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Di-μ-chlorido-bis[chlorido(di-2-pyridylmethanediol-κ^3N,N',O)cadmium(II)] trihydrate

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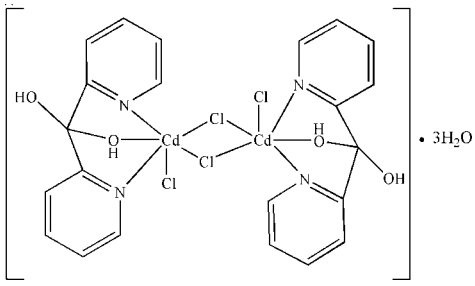
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.033; wR factor = 0.080; data-to-parameter ratio = 17.8.

In the title compound, $[Cd_2Cl_4(C_{11}H_{10}N_2O_2)_2]\cdot 3H_2O$, each metal atom is coordinated by an N,O,N'-chelated di-2-pyridylmethanediol ligand, two bridging chloride ligands and one terminal chloride ligand in a distorted octahedral geometry. Two isomers of centrosymmetric dinuclear complexes, α and β, are observed; the asymmetric unit contains two half-molecules of the complex and three water molecules. In the α isomer, the Cd···Cd distance and O—Cd—$Cl_{terminal}$ angle are 3.8048 (7) Å and 160.09 (5)°, respectively. In the β isomer, the same geometric parameters are 3.7281 (7) Å and 88.84 (6)°, respectively.

Related literature

One similar dinuclear Cd complex with Br has been reported by Zhu *et al.* (2000).



Experimental

Crystal data

$[Cd_2Cl_4(C_{11}H_{10}N_2O_2)_2]\cdot 3H_2O$
M_r = 825.07
Triclinic, $P\overline{1}$
a = 8.1634 (1) Å
b = 9.7180 (1) Å
c = 19.6761 (2) Å
α = 100.453 (7)°
β = 92.230 (11)°
γ = 106.272 (8)°
V = 1466.87 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.86 mm^{-1}
T = 293 (2) K
0.22 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.744, T_{max} = 0.989
(expected range = 0.519–0.689)
11364 measured reflections
6631 independent reflections
5655 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.080
S = 1.06
6631 reflections
373 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—Cl1	2.4983 (9)	Cd2—Cl3	2.4902 (10)
Cd1—O1	2.639 (2)	Cd2—O4	2.491 (2)
N2—Cd1—Cl1	109.16 (7)	N4—Cd2—Cl3	155.96 (8)
Cl1—Cd1—O1	160.09 (5)	Cl3—Cd2—O4	88.84 (6)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···O6^{i}	0.82	1.82	2.630 (3)	172
O2—H2A···O1^{ii}	0.82	2.01	2.818 (3)	171
O3—H3A···O7^{iii}	0.82	1.89	2.698 (5)	169
O4—H4B···O5	0.82	1.92	2.720 (4)	168
O5—H5B···Cl3^{iv}	0.84 (4)	2.66 (5)	3.324 (5)	137 (4)
O6—H6···Cl1	0.85 (4)	2.54 (5)	3.262 (3)	144 (5)
O6—H6B···Cl1^{v}	0.85 (4)	2.56 (4)	3.392 (3)	169 (4)
O7—H7C···Cl3^{vi}	0.85 (4)	2.50 (4)	3.308 (4)	159 (6)
O7—H7B···O5^{vi}	0.85 (5)	2.09 (5)	2.932 (6)	172 (6)

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: CV2294).

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Rigaku (2000). *CrystalClear*. Version 1.3. Rigaku Corporation, Tokyo, Japan.
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supplementary materials

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Di-μ-chlorido-bis[chlorido(di-2-pyridylmethanediol-κ^3N,N',O)cadmium(II)] trihydrate

Y.-M. Li, J.-L. Zhang and X.-W. Zhao

Comment

The coordination behavior of di-2-pyridylketone [$(C_5H_4N)_2CO$, dpk] and its hydrolyzed derivative, di-2-pyridylmethanediol [$(C_5H_4N)_2C(OH)_2$, dpd], have attracted much attention. Based on dpd, one dinuclear cadmium complex with Br has been reported (Zhu *et al.*, 2000). Herein we present the similar dinuclear cadmium compoud with Cl - the title compound, (I).

