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Di-μ_3-chlorido-tetra-μ_2-chlorido-dichlorido-tetrakis(*N*,*N*-diethylethane-1,2-diamine-κ^2N,N')-tetracadmium(II)

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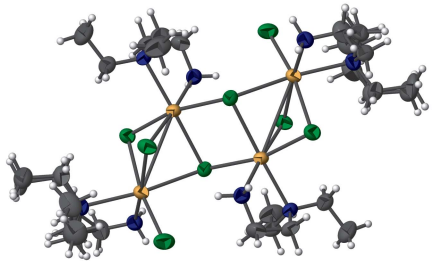
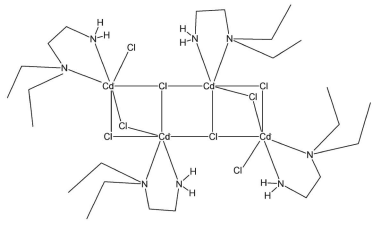
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Cd_4Cl_8(C_6H_{16}N_2)_4]$, the Cd^{2+} cations and Cl^- anions form M_4Cl_8 clusters with six of the Cl^- ions bridging Cd^{2+} cations and two being pendant. Each Cd^{2+} cation has distorted octahedral coordination completed by four Cl^- ions and two N atoms of the asymmetrical bidentate amino ligand. The cluster consists of pairs of face-sharing hexahedra linked by a shared edge.

3D view



Chemical scheme



Structure description

The coordination chemistry of cadmium is of interest to a wide range of disciplines ranging from toxicology to catalysis (Melnik *et al.*, 2009; Andersen *et al.*, 1984).

In the crystal structure, each complex unit has four amino ligands with two nitrogen atoms of each ligand coordinating to one Cd^{2+} ion (Fig. 1). The complex is centrosymmetric with the asymmetric unit consisting of half of the complex unit. One ligand of the asymmetric unit is disordered with two components of 0.553 (13) and 0.447 (13) occupancy.

The Cd^{2+} cations and Cl^- ions form Cd_4Cl_8 clusters with six bridging and two pendant Cl^- ions. Cd···Cl distances range from 2.5158 (19) to 2.8227 (18) Å in the cluster. A similar M_4Cl_8 core has been reported for an Ni^{II} complex (Kermagoret *et al.*, 2007). Each Cd^{2+} cation has a distorted octahedral coordination completed by four Cl^- ions and two nitrogen atoms of the bidentate amino ligand. The cluster consists of pairs of face-sharing hexahedra linked by a shared edge. The complex units are linked by intermolecular N—H···Cl contacts with N···Cl distances in the range 3.407 (6) to 3.548 (6) Å and N—H···Cl angles in the range 140.5 to 146.3° (Fig. 2, Table 1). Each complex unit donates four and accepts four N—H···Cl contacts with each pendant Cl^- accepting two bonds from different units.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2C···Cl4^{i}	0.89	2.82	3.548 (6)	141
N2—H2D···Cl4^{ii}	0.89	2.63	3.407 (6)	146
N4—H4D···Cl4^{iii}	0.89	2.71	3.463 (6)	143

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

Synthesis and crystallization

The cadmium complex was prepared by direct reaction of equimolar amounts of cadmium dichloride and *N*-diethylaminoethylamine in ethanol at room temperature. The white solid obtained was separated by filtration after three hours, washed with 5 ml cold ethanol and then three times (5 ml each) with diethyl ether. Based on the cadmium dichloride used, the yield was 85%. Crystallization from warm methanol solution in open air produced colourless crystals.

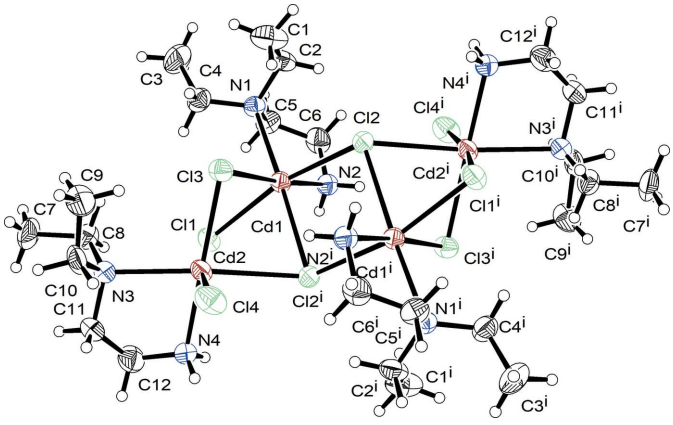


Figure 1
An *ORTEP* representation of the complex showing 50% probability ellipsoids (only the major component of the disordered ligand is shown). Symmetry code: (i) $1-x, 1-y, -z$.

