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Bis(μ-*N*,2-di-3-pyridylisoindoline-1-imine-κ²*N*,*N*′)bis[aqua(perchlorato-κ*O*)-cadmium(II)] bis(perchlorate) methanol disolvate

Li-Na Zhu,[a] Shan Gao[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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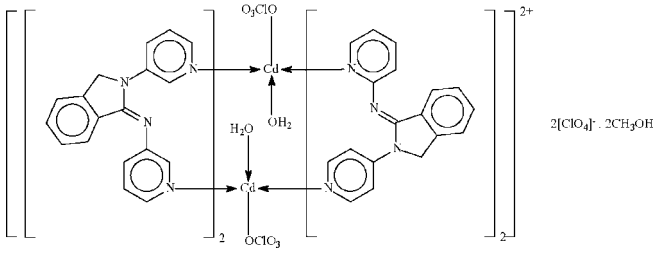
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.008 Å; R factor = 0.056; wR factor = 0.181; data-to-parameter ratio = 16.7.

The dinuclear dication in the title compound, $[Cd_2(ClO_4)_2(C_{17}H_{14}N_4)_4(H_2O)_2](ClO_4)_2\cdot 2CH_4O$, lies on a twofold rotation axis as the two *N*,2-di-3-pyridylisoindoline-1-imine *N*-heterocycles function in μ_2-bridging modes. Aside from the four N atoms, the Cd atom is also linked to the water and perchlorate O atoms, the O atoms being *cis* to each other in an octahedral geometry. The charge is balanced by two perchlorate ions; these interact weakly with the coordinated water and uncoordinated methanol molecules.

Related literature

For the only reference in the literature to *N*-[2,3-dihydro-2-(3-pyridinyl)-1*H*-isoindol-1-ylidene]-3-pyridinamine, see Vanden Eynde *et al.* (1992). The title compound was synthesized using the same procedure as for the 4-pyridyl analogue (Mulyana *et al.*, 2005); Mulyana *et al.* (2005) also report the crystal structure of the ethanol-coordinated $Cd(NO_3)_2$ adduct.



Experimental

Crystal data

$[Cd_2(ClO_4)_2(C_{17}H_{14}N_4)_4(H_2O)_2](ClO_4)_2\cdot 2CH_4O$
M_r = 1868.04
Orthorhombic, *Pbcn*
a = 21.0869 (6) Å
b = 14.8065 (4) Å
c = 24.5650 (6) Å
V = 7669.8 (4) Å³
Z = 4
Mo $K\alpha$ radiation
μ = 0.78 mm⁻¹
T = 295 (2) K
0.31 × 0.26 × 0.23 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.399, T_{max} = 0.842
70672 measured reflections
8748 independent reflections
4867 reflections with $I > 2\sigma(I)$
R_{int} = 0.077

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.181
S = 1.09
8748 reflections
525 parameters
17 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å⁻³
$\Delta\rho_{min}$ = −0.92 e Å⁻³

Table 1
Selected bond lengths (Å).

Cd1—O1	2.442 (3)	Cd1—N4^{i}	2.343 (4)
Cd1—O1*w*	2.306 (3)	Cd1—N5	2.378 (4)
Cd1—N1	2.354 (4)	Cd1—N8^{i}	2.319 (4)

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O3^{ii}	0.85	2.11	2.945 (6)	167
O1*W*—H1*W*2···O9	0.85	1.83	2.665 (7)	167
O9—H9*O*···O5	0.85	2.32	2.959 (9)	132

Symmetry code: (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2328).

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supplementary materials

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Bis(μ-*N*,2-di-3-pyridylisoindoline-1-imine-$\kappa^2 N,N'$)bis[aqua(perchlorato-κO)cadmium(II)] bis(perchlorate) methanol disolvate

L.-N. Zhu, S. Gao and S. W. Ng

Comment

The *N*-[2,3-dihydro-2-(4-pyridinyl)-1*H*-isoindol-1-ylidene]-4-pyridinamine *N*-heterocycle forms an ethanol-coordinated adduct with cadmium dinitrate; the compound exists as a linear chain as the ligand functions as a bridge through its pyridyl *N*-atoms (Mulyana *et al.*, 2005). *N*-[2,3-Dihydro-2-(3-pyridinyl)-1*H*-isoindol-1-ylidene]-3-pyridinamine forms a 2:1 adduct with cadmium perchlorate, but the position of the donor pyridyl *N*-atoms restricts the formation of a chain structure.

The dinuclear dication in $[Cd_2(C_{17}H_{14}N_4)_4(H_2O)_2(ClO_4)_2]\,2[ClO_4]\cdot 2(CH_3OH)$ lies about a twofold rotation axis. Aside from the four N atoms, the Cd is also linked to the water and perchlorate O atoms, the O atoms being *cis* to each other in the octahedral geometry (Table 1). The charge is balanced by two perchlorate ions; these interact weakly with the coordinated water and free methanol molecules (Table 2).