The structure of (I) contains two kinds of neutral conformational isomers, α-$Cd_2(C_{11}H_{10}N_2O_2)_2Cl_4$ and β-$Cd_2(C_{11}H_{10}N_2O_2)_2Cl_4$, and crystalline water molecules (Fig. 1). Each isomer is centrosymmetric. Both of them contain di-2-chloro bridging between the two metal atoms, and each metal atom is also bonded to a terminal chloro ligand and capped by the organic dpd ligand in an *N*,*N*′,*O* -tridentate mode, resulting in a distorted octahedral coordination environment. In α isomer, the terminal chloro atom is *trans* oriented to the oxygen atom of dpd with respect to the bridge plane and the Cl1—Cd1—O1 angle is 160.09 (5) ° (Table 1), while the Cl3—Cd2—O4 angle is 88.84 (6) ° in β isomer. The Cd···Cd distances are 3.8048 (7) and 3.7281 (7) Å, respectively, in α- and β-isomers.

The crystal structure is stabilized by O—H···O and O—H···Cl hydrogen bonds (Table 2, Fig. 2) involving the hydroxyl groups, crystalline water molecules and terminal Cl ligands.

Experimental

The title compound was synthesized by refluxing a 20 ml EtOH/H_2O solution (3:1, *v*/*v*) of $CdCl_2·2.5H_2O$ (0.458 g, 2 mmol), di-2-pyridylketone (0.185 g, 1 mmol) for 1 h with stirring. After cooling, the solution was filtered. Colourless prism crystals of (I) were obtained by slow evaporation of the colourless filtrate for several days. Yield: 60.6% based on di-2-pyridylketone (0.250 g). (Anal. Calcd. for $C_{22}H_{26}Cd_2Cl_4N_4O_7$: C, 32.03; H, 3.18; N 6.79. Found: C, 31.89; H, 3.23; N 6.65%). IR (KBr pellet, cm^{-1}): *ν*(OH) 3430, *ν*(C–O) 1600, *ν*(C═N, C═C) 1467, 1441, 1384.

Refinement

The C-bound H-atoms were positioned geometrically (C—H 0.93 Å), and treated as riding with $U_{iso}(H) = 1.2\ U_{eq}(C)$. H atoms of the water molecules were located in a difference Fourier map and isotropically refined with the O—H distance restrained to 0.85 (4) Å. The hydroxy H atoms were positioned geometrically (O—H 0.82 Å), and treated as riding with $U_{iso}(H) = 1.5\ U_{eq}(O)$.

Figures

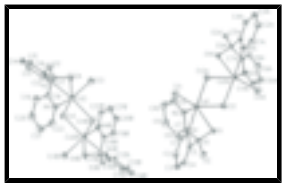


Fig. 1. The molecular structure of (I) showing the atomic numbering and 30% probability displacement ellipsoids [symmetry codes: (A) −*x*, −*y*, −*z*; (B) 2 − *x*, 1 − *y*, 1 − *z*]. The crystalline water molecules and H-atoms omitted for clarity.

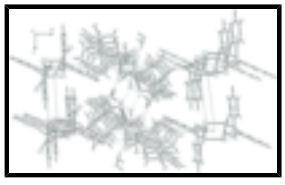


Fig. 2. A view of the crystal packing along the *b* axis. Hydrogen bonds are shown as dashed lines.

