

$k = -15$ → $15$

$l = -27$ → $27$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.028$  $wR(F^2) = 0.069$  $S = 1.05$ 

4833 reflections

237 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 1.0319P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.002$  $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.66 \text{ e } \text{\AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick,  
2008)

Extinction coefficient: 0

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1022 (4)	0.0007 (3)	0.59318 (17)	0.0415 (8)
H1	0.1309	-0.0205	0.5542	0.050*
C2	0.0277 (4)	-0.0083 (3)	0.68722 (18)	0.0457 (9)
H2	-0.0036	-0.0348	0.7247	0.055*
C3	0.0450 (4)	0.0970 (3)	0.67154 (16)	0.0380 (8)
H3	0.0275	0.1563	0.6969	0.046*
C4	0.5413 (4)	0.2881 (3)	0.57582 (18)	0.0416 (8)
H4	0.5389	0.2891	0.5316	0.050*
C5	0.6345 (5)	0.2923 (4)	0.6781 (2)	0.0559 (10)
H5	0.7043	0.2964	0.7172	0.067*
C6	0.4692 (4)	0.2792 (3)	0.66852 (18)	0.0484 (9)
H6	0.4053	0.2730	0.7008	0.058*
C7	-0.5008 (4)	0.4395 (3)	0.38982 (19)	0.0429 (8)
H7	-0.5052	0.4478	0.4333	0.051*
C8	-0.5764 (5)	0.4230 (3)	0.2874 (2)	0.0582 (11)
H8	-0.6402	0.4178	0.2470	0.070*
C9	-0.4130 (5)	0.4196 (3)	0.30070 (17)	0.0457 (9)
H9	-0.3428	0.4114	0.2707	0.055*
C10	0.3020 (4)	0.1635 (3)	0.43669 (16)	0.0384 (8)
H10	0.2958	0.2363	0.4245	0.046*
C11	0.3797 (6)	-0.0201 (3)	0.4151 (2)	0.0638 (12)
H11A	0.3284	-0.0347	0.4519	0.096*
H11B	0.4930	-0.0415	0.4239	0.096*

H11C	0.3249	-0.0605	0.3790	0.096*
C12	0.4289 (8)	0.1321 (5)	0.3439 (3)	0.096 (2)
H12A	0.3740	0.0932	0.3072	0.144*
H12B	0.5449	0.1192	0.3485	0.144*
H12C	0.4078	0.2086	0.3382	0.144*
Cd1	-0.10174 (3)	0.428101 (17)	0.415237 (10)	0.02728 (7)
Cd2	0.14449 (3)	0.254846 (17)	0.557490 (11)	0.02742 (7)
N1	0.0926 (3)	0.1030 (2)	0.61219 (12)	0.0322 (6)
N2	0.0649 (4)	-0.0674 (2)	0.63767 (16)	0.0480 (8)
H2A	0.0647	-0.1373	0.6353	0.058*
N3	0.4108 (3)	0.2763 (2)	0.60408 (13)	0.0319 (6)
N4	0.6769 (4)	0.2984 (3)	0.61908 (17)	0.0502 (8)
H4A	0.7747	0.3073	0.6108	0.060*
N5	-0.3653 (3)	0.4301 (2)	0.36550 (13)	0.0318 (6)
N6	-0.6315 (4)	0.4356 (3)	0.34380 (19)	0.0549 (9)
H6A	-0.7325	0.4402	0.3490	0.066*
N7	0.3690 (4)	0.0952 (2)	0.40063 (15)	0.0433 (7)
O1	0.2472 (3)	0.13812 (19)	0.48519 (11)	0.0423 (6)
Cl1	-0.04823 (9)	0.61386 (6)	0.35684 (4)	0.02980 (16)
Cl2	0.00339 (10)	0.31740 (6)	0.32819 (4)	0.03436 (17)
Cl3	-0.14308 (9)	0.25405 (6)	0.48437 (4)	0.03149 (17)
Cl4	0.19278 (8)	0.44090 (6)	0.48833 (3)	0.02730 (15)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.053 (2)	0.0290 (17)	0.042 (2)	-0.0073 (16)	0.0058 (16)	-0.0043 (15)
C2	0.045 (2)	0.052 (2)	0.038 (2)	-0.0087 (17)	0.0011 (16)	0.0146 (17)
C3	0.0392 (18)	0.0418 (19)	0.0326 (18)	-0.0001 (15)	0.0045 (14)	0.0006 (15)
C4	0.0326 (18)	0.046 (2)	0.048 (2)	0.0014 (16)	0.0132 (15)	0.0057 (17)
C5	0.043 (2)	0.066 (3)	0.054 (3)	-0.002 (2)	-0.0067 (18)	-0.003 (2)
C6	0.041 (2)	0.065 (3)	0.040 (2)	-0.0048 (18)	0.0077 (16)	-0.0007 (18)
C7	0.0342 (18)	0.044 (2)	0.052 (2)	-0.0048 (15)	0.0136 (16)	0.0018 (16)
C8	0.040 (2)	0.067 (3)	0.059 (3)	0.001 (2)	-0.0162 (19)	-0.002 (2)
C9	0.042 (2)	0.062 (2)	0.0334 (19)	-0.0014 (18)	0.0045 (15)	-0.0018 (17)
C10	0.047 (2)	0.0311 (17)	0.0377 (19)	0.0053 (15)	0.0091 (15)	-0.0054 (14)
C11	0.078 (3)	0.042 (2)	0.072 (3)	0.019 (2)	0.014 (2)	-0.007 (2)
C12	0.143 (5)	0.082 (4)	0.080 (4)	0.007 (4)	0.071 (4)	0.001 (3)
Cd1	0.02655 (12)	0.02762 (12)	0.02745 (13)	-0.00098 (9)	0.00362 (9)	-0.00129 (9)
Cd2	0.02759 (12)	0.02543 (12)	0.03022 (13)	0.00193 (9)	0.00767 (9)	0.00044 (9)
N1	0.0365 (14)	0.0279 (13)	0.0323 (15)	-0.0019 (11)	0.0058 (11)	0.0029 (11)
N2	0.0547 (19)	0.0268 (15)	0.060 (2)	-0.0064 (14)	0.0004 (16)	0.0056 (14)
N3	0.0283 (13)	0.0317 (14)	0.0369 (15)	0.0022 (11)	0.0090 (11)	0.0024 (11)
N4	0.0294 (16)	0.0476 (19)	0.074 (2)	-0.0023 (14)	0.0098 (15)	0.0005 (17)
N5	0.0266 (13)	0.0353 (14)	0.0334 (15)	-0.0027 (11)	0.0047 (11)	-0.0015 (11)
N6	0.0235 (15)	0.053 (2)	0.088 (3)	-0.0017 (14)	0.0089 (16)	0.0052 (18)
N7	0.0524 (18)	0.0368 (16)	0.0440 (17)	0.0076 (14)	0.0178 (14)	-0.0062 (13)
O1	0.0542 (15)	0.0369 (13)	0.0385 (14)	0.0081 (11)	0.0156 (11)	-0.0038 (10)