Experimental

The ligand was synthesized from *o*-phthalaldehyde and 3-aminopyridine (in place of 4-aminopyridine) according to the procedure described by Mulyana *et al.* (2005). An aqueous solution (5 ml) of cadmium perchlorate hexahydrate (0.210 g, 0.5 mmol) was added dropwise to an methanol solution (15 ml) containing *N*-[2,3-dihydro-2-(3-pyridinyl)-1*H*-isoindol-1-ylidene]-3-pyridinamine (0.286 g, 1 mmol). The resulting mixture was heated for 0.5 h. Colorless prismatic crystals were obtained from the solution after several days.

Refinement

The Cl–O distance in the free perchlorate was refined with a distance restraint of Cl–O = 1.440±0.005 Å and the C–O distance in the methanol molecule was restrained to 1.450±0.005 Å (somewhat tight restraints were used). The anisotropic displacement parameters of the methanol atoms were restrained to be nearly isotropic.

The carbon-bound H atoms were generated geometrically (C–H 0.93 – 0.96 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5U_{eq}(C). The water and methanolic H atoms were placed in chemically sensible positions on the basis of hydrogen bonding interactions but they were not refined; U(H) was set to 1.5U_{eq}(O).

Figures

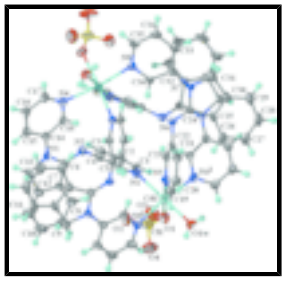


Fig. 1. Thermal ellipsoid plot of the dinuclear dication (the free perchlorate and methanol are omitted). Displacement ellipsoids are drawn at the 30% probability level, and H atoms are drawn as spheres of arbitrary radii. Symmetry code $i = 1 - x, y, 3/2 - z$.

Bis(μ-*N*,2-di-3-pyridylisoindoline-1-imine-κ^2*N*,*N*')bis[aqua(perchlorato-\ κ*O*)cadmium(II)] bis(perchlorate) methanol disolvate

Crystal data

$[Cd_2(ClO_4)_2(C_{17}H_{14}N_4)_4(H_2O)_2](ClO_4)_2{\cdot}2CH_4O$	$F_{000} = 3792$
$M_r = 1868.04$	$D_x = 1.618$ Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 36081 reflections
$a = 21.0869$ (6) Å	θ = 3.0–27.5º
$b = 14.8065$ (4) Å	μ = 0.78 mm^{-1}
$c = 24.5650$ (6) Å	$T = 295$ (2) K
$V = 7669.8$ (4) Å^3	Prism, colorless
$Z = 4$	0.31 × 0.26 × 0.23 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer	8748 independent reflections
Radiation source: fine-focus sealed tube	4867 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.077$
$T = 295(2)$ K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -27\rightarrow27$
$T_{min} = 0.399$, $T_{max} = 0.842$	$k = -19\rightarrow17$
70672 measured reflections	$l = -31\rightarrow31$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.056$	H-atom parameters constrained
$wR(F^2) = 0.181$	$w = 1/[\sigma^2(F_o^2) + (0.0926P)^2 + 0.6395P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
8748 reflections	$\Delta\rho_{max} = 0.82$ e Å^{-3}
525 parameters	$\Delta\rho_{min} = -0.92$ e Å^{-3}
17 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0010 (2)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.635902 (17)	0.65940 (2)	0.627490 (13)	0.05385 (17)
Cl1	0.74313 (8)	0.47014 (11)	0.60565 (7)	0.0835 (4)
Cl2	0.53500 (9)	0.81815 (11)	0.36251 (6)	0.0824 (4)
O1	0.7036 (2)	0.5440 (3)	0.58675 (14)	0.0824 (12)
O2	0.7426 (3)	0.4662 (4)	0.66334 (17)	0.1157 (17)
O3	0.7203 (3)	0.3871 (3)	0.5849 (2)	0.1266 (19)
O4	0.8058 (3)	0.4856 (4)	0.5878 (3)	0.157 (3)
O5	0.5253 (4)	0.8874 (4)	0.4008 (3)	0.166 (3)
O6	0.5543 (4)	0.8587 (5)	0.3128 (2)	0.163 (3)
O7	0.4781 (3)	0.7685 (6)	0.3600 (3)	0.203 (4)
O8	0.5853 (3)	0.7629 (4)	0.3823 (3)	0.161 (3)
O9	0.5898 (4)	0.8544 (4)	0.5059 (3)	0.153 (3)
H9o	0.5933	0.8495	0.4715	0.229*
O1w	0.67378 (17)	0.7619 (2)	0.56473 (13)	0.0669 (9)
H1w1	0.7050	0.7940	0.5754	0.100*
H1w2	0.6461	0.7963	0.5502	0.100*
N1	0.5972 (2)	0.5502 (3)	0.68868 (15)	0.0577 (10)
N2	0.5722 (2)	0.5292 (3)	0.83597 (15)	0.0610 (11)
N3	0.60584 (19)	0.5596 (3)	0.92480 (15)	0.0568 (10)
N4	0.4370 (2)	0.6175 (3)	0.93989 (15)	0.0571 (10)
N5	0.56585 (18)	0.7712 (3)	0.66228 (15)	0.0519 (9)
N6	0.39646 (18)	0.7952 (3)	0.69501 (15)	0.0555 (10)
N7	0.29018 (18)	0.7710 (3)	0.67160 (15)	0.0543 (10)
N8	0.2817 (2)	0.7036 (3)	0.81592 (16)	0.0630 (11)
C1	0.5938 (3)	0.4629 (3)	0.6737 (2)	0.0652 (13)
H1	0.5983	0.4486	0.6371	0.078*
C2	0.5841 (3)	0.3945 (4)	0.7100 (2)	0.0740 (15)
H2	0.5808	0.3351	0.6981	0.089*
C3	0.5791 (3)	0.4154 (4)	0.7651 (2)	0.0703 (15)
H3	0.5733	0.3697	0.7906	0.084*
C4	0.5828 (2)	0.5038 (3)	0.78171 (18)	0.0546 (11)
C5	0.5907 (2)	0.5696 (3)	0.74220 (18)	0.0545 (11)
H5	0.5916	0.6298	0.7529	0.065*
C6	0.6173 (3)	0.5363 (3)	0.87058 (19)	0.0557 (12)
C7	0.6870 (2)	0.5257 (3)	0.8650 (2)	0.0593 (12)
C8	0.7249 (3)	0.5074 (4)	0.8197 (2)	0.0717 (15)