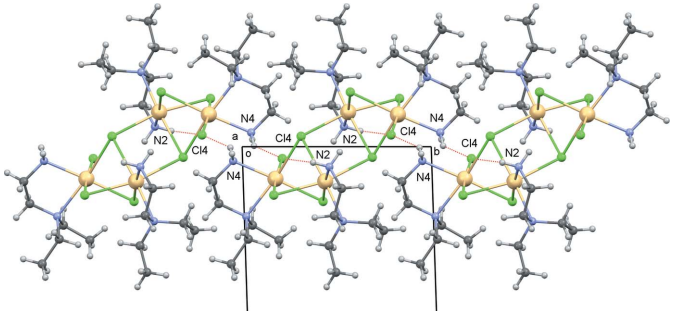


Figure 2
A segment of the crystal packing showing intermolecular N—H···Cl contacts as red dotted lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd_2Cl_4(C_6H_{16}N_2)_2]$
M_r	599.01
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	9.3622 (10), 9.4023 (10), 12.4248 (9)
α, β, γ (°)	87.667 (7), 86.171 (7), 81.993 (9)
V (Å^3)	1080.08 (18)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.46
Crystal size (mm)	0.26 × 0.17 × 0.06
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at home/near, Atlas
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min}, T_{max}	0.498, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15671, 5120, 3897
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.701
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.131, 1.07
No. of reflections	5120
No. of parameters	247
No. of restraints	390
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.01, −1.42

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *ORTEP-3 for Windows* (Farrugia, 2012).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The geometry and displacement parameters associated with the disordered atoms of the ligand were restrained during refinement.

Acknowledgements

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References

Andersen, O. (1984). *EHP, Environ. Health Perspect.* **54**, 249–266.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Kermagoret, A., Pattacini, R., Chavez Vasquez, P., Rogez, G., Welter, R. & Braunstein, P. (2007). *Angew. Chem. Int. Ed.* **46**, 6438–6441.
Melnik, M., Valent, A. & Kohutova, M. (2009). *Main Group Met. Chem.* **32**, 269–295.
Rigaku OD (2018). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2019). **4**, x191618 [https://doi.org/10.1107/S2414314619016183]