C11	0.0327 (4)	0.0265 (4)	0.0323 (4)	-0.0034 (3)	0.0117 (3)	-0.0020 (3)
C12	0.0418 (4)	0.0305 (4)	0.0335 (4)	-0.0011 (3)	0.0144 (3)	-0.0021 (3)
C13	0.0327 (4)	0.0306 (4)	0.0313 (4)	-0.0037 (3)	0.0057 (3)	0.0020 (3)
C14	0.0249 (3)	0.0298 (4)	0.0277 (4)	0.0005 (3)	0.0058 (3)	-0.0008 (3)

*Geometric parameters (Å, °)*

C1—N1	1.326 (4)	C10—H10	0.9300
C1—N2	1.330 (5)	C11—N7	1.450 (5)
C1—H1	0.9300	C11—H11A	0.9600
C2—C3	1.349 (5)	C11—H11B	0.9600
C2—N2	1.350 (5)	C11—H11C	0.9600
C2—H2	0.9300	C12—N7	1.440 (5)
C3—N1	1.374 (4)	C12—H12A	0.9600
C3—H3	0.9300	C12—H12B	0.9600
C4—N3	1.320 (4)	C12—H12C	0.9600
C4—N4	1.332 (5)	Cd1—N5	2.259 (3)
C4—H4	0.9300	Cd1—C12	2.5486 (9)
C5—N4	1.349 (5)	Cd1—C13	2.6426 (9)
C5—C6	1.357 (5)	Cd1—C11	2.6651 (9)
C5—H5	0.9300	Cd1—C14	2.6671 (11)
C6—N3	1.369 (4)	Cd1—C14 <sup>i</sup>	2.7920 (9)
C6—H6	0.9300	Cd2—N1	2.272 (3)
C7—N5	1.308 (4)	Cd2—N3	2.275 (3)
C7—N6	1.332 (5)	Cd2—O1	2.350 (2)
C7—H7	0.9300	Cd2—C13	2.6158 (12)
C8—C9	1.333 (5)	Cd2—C11 <sup>i</sup>	2.6400 (9)
C8—N6	1.350 (6)	Cd2—C14	2.7762 (9)
C8—H8	0.9300	N2—H2A	0.8600
C9—N5	1.368 (4)	N4—H4A	0.8600
C9—H9	0.9300	N6—H6A	0.8600
C10—O1	1.225 (4)	C11—Cd2 <sup>i</sup>	2.6400 (9)
C10—N7	1.313 (4)	C14—Cd1 <sup>i</sup>	2.7920 (9)
N1—C1—N2	110.5 (3)	C13—Cd1—C14	85.09 (3)
N1—C1—H1	124.7	C11—Cd1—C14	90.80 (3)
N2—C1—H1	124.7	N5—Cd1—C14 <sup>i</sup>	88.92 (7)
C3—C2—N2	106.3 (3)	C12—Cd1—C14 <sup>i</sup>	175.27 (2)
C3—C2—H2	126.9	C13—Cd1—C14 <sup>i</sup>	89.43 (3)
N2—C2—H2	126.9	C11—Cd1—C14 <sup>i</sup>	85.84 (3)
C2—C3—N1	109.4 (3)	C14—Cd1—C14 <sup>i</sup>	82.58 (3)
C2—C3—H3	125.3	N1—Cd2—N3	97.08 (9)
N1—C3—H3	125.3	N1—Cd2—O1	86.90 (9)
N3—C4—N4	110.9 (3)	N3—Cd2—O1	85.85 (9)
N3—C4—H4	124.6	N1—Cd2—C13	94.01 (7)
N4—C4—H4	124.6	N3—Cd2—C13	167.97 (7)
N4—C5—C6	105.8 (3)	O1—Cd2—C13	90.10 (7)
N4—C5—H5	127.1	N1—Cd2—C11 <sup>i</sup>	92.97 (7)