Di-μ-chlorido-bis[chlorido(di-2-pyridylmethanediol-κ^3*N*,*N*',*O*)cadmium(II)] trihydrate

Crystal data

$[Cd_2Cl_4(C_{11}H_{10}N_2O_2)_2]\cdot 3H_2O$	$Z = 2$
$M_r = 825.07$	$F_{000} = 812$
Triclinic, $P\overline{1}$	$D_x = 1.868$ Mg m^{-3}
$a = 8.1634$ (1) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 9.7180$ (1) Å	Cell parameters from 3698 reflections
$c = 19.6761$ (2) Å	$\theta = 3.2$–27.5º
$\alpha = 100.453$ (7)º	$\mu = 1.86$ mm^{-1}
$\beta = 92.230$ (11)º	$T = 293$ (2) K
$\gamma = 106.272$ (8)º	Prism, colourless
$V = 1466.87$ (8) Å^3	0.22 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer	6631 independent reflections
Radiation source: fine-focus sealed tube	5655 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 293$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.2$º
Absorption correction: multi-scan (CrystalClear; Rigaku, 2000)	$h = -10\rightarrow7$
$T_{min} = 0.744$, $T_{max} = 0.989$	$k = -11\rightarrow12$
11364 measured reflections	$l = -25\rightarrow25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.033$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.080$	$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 0.9676P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.004$
6631 reflections	$\Delta\rho_{max} = 0.78$ e Å^{-3}
373 parameters	$\Delta\rho_{min} = -0.80$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.12516 (3)	0.16234 (2)	0.069775 (11)	0.03408 (7)
Cd2	0.88520 (3)	0.34097 (3)	0.537679 (12)	0.04439 (8)
Cl1	0.34946 (12)	0.07703 (10)	0.12495 (5)	0.0496 (2)
Cl2	0.12820 (12)	0.08617 (8)	−0.06028 (4)	0.0454 (2)
Cl3	0.90828 (13)	0.13407 (11)	0.44696 (5)	0.0555 (2)
Cl4	1.19742 (11)	0.50737 (11)	0.55079 (4)	0.0497 (2)
C1	0.4615 (4)	0.4596 (4)	0.09048 (18)	0.0413 (7)
H9A	0.5216	0.3906	0.0833	0.050*
C2	0.5530 (4)	0.6055 (4)	0.10414 (19)	0.0462 (8)
H11A	0.6720	0.6344	0.1059	0.055*
C3	0.4642 (4)	0.7079 (4)	0.11517 (18)	0.0423 (7)
H16A	0.5227	0.8073	0.1245	0.051*
C4	0.2877 (4)	0.6612 (3)	0.11222 (16)	0.0344 (6)
H17A	0.2258	0.7288	0.1199	0.041*
C5	0.2041 (3)	0.5132 (3)	0.09775 (13)	0.0261 (5)
C6	0.0099 (3)	0.4529 (3)	0.09272 (14)	0.0258 (5)
C7	−0.0475 (4)	0.3887 (3)	0.15610 (14)	0.0278 (6)
C8	−0.1184 (4)	0.4594 (4)	0.20905 (16)	0.0383 (7)
H12A	−0.1306	0.5513	0.2079	0.046*
C9	−0.1709 (5)	0.3918 (4)	0.26377 (17)	0.0493 (9)
H10A	−0.2176	0.4379	0.3004	0.059*
C10	−0.1529 (5)	0.2552 (5)	0.26312 (19)	0.0571 (10)