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Crystal data

$[Cd_2Cl_4(C_6H_{16}N_2)_2]$
M_r = 599.01
Triclinic, $P\overline{1}$
a = 9.3622 (10) Å
b = 9.4023 (10) Å
c = 12.4248 (9) Å
α = 87.667 (7)°
β = 86.171 (7)°
γ = 81.993 (9)°
V = 1080.08 (18) Å^3
Z = 2
$F(000)$ = 592
D_x = 1.842 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3382 reflections
θ = 4.3–29.0°
μ = 2.46 mm^{-1}
T = 293 K
Plate, colourless
0.26 × 0.17 × 0.06 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at home/near, Atlas diffractometer
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)
T_{min} = 0.498, T_{max} = 1.000
15671 measured reflections
5120 independent reflections
3897 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 29.9°, θ_{min} = 2.2°
h = −12→12
k = −13→11
l = −16→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.131
S = 1.07
5120 reflections
247 parameters
390 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 6.2177P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −1.42 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in calculated positions and refined using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with displacement parameters 1.5 times U_{eq}(C). C—H distances for methylene groups were set to 0.97 Å and their U_{iso}(H) set to 1.2 times the U_{eq}(C). N—H distances for methylene groups were set to 0.89 Å and their U_{iso}(H) set to 1.2 times the U_{eq}(N).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3866 (10)	0.7344 (10)	0.3329 (9)	0.082 (3)	
H1A	0.465814	0.696964	0.284423	0.123*	
H1B	0.407495	0.704330	0.405591	0.123*	
H1C	0.372739	0.837455	0.326914	0.123*	
C2	0.2507 (8)	0.6784 (7)	0.3041 (7)	0.0558 (19)	
H2A	0.173933	0.708569	0.358127	0.067*	
H2B	0.221937	0.722091	0.235435	0.067*	
C3	0.2355 (13)	0.4747 (12)	0.4994 (6)	0.089 (3)	
H3A	0.142236	0.444258	0.496016	0.133*	
H3B	0.223962	0.575986	0.511236	0.133*	
H3C	0.284821	0.423647	0.557614	0.133*	
C4	0.3231 (8)	0.4433 (8)	0.3941 (5)	0.0545 (18)	
H4A	0.419740	0.466318	0.401386	0.065*	
H4B	0.331569	0.340956	0.382622	0.065*	
C5	0.1245 (7)	0.4757 (8)	0.2735 (5)	0.0514 (17)	
H5A	0.132528	0.371930	0.281572	0.062*	
H5B	0.051170	0.516084	0.326825	0.062*	
C6	0.0763 (8)	0.5190 (9)	0.1657 (6)	0.060 (2)	
H6A	0.063721	0.622981	0.158022	0.073*	
H6B	−0.016600	0.487290	0.157711	0.073*	
N1	0.2651 (5)	0.5211 (5)	0.2966 (4)	0.0394 (12)	
C7	0.714 (4)	−0.077 (3)	0.4663 (12)	0.073 (6)	0.553 (13)
H7A	0.635299	−0.063720	0.520053	0.110*	0.553 (13)
H7B	0.730646	−0.176329	0.446588	0.110*	0.553 (13)
H7C	0.799720	−0.052313	0.494931	0.110*	0.553 (13)
C8	0.6775 (13)	0.0172 (16)	0.3676 (9)	0.048 (3)	0.553 (13)
H8A	0.588856	−0.007556	0.341762	0.057*	0.553 (13)
H8B	0.657684	0.116019	0.389934	0.057*	0.553 (13)
C9	0.926 (2)	0.1786 (15)	0.3716 (14)	0.072 (5)	0.553 (13)
H9A	1.021730	0.188722	0.390221	0.108*	0.553 (13)
H9B	0.889663	0.258784	0.326183	0.108*	0.553 (13)
H9C	0.863855	0.175657	0.436148	0.108*	0.553 (13)
C10	0.9295 (11)	0.0413 (15)	0.3123 (12)	0.060 (4)	0.553 (13)
H10A	0.969293	−0.038212	0.358338	0.072*	0.553 (13)
H10B	0.995039	0.044716	0.248637	0.072*	0.553 (13)
C11	0.8223 (14)	−0.1326 (11)	0.2264 (10)	0.056 (3)	0.553 (13)
H11A	0.922980	−0.142333	0.200069	0.067*	0.553 (13)
H11B	0.813489	−0.206590	0.282200	0.067*	0.553 (13)
C12	0.7378 (10)	−0.1610 (8)	0.1385 (7)	0.064 (2)	0.553 (13)