H8	0.7072	0.4978	0.7855	0.086*
C9	0.7896 (3)	0.5042 (4)	0.8275 (3)	0.0794 (17)
H9	0.8158	0.4915	0.7980	0.095*
C10	0.8163 (3)	0.5192 (4)	0.8776 (3)	0.093 (2)
H10	0.8602	0.5174	0.8813	0.112*
C11	0.7794 (3)	0.5368 (4)	0.9225 (3)	0.0842 (18)
H11	0.7976	0.5460	0.9565	0.101*
C12	0.7141 (3)	0.5403 (3)	0.9154 (2)	0.0671 (14)
C13	0.6648 (3)	0.5607 (4)	0.9568 (2)	0.0672 (14)
H13	0.6641	0.5151	0.9852	0.081*
H13B	0.6718	0.6194	0.9733	0.081*
C14	0.5484 (2)	0.5836 (3)	0.94858 (18)	0.0533 (11)
C15	0.5449 (3)	0.6060 (3)	1.00350 (19)	0.0643 (13)
H15	0.5811	0.6041	1.0252	0.077*
C16	0.4877 (3)	0.6309 (3)	1.0255 (2)	0.0665 (14)
H16	0.4845	0.6431	1.0625	0.080*
C17	0.4347 (3)	0.6380 (3)	0.9925 (2)	0.0651 (14)
H17	0.3966	0.6575	1.0075	0.078*
C18	0.4921 (2)	0.5902 (3)	0.91875 (18)	0.0538 (11)
H18	0.4930	0.5746	0.8821	0.065*
C19	0.5831 (2)	0.8585 (3)	0.6609 (2)	0.0601 (13)
H19	0.6250	0.8727	0.6529	0.072*
C20	0.5412 (3)	0.9274 (4)	0.6710 (2)	0.0672 (14)
H20	0.5552	0.9869	0.6709	0.081*
C21	0.4790 (2)	0.9087 (3)	0.68110 (19)	0.0600 (12)
H21	0.4503	0.9552	0.6873	0.072*
C22	0.4592 (2)	0.8191 (3)	0.68203 (16)	0.0502 (11)
C23	0.5045 (2)	0.7530 (3)	0.67357 (17)	0.0507 (11)
H23	0.4921	0.6928	0.6758	0.061*
C24	0.3530 (2)	0.7902 (3)	0.65882 (18)	0.0521 (11)
C25	0.3553 (2)	0.8023 (3)	0.59882 (18)	0.0566 (12)
C26	0.4052 (3)	0.8169 (4)	0.5640 (2)	0.0687 (14)
H26	0.4465	0.8206	0.5772	0.082*
C27	0.3930 (4)	0.8260 (4)	0.5089 (2)	0.0832 (18)
H27	0.4262	0.8356	0.4847	0.100*
C28	0.3314 (4)	0.8208 (4)	0.4899 (2)	0.097 (2)
H28	0.3239	0.8272	0.4528	0.116*
C29	0.2814 (4)	0.8065 (4)	0.5238 (2)	0.0857 (19)
H29	0.2402	0.8047	0.5104	0.103*
C30	0.2936 (3)	0.7948 (3)	0.5790 (2)	0.0650 (14)
C31	0.2486 (3)	0.7760 (4)	0.62388 (18)	0.0658 (14)
H31	0.2178	0.8242	0.6276	0.079*
H31B	0.2264	0.7194	0.6181	0.079*
C32	0.2651 (2)	0.7455 (3)	0.72242 (19)	0.0552 (11)
C33	0.2017 (2)	0.7243 (4)	0.7285 (2)	0.0661 (13)
H33	0.1740	0.7308	0.6993	0.079*
C34	0.1797 (3)	0.6936 (4)	0.7776 (3)	0.0788 (16)
H34	0.1369	0.6800	0.7819	0.095*
C35	0.2207 (3)	0.6831 (4)	0.8204 (2)	0.0742 (15)