H6A	−0.1893	0.2063	0.2988	0.068*
C11	−0.0806 (6)	0.1923 (4)	0.20897 (19)	0.0555 (10)
H2B	−0.0692	0.0996	0.2087	0.067*
C12	1.0703 (4)	0.2108 (4)	0.65684 (18)	0.0434 (7)
H7A	1.1651	0.2332	0.6317	0.052*
C13	1.0857 (5)	0.1573 (4)	0.71639 (18)	0.0474 (8)
H13A	1.1885	0.1435	0.7312	0.057*
C14	0.9443 (5)	0.1247 (4)	0.75334 (18)	0.0476 (8)
H8A	0.9519	0.0919	0.7946	0.057*
C15	0.7918 (5)	0.1410 (4)	0.72893 (17)	0.0439 (8)
H15A	0.6946	0.1165	0.7525	0.053*
C16	0.7863 (4)	0.1945 (3)	0.66889 (15)	0.0360 (7)
C17	0.6250 (4)	0.2239 (4)	0.64035 (16)	0.0403 (7)
C18	0.6458 (4)	0.3874 (4)	0.65905 (16)	0.0376 (7)
C19	0.5705 (5)	0.4500 (4)	0.71349 (18)	0.0491 (8)
H5A	0.5014	0.3921	0.7403	0.059*
C20	0.5994 (5)	0.5989 (5)	0.7273 (2)	0.0571 (10)
H4A	0.5507	0.6435	0.7637	0.069*
C21	0.7017 (6)	0.6814 (5)	0.6863 (2)	0.0626 (11)
H1A	0.7212	0.7823	0.6940	0.075*
C22	0.7744 (6)	0.6122 (5)	0.6337 (2)	0.0588 (10)
H3B	0.8445	0.6683	0.6066	0.071*
N1	0.2894 (3)	0.4120 (3)	0.08710 (13)	0.0313 (5)
N2	−0.0253 (4)	0.2578 (3)	0.15643 (13)	0.0371 (6)
N3	0.9250 (4)	0.2317 (3)	0.63383 (13)	0.0392 (6)
N4	0.7482 (4)	0.4674 (3)	0.62011 (15)	0.0461 (7)
O1	−0.0368 (3)	0.3405 (2)	0.03214 (10)	0.0312 (4)
H1B	−0.1361	0.2908	0.0325	0.047*
O2	−0.0707 (3)	0.5609 (2)	0.08952 (11)	0.0346 (5)
H2A	−0.0454	0.5959	0.0551	0.052*
O3	0.4792 (3)	0.1514 (3)	0.66786 (13)	0.0513 (6)
H3A	0.4639	0.0629	0.6571	0.077*
O4	0.6143 (3)	0.1775 (3)	0.56695 (11)	0.0463 (6)
H4B	0.5195	0.1736	0.5499	0.069*
O5	0.3165 (5)	0.1509 (6)	0.4914 (2)	0.0882 (11)
H5	0.323 (9)	0.241 (2)	0.504 (3)	0.12 (3)*
H5B	0.219 (3)	0.094 (5)	0.494 (3)	0.10 (3)*
O6	0.6482 (4)	0.1664 (3)	0.02199 (17)	0.0596 (7)
H6	0.612 (7)	0.137 (6)	0.0581 (18)	0.11 (3)*
H6B	0.646 (7)	0.096 (4)	−0.011 (2)	0.11 (2)*
O7	0.4677 (5)	0.8691 (4)	0.62350 (19)	0.0735 (9)
H7C	0.369 (4)	0.844 (8)	0.601 (3)	0.14 (3)*
H7B	0.530 (10)	0.855 (10)	0.591 (3)	0.17 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03876 (13)	0.02852 (11)	0.03738 (12)	0.01258 (9)	0.00889 (9)	0.00729 (9)