H12A	0.785831	−0.246872	0.103918	0.076*	0.553 (13)
H12B	0.644811	−0.182497	0.169054	0.076*	0.553 (13)
N3	0.7854 (6)	0.0103 (6)	0.2774 (4)	0.0485 (13)	0.553 (13)
C7A	0.717 (5)	−0.036 (4)	0.4747 (16)	0.086 (10)	0.447 (13)
H7D	0.660368	0.008251	0.534889	0.129*	0.447 (13)
H7E	0.682484	−0.124036	0.459786	0.129*	0.447 (13)
H7F	0.816379	−0.055382	0.491673	0.129*	0.447 (13)
C8A	0.703 (2)	0.0650 (18)	0.3765 (11)	0.054 (4)	0.447 (13)
H8C	0.601901	0.086166	0.361723	0.065*	0.447 (13)
H8D	0.735526	0.154681	0.393546	0.065*	0.447 (13)
C9A	1.006 (2)	0.109 (2)	0.320 (2)	0.086 (6)	0.447 (13)
H9D	1.108561	0.084451	0.324111	0.129*	0.447 (13)
H9E	0.987038	0.186474	0.267480	0.129*	0.447 (13)
H9F	0.963054	0.138641	0.388936	0.129*	0.447 (13)
C10A	0.9423 (11)	−0.0202 (18)	0.2858 (17)	0.066 (4)	0.447 (13)
H10C	0.987562	−0.050771	0.216465	0.079*	0.447 (13)
H10D	0.963571	−0.098619	0.337960	0.079*	0.447 (13)
C11A	0.7214 (17)	−0.1211 (14)	0.2495 (9)	0.049 (3)	0.447 (13)
H11C	0.764720	−0.201795	0.292893	0.059*	0.447 (13)
H11D	0.618980	−0.105711	0.270666	0.059*	0.447 (13)
C12A	0.7378 (10)	−0.1610 (8)	0.1385 (7)	0.064 (2)	0.447 (13)
H12C	0.673030	−0.231003	0.129259	0.076*	0.447 (13)
H12D	0.835534	−0.209166	0.125144	0.076*	0.447 (13)
N3A	0.7854 (6)	0.0103 (6)	0.2774 (4)	0.0485 (13)	0.447 (13)
N2	0.1805 (6)	0.4578 (6)	0.0801 (4)	0.0433 (13)	
H2C	0.174767	0.515162	0.021306	0.052*	
H2D	0.159441	0.372377	0.063023	0.052*	
N4	0.7120 (7)	−0.0498 (6)	0.0565 (5)	0.0477 (14)	
H4C	0.627621	−0.054594	0.028690	0.057*	
H4D	0.781024	−0.062664	0.003613	0.057*	
Cl1	0.41595 (19)	0.15941 (18)	0.19230 (15)	0.0480 (4)	
Cl2	0.44096 (18)	0.68635 (17)	0.04175 (13)	0.0431 (4)	
Cl3	0.66065 (18)	0.41883 (19)	0.21743 (14)	0.0473 (4)	
Cl4	0.9546 (2)	0.2105 (2)	0.04702 (19)	0.0635 (5)	
Cd1	0.40910 (5)	0.43345 (5)	0.13790 (4)	0.03912 (14)	
Cd2	0.70911 (5)	0.17078 (5)	0.12779 (4)	0.04159 (15)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.085 (7)	0.066 (6)	0.097 (7)	−0.025 (5)	0.027 (6)	−0.028 (5)
C2	0.059 (5)	0.041 (4)	0.064 (4)	−0.002 (3)	0.017 (4)	−0.010 (3)
C3	0.109 (8)	0.107 (8)	0.044 (5)	−0.001 (6)	0.013 (5)	0.000 (5)
C4	0.056 (4)	0.064 (5)	0.042 (4)	−0.005 (4)	0.001 (3)	−0.002 (3)
C5	0.040 (4)	0.064 (4)	0.049 (4)	−0.008 (3)	0.013 (3)	−0.005 (3)
C6	0.040 (4)	0.068 (5)	0.068 (5)	0.007 (3)	0.001 (4)	0.001 (4)
N1	0.037 (3)	0.043 (3)	0.038 (3)	−0.007 (2)	0.004 (2)	−0.002 (2)
C7	0.102 (12)	0.076 (13)	0.043 (9)	−0.022 (11)	−0.010 (9)	0.023 (8)

C8	0.051 (6)	0.051 (7)	0.044 (6)	−0.018 (5)	−0.003 (5)	0.005 (5)
C9	0.076 (11)	0.056 (9)	0.091 (12)	−0.023 (8)	−0.033 (9)	−0.003 (8)
C10	0.057 (7)	0.059 (8)	0.055 (7)	0.024 (6)	−0.002 (6)	0.016 (6)
C11	0.065 (6)	0.039 (5)	0.058 (6)	0.007 (5)	−0.004 (5)	−0.001 (5)
C12	0.076 (5)	0.047 (4)	0.070 (4)	−0.014 (4)	−0.012 (4)	0.000 (3)
N3	0.063 (3)	0.039 (3)	0.042 (3)	0.001 (2)	−0.006 (3)	−0.001 (2)
C7A	0.109 (16)	0.080 (18)	0.061 (13)	0.007 (15)	0.009 (12)	0.006 (11)
C8A	0.065 (8)	0.049 (8)	0.049 (7)	−0.011 (7)	−0.007 (7)	0.005 (6)
C9A	0.082 (14)	0.087 (14)	0.093 (14)	−0.018 (11)	−0.018 (12)	−0.005 (12)
C10A	0.059 (7)	0.058 (8)	0.069 (8)	0.019 (7)	0.002 (7)	0.014 (7)
C11A	0.055 (6)	0.039 (6)	0.051 (6)	−0.008 (5)	0.006 (6)	−0.001 (5)
C12A	0.076 (5)	0.047 (4)	0.070 (4)	−0.014 (4)	−0.012 (4)	0.000 (3)
N3A	0.063 (3)	0.039 (3)	0.042 (3)	0.001 (2)	−0.006 (3)	−0.001 (2)
N2	0.044 (3)	0.043 (3)	0.044 (3)	−0.008 (2)	−0.001 (2)	−0.001 (2)
N4	0.054 (4)	0.045 (3)	0.042 (3)	0.001 (3)	−0.004 (3)	−0.005 (2)
Cl1	0.0453 (9)	0.0411 (8)	0.0549 (10)	−0.0014 (7)	0.0034 (8)	0.0047 (7)
Cl2	0.0476 (9)	0.0430 (8)	0.0370 (8)	−0.0030 (7)	0.0026 (7)	0.0002 (6)
Cl3	0.0386 (9)	0.0483 (9)	0.0544 (10)	0.0014 (7)	−0.0098 (7)	−0.0096 (7)
Cl4	0.0472 (10)	0.0562 (11)	0.0829 (14)	−0.0023 (8)	0.0150 (10)	0.0002 (10)
Cd1	0.0324 (3)	0.0429 (3)	0.0388 (3)	0.00378 (19)	0.00272 (19)	−0.00057 (19)
Cd2	0.0398 (3)	0.0354 (3)	0.0466 (3)	0.00223 (19)	0.0016 (2)	0.0013 (2)