H35	0.2054	0.6610	0.8533	0.089*
C36	0.3031 (2)	0.7365 (3)	0.76821 (18)	0.0558 (11)
H36	0.3454	0.7541	0.7658	0.067*
C37	0.5692 (4)	0.9435 (5)	0.5193 (3)	0.136 (3)
H37A	0.5237	0.9447	0.5213	0.203*
H37B	0.5832	0.9849	0.4917	0.203*
H37C	0.5867	0.9609	0.5538	0.203*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0483 (2)	0.0615 (3)	0.0518 (2)	0.00206 (16)	0.00526 (15)	−0.00315 (15)
Cl1	0.0760 (10)	0.0842 (11)	0.0903 (10)	0.0239 (9)	0.0060 (8)	0.0004 (8)
Cl2	0.0913 (12)	0.0785 (10)	0.0773 (9)	−0.0042 (9)	0.0064 (8)	−0.0024 (7)
O1	0.090 (3)	0.083 (3)	0.074 (2)	0.048 (2)	0.003 (2)	−0.0037 (19)
O2	0.126 (4)	0.143 (4)	0.078 (3)	0.018 (3)	−0.019 (3)	0.010 (3)
O3	0.154 (5)	0.081 (3)	0.145 (4)	0.017 (3)	−0.030 (4)	−0.029 (3)
O4	0.087 (4)	0.156 (5)	0.229 (7)	0.043 (4)	0.061 (4)	0.057 (5)
O5	0.188 (7)	0.143 (5)	0.165 (6)	0.017 (5)	0.012 (5)	−0.068 (5)
O6	0.189 (7)	0.193 (7)	0.108 (4)	0.027 (5)	0.022 (5)	0.048 (4)
O7	0.175 (7)	0.217 (9)	0.218 (7)	−0.110 (7)	−0.058 (6)	0.009 (6)
O8	0.125 (5)	0.157 (6)	0.200 (6)	0.055 (4)	0.045 (4)	0.088 (5)
O9	0.195 (6)	0.112 (4)	0.151 (5)	−0.011 (4)	−0.085 (4)	0.014 (3)
O1w	0.064 (2)	0.069 (2)	0.067 (2)	−0.0084 (18)	0.0102 (17)	0.0027 (17)
N1	0.060 (3)	0.058 (2)	0.055 (2)	0.006 (2)	0.0026 (19)	0.0016 (18)
N2	0.055 (3)	0.071 (3)	0.057 (2)	0.010 (2)	−0.0024 (19)	0.0027 (19)
N3	0.049 (2)	0.067 (3)	0.055 (2)	−0.003 (2)	−0.0071 (18)	0.0079 (18)
N4	0.061 (3)	0.054 (2)	0.056 (2)	0.004 (2)	0.0051 (19)	0.0052 (18)
N5	0.043 (2)	0.053 (2)	0.060 (2)	0.0064 (18)	0.0048 (17)	−0.0044 (17)
N6	0.041 (2)	0.073 (3)	0.053 (2)	0.002 (2)	−0.0021 (17)	0.0018 (18)
N7	0.043 (2)	0.060 (2)	0.060 (2)	0.0029 (18)	−0.0110 (17)	−0.0008 (18)
N8	0.049 (3)	0.078 (3)	0.062 (2)	0.003 (2)	0.0024 (19)	0.004 (2)
C1	0.071 (4)	0.060 (3)	0.065 (3)	0.001 (3)	0.009 (3)	−0.008 (2)
C2	0.076 (4)	0.058 (3)	0.087 (4)	0.002 (3)	0.003 (3)	−0.011 (3)
C3	0.071 (4)	0.061 (3)	0.080 (4)	0.010 (3)	0.004 (3)	0.012 (3)
C4	0.048 (3)	0.063 (3)	0.052 (2)	0.002 (2)	−0.001 (2)	0.002 (2)
C5	0.050 (3)	0.056 (3)	0.058 (3)	0.003 (2)	0.006 (2)	−0.003 (2)
C6	0.054 (3)	0.052 (3)	0.061 (3)	0.004 (2)	0.000 (2)	0.016 (2)
C7	0.048 (3)	0.046 (3)	0.083 (3)	0.003 (2)	−0.002 (2)	0.010 (2)
C8	0.062 (4)	0.065 (4)	0.088 (4)	0.005 (3)	0.007 (3)	0.011 (3)
C9	0.055 (4)	0.065 (4)	0.118 (5)	0.013 (3)	0.015 (3)	0.018 (3)
C10	0.053 (4)	0.067 (4)	0.159 (7)	0.002 (3)	−0.005 (4)	0.020 (4)
C11	0.059 (4)	0.071 (4)	0.123 (5)	0.001 (3)	−0.023 (4)	−0.001 (3)
C12	0.054 (3)	0.054 (3)	0.093 (4)	0.004 (2)	−0.009 (3)	0.010 (3)
C13	0.058 (3)	0.070 (3)	0.073 (3)	−0.002 (3)	−0.019 (3)	0.006 (3)
C14	0.058 (3)	0.048 (3)	0.054 (3)	−0.003 (2)	−0.003 (2)	0.009 (2)
C15	0.075 (4)	0.058 (3)	0.060 (3)	−0.002 (3)	−0.011 (3)	0.005 (2)
C16	0.088 (4)	0.060 (3)	0.052 (3)	0.008 (3)	0.000 (3)	0.001 (2)