Cd2	0.04591 (15)	0.05942 (17)	0.03354 (13)	0.01892 (12)	0.01373 (10)	0.01615 (11)
Cl1	0.0498 (5)	0.0502 (5)	0.0578 (5)	0.0239 (4)	0.0051 (4)	0.0190 (4)
Cl2	0.0534 (5)	0.0352 (4)	0.0396 (4)	−0.0006 (3)	0.0168 (4)	0.0065 (3)
Cl3	0.0609 (6)	0.0567 (5)	0.0496 (5)	0.0190 (4)	0.0167 (4)	0.0072 (4)
Cl4	0.0445 (5)	0.0677 (6)	0.0401 (4)	0.0151 (4)	0.0053 (3)	0.0207 (4)
C1	0.0272 (15)	0.0465 (18)	0.057 (2)	0.0179 (14)	0.0084 (14)	0.0147 (15)
C2	0.0229 (15)	0.052 (2)	0.061 (2)	0.0038 (14)	0.0080 (14)	0.0173 (17)
C3	0.0339 (17)	0.0360 (17)	0.054 (2)	0.0022 (13)	0.0032 (14)	0.0130 (14)
C4	0.0340 (15)	0.0299 (14)	0.0400 (16)	0.0105 (12)	0.0053 (13)	0.0061 (12)
C5	0.0243 (13)	0.0295 (13)	0.0259 (13)	0.0084 (11)	0.0041 (10)	0.0081 (10)
C6	0.0267 (13)	0.0261 (13)	0.0270 (13)	0.0109 (11)	0.0043 (10)	0.0061 (10)
C7	0.0248 (13)	0.0312 (14)	0.0273 (13)	0.0068 (11)	0.0037 (11)	0.0074 (11)
C8	0.0411 (17)	0.0418 (17)	0.0362 (16)	0.0185 (14)	0.0108 (13)	0.0067 (13)
C9	0.053 (2)	0.066 (2)	0.0335 (17)	0.0239 (18)	0.0173 (15)	0.0089 (16)
C10	0.071 (3)	0.071 (3)	0.0400 (19)	0.025 (2)	0.0247 (18)	0.0274 (18)
C11	0.081 (3)	0.051 (2)	0.049 (2)	0.029 (2)	0.023 (2)	0.0278 (17)
C12	0.0378 (18)	0.0492 (19)	0.0459 (18)	0.0172 (15)	0.0091 (14)	0.0083 (15)
C13	0.053 (2)	0.050 (2)	0.049 (2)	0.0278 (17)	0.0050 (16)	0.0127 (16)
C14	0.065 (2)	0.0461 (19)	0.0416 (18)	0.0259 (17)	0.0062 (17)	0.0171 (15)
C15	0.052 (2)	0.0460 (19)	0.0406 (17)	0.0201 (16)	0.0167 (15)	0.0148 (14)
C16	0.0388 (17)	0.0394 (16)	0.0323 (15)	0.0141 (14)	0.0103 (13)	0.0080 (12)
C17	0.0359 (17)	0.0533 (19)	0.0336 (15)	0.0144 (15)	0.0119 (13)	0.0096 (14)
C18	0.0332 (16)	0.0513 (19)	0.0330 (15)	0.0178 (14)	0.0051 (12)	0.0114 (13)
C19	0.045 (2)	0.064 (2)	0.0419 (18)	0.0218 (18)	0.0113 (15)	0.0092 (16)
C20	0.056 (2)	0.070 (3)	0.050 (2)	0.031 (2)	0.0089 (18)	0.0038 (19)
C21	0.070 (3)	0.055 (2)	0.068 (3)	0.029 (2)	0.004 (2)	0.010 (2)
C22	0.068 (3)	0.059 (2)	0.059 (2)	0.025 (2)	0.016 (2)	0.0250 (19)
N1	0.0268 (12)	0.0321 (12)	0.0392 (13)	0.0140 (10)	0.0066 (10)	0.0084 (10)
N2	0.0449 (15)	0.0359 (13)	0.0357 (13)	0.0155 (12)	0.0121 (11)	0.0132 (11)
N3	0.0405 (15)	0.0449 (15)	0.0354 (13)	0.0156 (12)	0.0108 (11)	0.0100 (11)
N4	0.0534 (18)	0.0530 (17)	0.0403 (15)	0.0225 (14)	0.0147 (13)	0.0177 (13)
O1	0.0290 (10)	0.0350 (10)	0.0278 (10)	0.0071 (8)	0.0040 (8)	0.0048 (8)
O2	0.0330 (11)	0.0394 (11)	0.0423 (12)	0.0212 (9)	0.0114 (9)	0.0174 (9)
O3	0.0374 (13)	0.0594 (15)	0.0582 (15)	0.0116 (11)	0.0201 (11)	0.0154 (12)
O4	0.0367 (13)	0.0643 (16)	0.0358 (12)	0.0143 (11)	0.0071 (10)	0.0045 (11)
O5	0.0504 (19)	0.134 (4)	0.094 (3)	0.031 (2)	0.0098 (19)	0.049 (3)
O6	0.0455 (15)	0.0456 (15)	0.076 (2)	0.0007 (12)	0.0092 (14)	0.0007 (14)
O7	0.073 (2)	0.069 (2)	0.068 (2)	0.0071 (18)	−0.0006 (18)	0.0113 (16)