Geometric parameters (Å, º)

C1—C2	1.512 (10)	C12—H12A	0.9700
C1—H1A	0.9600	C12—H12B	0.9700
C1—H1B	0.9600	N3—Cd2	2.427 (5)
C1—H1C	0.9600	C7A—C8A	1.516 (11)
C2—N1	1.473 (7)	C7A—H7D	0.9600
C2—H2A	0.9700	C7A—H7E	0.9600
C2—H2B	0.9700	C7A—H7F	0.9600
C3—C4	1.514 (9)	C8A—N3A	1.479 (9)
C3—H3A	0.9600	C8A—H8C	0.9700
C3—H3B	0.9600	C8A—H8D	0.9700
C3—H3C	0.9600	C9A—C10A	1.514 (12)
C4—N1	1.484 (8)	C9A—H9D	0.9600
C4—H4A	0.9700	C9A—H9E	0.9600
C4—H4B	0.9700	C9A—H9F	0.9600
C5—C6	1.465 (9)	C10A—N3A	1.467 (10)
C5—N1	1.488 (7)	C10A—H10C	0.9700
C5—H5A	0.9700	C10A—H10D	0.9700
C5—H5B	0.9700	C11A—C12A	1.436 (10)
C6—N2	1.473 (9)	C11A—N3A	1.508 (9)
C6—H6A	0.9700	C11A—H11C	0.9700
C6—H6B	0.9700	C11A—H11D	0.9700
N1—Cd1	2.419 (5)	C12A—N4	1.437 (9)
C7—C8	1.516 (11)	C12A—H12C	0.9700
C7—H7A	0.9600	C12A—H12D	0.9700

C7—H7B	0.9600	N3A—Cd2	2.427 (5)
C7—H7C	0.9600	N2—Cd1	2.282 (6)
C8—N3	1.455 (9)	N2—H2C	0.8900
C8—H8A	0.9700	N2—H2D	0.8900
C8—H8B	0.9700	N4—Cd2	2.285 (6)
C9—C10	1.507 (12)	N4—H4C	0.8900
C9—H9A	0.9600	N4—H4D	0.8900
C9—H9B	0.9600	Cl1—Cd1	2.6302 (17)
C9—H9C	0.9600	Cl1—Cd2	2.8227 (18)
C10—N3	1.514 (10)	Cl2—Cd1	2.6625 (17)
C10—H10A	0.9700	Cl2—Cd1^{i}	2.7509 (16)
C10—H10B	0.9700	Cl2—Cd2^{i}	2.8027 (17)
C11—C12	1.445 (10)	Cl3—Cd2	2.5952 (18)
C11—N3	1.495 (9)	Cl3—Cd1	2.5983 (18)
C11—H11A	0.9700	Cl4—Cd2	2.5158 (19)
C11—H11B	0.9700	Cd1—Cd2	3.4713 (8)
C12—N4	1.437 (9)		