C17	0.077 (4)	0.059 (3)	0.059 (3)	0.009 (3)	0.008 (3)	0.004 (2)
C18	0.052 (3)	0.059 (3)	0.051 (2)	0.002 (2)	0.004 (2)	0.007 (2)
C19	0.049 (3)	0.056 (3)	0.076 (3)	0.001 (2)	0.005 (2)	0.000 (2)
C20	0.068 (4)	0.057 (3)	0.077 (3)	0.002 (3)	0.006 (3)	0.003 (2)
C21	0.052 (3)	0.056 (3)	0.072 (3)	0.007 (2)	0.004 (2)	0.003 (2)
C22	0.047 (3)	0.062 (3)	0.041 (2)	0.003 (2)	−0.0047 (19)	0.0064 (19)
C23	0.044 (3)	0.056 (3)	0.052 (2)	0.003 (2)	0.0015 (19)	0.002 (2)
C24	0.052 (3)	0.050 (3)	0.054 (3)	0.005 (2)	−0.008 (2)	0.000 (2)
C25	0.072 (4)	0.050 (3)	0.048 (2)	0.004 (2)	−0.012 (2)	0.001 (2)
C26	0.084 (4)	0.066 (3)	0.057 (3)	−0.001 (3)	−0.006 (3)	0.003 (2)
C27	0.114 (5)	0.080 (4)	0.055 (3)	−0.001 (4)	−0.003 (3)	0.005 (3)
C28	0.145 (7)	0.095 (5)	0.051 (3)	−0.002 (5)	−0.029 (4)	0.007 (3)
C29	0.105 (5)	0.085 (4)	0.067 (4)	−0.006 (4)	−0.036 (4)	0.003 (3)
C30	0.079 (4)	0.054 (3)	0.062 (3)	0.003 (3)	−0.024 (3)	−0.004 (2)
C31	0.061 (3)	0.065 (3)	0.071 (3)	0.006 (3)	−0.027 (3)	−0.006 (2)
C32	0.048 (3)	0.048 (3)	0.069 (3)	0.006 (2)	−0.003 (2)	−0.004 (2)
C33	0.047 (3)	0.073 (4)	0.078 (3)	0.003 (3)	−0.013 (3)	−0.001 (3)
C34	0.048 (3)	0.084 (4)	0.105 (5)	−0.003 (3)	0.007 (3)	0.000 (3)
C35	0.050 (3)	0.089 (4)	0.083 (4)	−0.004 (3)	0.009 (3)	0.006 (3)
C36	0.046 (3)	0.065 (3)	0.057 (3)	0.001 (2)	−0.005 (2)	0.003 (2)
C37	0.123 (6)	0.141 (6)	0.143 (6)	0.005 (5)	−0.011 (5)	0.021 (5)

Geometric parameters (Å, °)