Geometric parameters (Å, °)

Cd1—N2	2.346 (3)	C11—N2	1.339 (4)
Cd1—N1	2.375 (2)	C11—H2B	0.9300
Cd1—Cl1	2.4983 (9)	C12—N3	1.334 (4)
Cd1—O1	2.639 (2)	C12—C13	1.380 (5)
Cd1—Cl2	2.5348 (8)	C12—H7A	0.9300
Cd1—Cl2^{i}	2.6744 (8)	C13—C14	1.381 (5)
Cd2—N4	2.362 (3)	C13—H13A	0.9300
Cd2—N3	2.385 (3)	C14—C15	1.377 (5)

Cd2—Cl3	2.4902 (10)	C14—H8A	0.9300
Cd2—O4	2.491 (2)	C15—C16	1.378 (4)
Cd2—Cl4	2.5818 (10)	C15—H15A	0.9300
Cd2—Cl4^{ii}	2.6560 (9)	C16—N3	1.346 (4)
Cl2—Cd1^{i}	2.6744 (8)	C16—C17	1.531 (5)
Cl4—Cd2^{ii}	2.6560 (9)	C17—O3	1.387 (4)
C1—N1	1.345 (4)	C17—O4	1.424 (4)
C1—C2	1.376 (5)	C17—C18	1.523 (5)
C1—H9A	0.9300	C18—N4	1.339 (4)
C2—C3	1.378 (5)	C18—C19	1.386 (5)
C2—H11A	0.9300	C19—C20	1.373 (6)
C3—C4	1.380 (4)	C19—H5A	0.9300
C3—H16A	0.9300	C20—C21	1.380 (6)
C4—C5	1.379 (4)	C20—H4A	0.9300
C4—H17A	0.9300	C21—C22	1.376 (6)
C5—N1	1.348 (3)	C21—H1A	0.9300
C5—C6	1.521 (4)	C22—N4	1.337 (5)
C6—O2	1.396 (3)	C22—H3B	0.9300
C6—O1	1.420 (3)	O1—H1B	0.8200
C6—C7	1.526 (4)	O2—H2A	0.8200
C7—N2	1.336 (4)	O3—H3A	0.8200
C7—C8	1.379 (4)	O4—H4B	0.8200
C8—C9	1.382 (5)	O5—H5	0.85 (4)
C8—H12A	0.9300	O5—H5B	0.84 (3)
C9—C10	1.374 (5)	O6—H6	0.85 (4)
C9—H10A	0.9300	O6—H6B	0.85 (4)
C10—C11	1.369 (5)	O7—H7C	0.85 (4)
C10—H6A	0.9300	O7—H7B	0.85 (5)
N2—Cd1—N1	81.85 (8)	C9—C10—H6A	120.6
N2—Cd1—Cl1	109.16 (7)	N2—C11—C10	123.1 (3)
N1—Cd1—Cl1	96.06 (6)	N2—C11—H2B	118.4
N2—Cd1—Cl2	143.92 (7)	C10—C11—H2B	118.4
N1—Cd1—Cl2	100.22 (6)	N3—C12—C13	122.7 (3)
Cl1—Cd1—Cl2	106.43 (3)	N3—C12—H7A	118.6
N2—Cd1—O1	65.70 (7)	C13—C12—H7A	118.6
N1—Cd1—O1	64.51 (7)	C12—C13—C14	118.1 (3)
Cl1—Cd1—O1	160.09 (5)	C12—C13—H13A	120.9
Cl2—Cd1—O1	82.55 (5)	C14—C13—H13A	120.9
N2—Cd1—Cl2^{i}	84.56 (7)	C15—C14—C13	119.8 (3)
N1—Cd1—Cl2^{i}	164.27 (6)	C15—C14—H8A	120.1
Cl1—Cd1—Cl2^{i}	95.85 (3)	C13—C14—H8A	120.1
Cl2—Cd1—Cl2^{i}	86.19 (3)	C14—C15—C16	118.7 (3)
O1—Cd1—Cl2^{i}	102.56 (5)	C14—C15—H15A	120.7
N4—Cd2—N3	80.74 (9)	C16—C15—H15A	120.7
N4—Cd2—Cl3	155.96 (8)	N3—C16—C15	122.1 (3)
N3—Cd2—Cl3	95.66 (7)	N3—C16—C17	115.8 (3)
N4—Cd2—O4	67.82 (9)	C15—C16—C17	122.1 (3)