C2—C1—H1A	109.5	C10A—C9A—H9D	109.5
C2—C1—H1B	109.5	C10A—C9A—H9E	109.5
H1A—C1—H1B	109.5	H9D—C9A—H9E	109.5
C2—C1—H1C	109.5	C10A—C9A—H9F	109.5
H1A—C1—H1C	109.5	H9D—C9A—H9F	109.5
H1B—C1—H1C	109.5	H9E—C9A—H9F	109.5
N1—C2—C1	114.4 (6)	N3A—C10A—C9A	112.3 (11)
N1—C2—H2A	108.7	N3A—C10A—H10C	109.1
C1—C2—H2A	108.7	C9A—C10A—H10C	109.1
N1—C2—H2B	108.7	N3A—C10A—H10D	109.1
C1—C2—H2B	108.7	C9A—C10A—H10D	109.1
H2A—C2—H2B	107.6	H10C—C10A—H10D	107.9
C4—C3—H3A	109.5	C12A—C11A—N3A	116.9 (8)
C4—C3—H3B	109.5	C12A—C11A—H11C	108.1
H3A—C3—H3B	109.5	N3A—C11A—H11C	108.1
C4—C3—H3C	109.5	C12A—C11A—H11D	108.1
H3A—C3—H3C	109.5	N3A—C11A—H11D	108.1
H3B—C3—H3C	109.5	H11C—C11A—H11D	107.3
N1—C4—C3	116.0 (6)	C11A—C12A—N4	118.4 (8)
N1—C4—H4A	108.3	C11A—C12A—H12C	107.7
C3—C4—H4A	108.3	N4—C12A—H12C	107.7
N1—C4—H4B	108.3	C11A—C12A—H12D	107.7
C3—C4—H4B	108.3	N4—C12A—H12D	107.7
H4A—C4—H4B	107.4	H12C—C12A—H12D	107.1
C6—C5—N1	114.4 (6)	C10A—N3A—C8A	114.8 (10)
C6—C5—H5A	108.7	C10A—N3A—C11A	112.0 (9)
N1—C5—H5A	108.7	C8A—N3A—C11A	106.0 (8)
C6—C5—H5B	108.7	C10A—N3A—Cd2	114.9 (9)
N1—C5—H5B	108.7	C8A—N3A—Cd2	107.9 (8)
H5A—C5—H5B	107.6	C11A—N3A—Cd2	99.9 (6)