Cd1—O1	2.442 (3)	C9—C10	1.373 (8)
Cd1—O1w	2.306 (3)	C9—H9	0.9300
Cd1—N1	2.354 (4)	C10—C11	1.374 (9)
Cd1—N4^{i}	2.343 (4)	C10—H10	0.9300
Cd1—N5	2.378 (4)	C11—C12	1.389 (8)
Cd1—N8^{i}	2.319 (4)	C11—H11	0.9300
Cl1—O4	1.410 (6)	C12—C13	1.485 (8)
Cl1—O3	1.415 (5)	C13—H13	0.9700
Cl1—O2	1.418 (4)	C13—H13B	0.9700
Cl1—O1	1.450 (4)	C14—C15	1.391 (6)
Cl2—O5	1.406 (4)	C14—C18	1.399 (7)
Cl2—O7	1.408 (4)	C15—C16	1.373 (7)
Cl2—O6	1.419 (4)	C15—H15	0.9300
Cl2—O8	1.425 (4)	C16—C17	1.383 (7)
O9—C37	1.428 (5)	C16—H16	0.9300
O9—H9o	0.85	C17—H17	0.9300
O1w—H1w1	0.85	C18—H18	0.9300
O1w—H1w2	0.85	C19—C20	1.372 (7)
N1—C1	1.344 (6)	C19—H19	0.9300
N1—C5	1.353 (5)	C20—C21	1.362 (7)
N2—C6	1.280 (6)	C20—H20	0.9300
N2—C4	1.403 (6)	C21—C22	1.392 (7)
N3—C14	1.391 (6)	C21—H21	0.9300
N3—C6	1.397 (6)	C22—C23	1.385 (6)
N3—C13	1.472 (6)	C23—H23	0.9300

N4—C17	1.329 (6)	C24—C25	1.485 (7)
N4—C18	1.334 (6)	C25—C26	1.372 (7)
N4—Cd1^{i}	2.343 (4)	C25—C30	1.394 (7)
N5—C19	1.342 (6)	C26—C27	1.385 (7)
N5—C23	1.350 (6)	C26—H26	0.9300
N6—C24	1.279 (6)	C27—C28	1.382 (11)
N6—C22	1.405 (6)	C27—H27	0.9300
N7—C24	1.391 (6)	C28—C29	1.360 (10)
N7—C32	1.407 (6)	C28—H28	0.9300
N7—C31	1.466 (5)	C29—C30	1.393 (7)
N8—C35	1.327 (7)	C29—H29	0.9300
N8—C36	1.347 (6)	C30—C31	1.481 (7)
N8—Cd1^{i}	2.319 (4)	C31—H31	0.9700
C1—C2	1.364 (7)	C31—H31B	0.9700
C1—H1	0.9300	C32—C33	1.381 (7)
C2—C3	1.393 (7)	C32—C36	1.387 (6)
C2—H2	0.9300	C33—C34	1.371 (8)
C3—C4	1.373 (7)	C33—H33	0.9300
C3—H3	0.9300	C34—C35	1.370 (8)
C4—C5	1.385 (6)	C34—H34	0.9300
C5—H5	0.9300	C35—H35	0.9300
C6—C7	1.484 (7)	C36—H36	0.9300
C7—C12	1.381 (7)	C37—H37A	0.9600
C7—C8	1.397 (7)	C37—H37B	0.9600
C8—C9	1.378 (8)	C37—H37C	0.9600
C8—H8	0.9300		
O1w—Cd1—N8^{i}	87.44 (14)	C7—C12—C13	110.9 (5)
O1w—Cd1—N4^{i}	85.96 (13)	C11—C12—C13	128.0 (6)
N8^{i}—Cd1—N4^{i}	171.83 (14)	N3—C13—C12	102.9 (4)
O1w—Cd1—N1	177.61 (12)	N3—C13—H13	111.2
N8^{i}—Cd1—N1	94.06 (15)	C12—C13—H13	111.2
N4^{i}—Cd1—N1	92.38 (14)	N3—C13—H13B	111.2
O1w—Cd1—N5	89.83 (13)	C12—C13—H13B	111.2
N8^{i}—Cd1—N5	93.05 (14)	H13—C13—H13B	109.1
N4^{i}—Cd1—N5	91.76 (14)	N3—C14—C15	121.0 (4)
N1—Cd1—N5	91.94 (14)	N3—C14—C18	122.5 (4)
O1w—Cd1—O1	89.10 (13)	C15—C14—C18	116.5 (5)
N8^{i}—Cd1—O1	90.30 (15)	C16—C15—C14	119.5 (5)
N4^{i}—Cd1—O1	84.78 (14)	C16—C15—H15	120.3
N1—Cd1—O1	89.04 (14)	C14—C15—H15	120.3
N5—Cd1—O1	176.44 (13)	C15—C16—C17	120.0 (5)
O4—Cl1—O3	110.3 (4)	C15—C16—H16	120.0
O4—Cl1—O2	109.0 (4)	C17—C16—H16	120.0
O3—Cl1—O2	108.7 (3)	N4—C17—C16	121.5 (5)
O4—Cl1—O1	108.4 (3)	N4—C17—H17	119.2
O3—Cl1—O1	110.1 (3)	C16—C17—H17	119.2