C6—C5—H5	127.1	N3—Cd2—C11 <sup>i</sup>	90.51 (7)
C5—C6—N3	109.6 (3)	O1—Cd2—C11 <sup>i</sup>	176.31 (6)
C5—C6—H6	125.2	Cl3—Cd2—C11 <sup>i</sup>	93.58 (3)
N3—C6—H6	125.2	N1—Cd2—Cl4	177.38 (7)
N5—C7—N6	110.7 (3)	N3—Cd2—Cl4	85.51 (7)
N5—C7—H7	124.6	O1—Cd2—Cl4	93.66 (6)
N6—C7—H7	124.6	Cl3—Cd2—Cl4	83.44 (3)
C9—C8—N6	106.9 (4)	C11 <sup>i</sup> —Cd2—Cl4	86.65 (3)
C9—C8—H8	126.5	C1—N1—C3	105.4 (3)
N6—C8—H8	126.5	C1—N1—Cd2	126.9 (2)
C8—C9—N5	109.0 (4)	C3—N1—Cd2	127.7 (2)
C8—C9—H9	125.5	C1—N2—C2	108.4 (3)
N5—C9—H9	125.5	C1—N2—H2A	125.8
O1—C10—N7	124.7 (3)	C2—N2—H2A	125.8
O1—C10—H10	117.7	C4—N3—C6	105.3 (3)
N7—C10—H10	117.7	C4—N3—Cd2	128.2 (2)
N7—C11—H11A	109.5	C6—N3—Cd2	126.5 (2)
N7—C11—H11B	109.5	C4—N4—C5	108.3 (3)
H11A—C11—H11B	109.5	C4—N4—H4A	125.8
N7—C11—H11C	109.5	C5—N4—H4A	125.8
H11A—C11—H11C	109.5	C7—N5—C9	105.9 (3)
H11B—C11—H11C	109.5	C7—N5—Cd1	129.7 (2)
N7—C12—H12A	109.5	C9—N5—Cd1	124.4 (2)
N7—C12—H12B	109.5	C7—N6—C8	107.4 (3)
H12A—C12—H12B	109.5	C7—N6—H6A	126.3
N7—C12—H12C	109.5	C8—N6—H6A	126.3
H12A—C12—H12C	109.5	C10—N7—C12	120.9 (4)
H12B—C12—H12C	109.5	C10—N7—C11	121.3 (3)
N5—Cd1—Cl2	94.83 (7)	C12—N7—C11	117.7 (3)
N5—Cd1—Cl3	93.76 (7)	C10—O1—Cd2	127.5 (2)
Cl2—Cd1—Cl3	93.18 (3)	Cd2 <sup>i</sup> —C11—Cd1	96.66 (3)
N5—Cd1—C11	89.68 (7)	Cd2—Cl3—Cd1	97.92 (3)
Cl2—Cd1—C11	91.30 (3)	Cd1—Cl4—Cd2	93.53 (3)
Cl3—Cd1—C11	174.11 (2)	Cd1—Cl4—Cd1 <sup>i</sup>	97.42 (3)
N5—Cd1—Cl4	171.43 (7)	Cd2—Cl4—Cd1 <sup>i</sup>	90.75 (3)
Cl2—Cd1—Cl4	93.71 (3)		

Symmetry code: (i)  $-x, -y+1, -z+1$ .

*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>
N2—H2A $\cdots$ Cl2 <sup>ii</sup>	0.86	2.44	3.226 (3)	152
N4—H4A $\cdots$ C11 <sup>iii</sup>	0.86	2.45	3.212 (3)	148
N6—H6A $\cdots$ Cl2 <sup>iv</sup>	0.86	2.63	3.314 (3)	137

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