N3—Cd2—O4	66.64 (9)	O3—C17—O4	111.8 (3)
Cl3—Cd2—O4	88.84 (6)	O3—C17—C18	108.1 (3)
N4—Cd2—Cl4	104.22 (8)	O4—C17—C18	110.1 (3)
N3—Cd2—Cl4	94.53 (7)	O3—C17—C16	112.1 (3)
Cl3—Cd2—Cl4	99.75 (3)	O4—C17—C16	105.7 (2)
O4—Cd2—Cl4	160.13 (6)	C18—C17—C16	109.1 (3)
N4—Cd2—Cl4^{ii}	86.73 (7)	N4—C18—C19	122.3 (3)
N3—Cd2—Cl4^{ii}	167.44 (7)	N4—C18—C17	114.6 (3)
Cl3—Cd2—Cl4^{ii}	95.49 (3)	C19—C18—C17	123.1 (3)
O4—Cd2—Cl4^{ii}	107.86 (6)	C20—C19—C18	118.9 (3)
Cl4—Cd2—Cl4^{ii}	89.25 (3)	C20—C19—H5A	120.5
Cd1—Cl2—Cd1^{i}	93.81 (3)	C18—C19—H5A	120.5
Cd2—Cl4—Cd2^{ii}	90.75 (3)	C19—C20—C21	119.0 (4)
N1—C1—C2	123.1 (3)	C19—C20—H4A	120.5
N1—C1—H9A	118.4	C21—C20—H4A	120.5
C2—C1—H9A	118.4	C22—C21—C20	118.9 (4)
C1—C2—C3	118.5 (3)	C22—C21—H1A	120.5
C1—C2—H11A	120.7	C20—C21—H1A	120.5
C3—C2—H11A	120.7	N4—C22—C21	122.6 (4)
C2—C3—C4	119.3 (3)	N4—C22—H3B	118.7
C2—C3—H16A	120.4	C21—C22—H3B	118.7
C4—C3—H16A	120.4	C1—N1—C5	117.8 (3)
C5—C4—C3	119.2 (3)	C1—N1—Cd1	124.7 (2)
C5—C4—H17A	120.4	C5—N1—Cd1	117.38 (18)
C3—C4—H17A	120.4	C7—N2—C11	118.0 (3)
N1—C5—C4	122.1 (3)	C7—N2—Cd1	118.51 (18)
N1—C5—C6	115.4 (2)	C11—N2—Cd1	123.4 (2)
C4—C5—C6	122.5 (2)	C12—N3—C16	118.6 (3)
O2—C6—O1	111.5 (2)	C12—N3—Cd2	126.5 (2)
O2—C6—C5	112.1 (2)	C16—N3—Cd2	114.8 (2)
O1—C6—C5	105.9 (2)	C22—N4—C18	118.3 (3)
O2—C6—C7	106.8 (2)	C22—N4—Cd2	125.1 (2)
O1—C6—C7	109.6 (2)	C18—N4—Cd2	116.5 (2)
C5—C6—C7	110.9 (2)	C6—O1—Cd1	98.73 (14)
N2—C7—C8	122.2 (3)	C6—O1—H1B	109.5
N2—C7—C6	115.0 (2)	Cd1—O1—H1B	99.5
C8—C7—C6	122.8 (3)	C6—O2—H2A	109.5
C7—C8—C9	119.1 (3)	C17—O3—H3A	109.5
C7—C8—H12A	120.5	C17—O4—Cd2	101.91 (18)
C9—C8—H12A	120.5	C17—O4—H4B	109.5
C10—C9—C8	118.8 (3)	Cd2—O4—H4B	122.8
C10—C9—H10A	120.6	H5—O5—H5B	113 (6)
C8—C9—H10A	120.6	H6—O6—H6B	112 (5)
C11—C10—C9	118.8 (3)	H7C—O7—H7B	101 (7)
C11—C10—H6A	120.6		