O2—Cl1—O1	110.2 (3)	N4—C18—C14	123.8 (4)
O5—Cl2—O7	106.6 (5)	N4—C18—H18	118.1
O5—Cl2—O6	107.9 (5)	C14—C18—H18	118.1
O7—Cl2—O6	115.3 (5)	N5—C19—C20	122.5 (5)
O5—Cl2—O8	107.4 (5)	N5—C19—H19	118.7
O7—Cl2—O8	110.4 (5)	C20—C19—H19	118.7
O6—Cl2—O8	108.8 (4)	C21—C20—C19	120.1 (5)
Cl1—O1—Cd1	137.1 (2)	C21—C20—H20	120.0
C37—O9—H9o	109.4	C19—C20—H20	120.0
Cd1—O1w—H1w1	115.3	C20—C21—C22	119.1 (5)
Cd1—O1w—H1w2	115.9	C20—C21—H21	120.5
H1w1—O1w—H1w2	109.0	C22—C21—H21	120.5
C1—N1—C5	117.7 (4)	C23—C22—C21	117.7 (4)
C1—N1—Cd1	120.3 (3)	C23—C22—N6	120.4 (4)
C5—N1—Cd1	120.6 (3)	C21—C22—N6	121.8 (4)
C6—N2—C4	122.3 (4)	N5—C23—C22	123.4 (4)
C14—N3—C6	127.9 (4)	N5—C23—H23	118.3
C14—N3—C13	120.6 (4)	C22—C23—H23	118.3
C6—N3—C13	111.5 (4)	N6—C24—N7	122.5 (4)
C17—N4—C18	118.7 (4)	N6—C24—C25	131.2 (5)
C17—N4—Cd1^{i}	127.0 (4)	N7—C24—C25	106.3 (4)
C18—N4—Cd1^{i}	112.1 (3)	C26—C25—C30	120.8 (5)
C19—N5—C23	117.2 (4)	C26—C25—C24	131.5 (5)
C19—N5—Cd1	119.6 (3)	C30—C25—C24	107.8 (4)
C23—N5—Cd1	122.0 (3)	C25—C26—C27	118.8 (6)
C24—N6—C22	122.1 (4)	C25—C26—H26	120.6
C24—N7—C32	127.8 (4)	C27—C26—H26	120.6
C24—N7—C31	112.3 (4)	C28—C27—C26	120.0 (7)
C32—N7—C31	119.9 (4)	C28—C27—H27	120.0
C35—N8—C36	118.7 (5)	C26—C27—H27	120.0
C35—N8—Cd1^{i}	127.7 (4)	C29—C28—C27	122.0 (6)
C36—N8—Cd1^{i}	111.9 (3)	C29—C28—H28	119.0
N1—C1—C2	122.9 (5)	C27—C28—H28	119.0
N1—C1—H1	118.6	C28—C29—C30	118.2 (6)
C2—C1—H1	118.6	C28—C29—H29	120.9
C1—C2—C3	118.8 (5)	C30—C29—H29	120.9
C1—C2—H2	120.6	C29—C30—C25	120.2 (6)
C3—C2—H2	120.6	C29—C30—C31	129.0 (5)
C4—C3—C2	119.7 (5)	C25—C30—C31	110.8 (4)
C4—C3—H3	120.1	N7—C31—C30	102.7 (4)
C2—C3—H3	120.1	N7—C31—H31	111.2
C3—C4—C5	118.0 (4)	C30—C31—H31	111.2
C3—C4—N2	121.9 (4)	N7—C31—H31B	111.2
C5—C4—N2	119.8 (5)	C30—C31—H31B	111.2
N1—C5—C4	122.9 (4)	H31—C31—H31B	109.1
N1—C5—H5	118.5	C33—C32—C36	116.7 (5)
C4—C5—H5	118.5	C33—C32—N7	121.3 (4)
N2—C6—N3	121.6 (5)	C36—C32—N7	121.9 (4)