C5—C6—N2	111.8 (6)	C6—N2—Cd1	109.8 (4)
C5—C6—H6A	109.3	C6—N2—H2C	109.7
N2—C6—H6A	109.3	Cd1—N2—H2C	109.7
C5—C6—H6B	109.3	C6—N2—H2D	109.7
N2—C6—H6B	109.3	Cd1—N2—H2D	109.7
H6A—C6—H6B	107.9	H2C—N2—H2D	108.2
C2—N1—C4	113.0 (5)	C12A—N4—Cd2	110.2 (4)
C2—N1—C5	110.5 (5)	C12—N4—Cd2	110.2 (4)
C4—N1—C5	110.6 (5)	C12—N4—H4C	109.6
C2—N1—Cd1	112.9 (4)	Cd2—N4—H4C	109.6
C4—N1—Cd1	109.5 (4)	C12—N4—H4D	109.6
C5—N1—Cd1	99.5 (4)	Cd2—N4—H4D	109.6
C8—C7—H7A	109.5	H4C—N4—H4D	108.1
C8—C7—H7B	109.5	Cd1—Cl1—Cd2	78.99 (5)
H7A—C7—H7B	109.5	Cd1—Cl2—Cd1^{i}	93.97 (5)
C8—C7—H7C	109.5	Cd1—Cl2—Cd2^{i}	128.87 (7)
H7A—C7—H7C	109.5	Cd1^{i}—Cl2—Cd2^{i}	77.36 (4)
H7B—C7—H7C	109.5	Cd2—Cl3—Cd1	83.89 (5)
N3—C8—C7	117.1 (11)	N2—Cd1—N1	78.02 (18)
N3—C8—H8A	108.0	N2—Cd1—Cl3	175.17 (15)
C7—C8—H8A	108.0	N1—Cd1—Cl3	97.32 (13)
N3—C8—H8B	108.0	N2—Cd1—Cl1	94.40 (15)
C7—C8—H8B	108.0	N1—Cd1—Cl1	95.61 (12)
H8A—C8—H8B	107.3	Cl3—Cd1—Cl1	87.24 (6)
C10—C9—H9A	109.5	N2—Cd1—Cl2	88.67 (14)
C10—C9—H9B	109.5	N1—Cd1—Cl2	98.15 (12)
H9A—C9—H9B	109.5	Cl3—Cd1—Cl2	90.80 (6)
C10—C9—H9C	109.5	Cl1—Cd1—Cl2	166.24 (5)
H9A—C9—H9C	109.5	N2—Cd1—Cl2^{i}	99.30 (14)
H9B—C9—H9C	109.5	N1—Cd1—Cl2^{i}	174.93 (12)
C9—C10—N3	115.6 (9)	Cl3—Cd1—Cl2^{i}	85.45 (5)
C9—C10—H10A	108.4	Cl1—Cd1—Cl2^{i}	80.24 (5)
N3—C10—H10A	108.4	Cl2—Cd1—Cl2^{i}	86.03 (5)
C9—C10—H10B	108.4	N2—Cd1—Cd2	136.10 (14)
N3—C10—H10B	108.4	N1—Cd1—Cd2	127.43 (12)
H10A—C10—H10B	107.4	Cl3—Cd1—Cd2	48.02 (4)
C12—C11—N3	117.2 (7)	Cl1—Cd1—Cd2	52.96 (4)
C12—C11—H11A	108.0	Cl2—Cd1—Cd2	116.86 (4)
N3—C11—H11A	108.0	Cl2^{i}—Cd1—Cd2	51.98 (4)
C12—C11—H11B	108.0	N4—Cd2—N3	78.04 (19)
N3—C11—H11B	108.0	N4—Cd2—N3A	78.04 (19)
H11A—C11—H11B	107.2	N4—Cd2—Cl4	95.52 (17)
N4—C12—C11	117.4 (8)	N3—Cd2—Cl4	98.54 (15)
N4—C12—H12A	108.0	N3A—Cd2—Cl4	98.54 (15)
C11—C12—H12A	108.0	N4—Cd2—Cl3	170.42 (17)
N4—C12—H12B	108.0	N3—Cd2—Cl3	102.29 (13)
C11—C12—H12B	108.0	N3A—Cd2—Cl3	102.29 (13)
H12A—C12—H12B	107.2	Cl4—Cd2—Cl3	93.90 (6)

C8—N3—C11	115.9 (8)	N4—Cd2—Cl2^{i}	93.02 (15)
C8—N3—C10	111.3 (8)	N3—Cd2—Cl2^{i}	164.69 (14)
C11—N3—C10	103.2 (7)	Cl4—Cd2—Cl2^{i}	94.66 (6)
C8—N3—Cd2	112.4 (7)	Cl3—Cd2—Cl2^{i}	84.45 (5)
C11—N3—Cd2	103.4 (5)	N4—Cd2—Cl1	87.06 (16)
C10—N3—Cd2	110.0 (6)	N3—Cd2—Cl1	90.86 (14)
C8A—C7A—H7D	109.5	N3A—Cd2—Cl1	90.86 (14)
C8A—C7A—H7E	109.5	Cl4—Cd2—Cl1	170.58 (6)
H7D—C7A—H7E	109.5	Cl3—Cd2—Cl1	83.36 (5)
C8A—C7A—H7F	109.5	Cl2^{i}—Cd2—Cl1	76.14 (5)
H7D—C7A—H7F	109.5	N4—Cd2—Cd1	123.88 (16)
H7E—C7A—H7F	109.5	N3—Cd2—Cd1	124.95 (13)
N3A—C8A—C7A	115.2 (11)	N3A—Cd2—Cd1	124.95 (13)
N3A—C8A—H8C	108.5	Cl4—Cd2—Cd1	124.18 (5)
C7A—C8A—H8C	108.5	Cl3—Cd2—Cd1	48.10 (4)
N3A—C8A—H8D	108.5	Cl2^{i}—Cd2—Cd1	50.65 (3)
C7A—C8A—H8D	108.5	Cl1—Cd2—Cd1	48.05 (4)
H8C—C8A—H8D	107.5		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*C*···Cl4^{i}	0.89	2.82	3.548 (6)	141
N2—H2*D*···Cl4^{ii}	0.89	2.63	3.407 (6)	146
N4—H4*D*···Cl4^{iii}	0.89	2.71	3.463 (6)	143

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) *x*−1, *y*, *z*; (iii) −*x*+2, −*y*, −*z*.