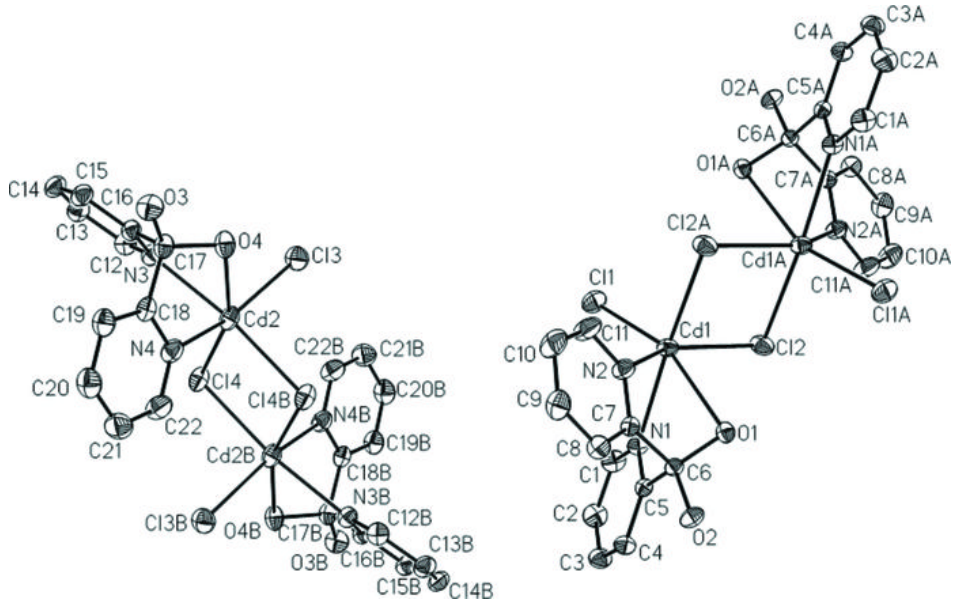
Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1B···O6^{iii}	0.82	1.82	2.630 (3)	172
O2—H2A···O1^{iv}	0.82	2.01	2.818 (3)	171
O3—H3A···O7^{v}	0.82	1.89	2.698 (5)	169
O4—H4B···O5	0.82	1.92	2.720 (4)	168
O5—H5B···Cl3^{vi}	0.84 (4)	2.66 (5)	3.324 (5)	137 (4)
O6—H6···Cl1	0.85 (4)	2.54 (5)	3.262 (3)	144 (5)
O6—H6B···Cl1^{vii}	0.85 (4)	2.56 (4)	3.392 (3)	169 (4)
O7—H7C···Cl3^{viii}	0.85 (4)	2.50 (4)	3.308 (4)	159 (6)
O7—H7B···O5^{viii}	0.85 (5)	2.09 (5)	2.932 (6)	172 (6)

Symmetry codes: (iii) $x-1, y, z$; (iv) $-x, -y+1, -z$; (v) $x, y-1, z$; (vi) $-x+1, -y, -z+1$; (vii) $-x+1, -y, -z$; (viii) $-x+1, -y+1, -z+1$.

Fig. 1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Cd2B
C18B
N3B
Cl3B
O4B
C17B
C12B
C13B
O3B
C16B
C15B
C14B

Fig. 2