N2—C6—C7	131.8 (5)	C34—C33—C32	119.9 (5)
N3—C6—C7	106.6 (4)	C34—C33—H33	120.0
C12—C7—C8	120.6 (5)	C32—C33—H33	120.0
C12—C7—C6	108.1 (4)	C35—C34—C33	119.9 (5)
C8—C7—C6	131.3 (5)	C35—C34—H34	120.0
C9—C8—C7	117.5 (6)	C33—C34—H34	120.0
C9—C8—H8	121.2	N8—C35—C34	121.5 (5)
C7—C8—H8	121.2	N8—C35—H35	119.2
C10—C9—C8	121.8 (6)	C34—C35—H35	119.2
C10—C9—H9	119.1	N8—C36—C32	123.1 (5)
C8—C9—H9	119.1	N8—C36—H36	118.4
C9—C10—C11	121.1 (6)	C32—C36—H36	118.4
C9—C10—H10	119.5	O9—C37—H37A	109.5
C11—C10—H10	119.5	O9—C37—H37B	109.5
C10—C11—C12	118.0 (6)	H37A—C37—H37B	109.5
C10—C11—H11	121.0	O9—C37—H37C	109.5
C12—C11—H11	121.0	H37A—C37—H37C	109.5
C7—C12—C11	121.0 (6)	H37B—C37—H37C	109.5
O4—Cl1—O1—Cd1	−120.7 (5)	C13—N3—C14—C18	175.0 (4)
O3—Cl1—O1—Cd1	118.4 (4)	N3—C14—C15—C16	178.8 (5)
O2—Cl1—O1—Cd1	−1.5 (5)	C18—C14—C15—C16	1.4 (7)
O1w—Cd1—O1—Cl1	140.1 (4)	C14—C15—C16—C17	−3.2 (8)
N8^{i}—Cd1—O1—Cl1	52.7 (4)	C18—N4—C17—C16	−0.5 (7)
N4^{i}—Cd1—O1—Cl1	−133.8 (4)	Cd1^{i}—N4—C17—C16	−162.4 (4)
N1—Cd1—O1—Cl1	−41.4 (4)	C15—C16—C17—N4	2.8 (8)
N8^{i}—Cd1—N1—C1	−120.6 (4)	C17—N4—C18—C14	−1.4 (7)
N4^{i}—Cd1—N1—C1	54.3 (4)	Cd1^{i}—N4—C18—C14	163.0 (4)
N5—Cd1—N1—C1	146.2 (4)	N3—C14—C18—N4	−176.4 (4)
O1—Cd1—N1—C1	−30.4 (4)	C15—C14—C18—N4	1.0 (7)
N8^{i}—Cd1—N1—C5	45.4 (4)	C23—N5—C19—C20	0.6 (7)
N4^{i}—Cd1—N1—C5	−139.6 (4)	Cd1—N5—C19—C20	167.9 (4)
N5—Cd1—N1—C5	−47.8 (4)	N5—C19—C20—C21	−2.2 (8)
O1—Cd1—N1—C5	135.6 (4)	C19—C20—C21—C22	1.2 (8)
O1w—Cd1—N5—C19	−31.4 (4)	C20—C21—C22—C23	1.3 (7)
N8^{i}—Cd1—N5—C19	56.0 (4)	C20—C21—C22—N6	176.6 (4)
N4^{i}—Cd1—N5—C19	−117.4 (4)	C24—N6—C22—C23	−96.3 (5)
N1—Cd1—N5—C19	150.2 (4)	C24—N6—C22—C21	88.4 (6)
O1w—Cd1—N5—C23	135.2 (3)	C19—N5—C23—C22	2.0 (6)
N8^{i}—Cd1—N5—C23	−137.3 (3)	Cd1—N5—C23—C22	−165.0 (3)
N4^{i}—Cd1—N5—C23	49.3 (3)	C21—C22—C23—N5	−2.9 (6)
N1—Cd1—N5—C23	−43.2 (3)	N6—C22—C23—N5	−178.4 (4)
C5—N1—C1—C2	0.1 (8)	C22—N6—C24—N7	−176.8 (4)
Cd1—N1—C1—C2	166.6 (4)	C22—N6—C24—C25	2.9 (8)
N1—C1—C2—C3	−1.8 (9)	C32—N7—C24—N6	−7.1 (8)
C1—C2—C3—C4	1.2 (8)	C31—N7—C24—N6	175.5 (5)
C2—C3—C4—C5	0.8 (8)	C32—N7—C24—C25	173.2 (4)
C2—C3—C4—N2	174.0 (5)	C31—N7—C24—C25	−4.3 (5)

C6—N2—C4—C3	92.8 (6)	N6—C24—C25—C26	4.6 (9)
C6—N2—C4—C5	−94.2 (6)	N7—C24—C25—C26	−175.7 (5)
C1—N1—C5—C4	2.1 (7)	N6—C24—C25—C30	−176.5 (5)
Cd1—N1—C5—C4	−164.3 (4)	N7—C24—C25—C30	3.2 (5)
C3—C4—C5—N1	−2.5 (7)	C30—C25—C26—C27	1.4 (8)
N2—C4—C5—N1	−175.8 (4)	C24—C25—C26—C27	−179.8 (5)
C4—N2—C6—N3	−178.5 (4)	C25—C26—C27—C28	0.3 (9)
C4—N2—C6—C7	3.1 (9)	C26—C27—C28—C29	−0.2 (10)
C14—N3—C6—N2	−4.5 (8)	C27—C28—C29—C30	−1.6 (10)
C13—N3—C6—N2	178.3 (5)	C28—C29—C30—C25	3.2 (9)
C14—N3—C6—C7	174.3 (4)	C28—C29—C30—C31	−178.1 (6)
C13—N3—C6—C7	−2.9 (5)	C26—C25—C30—C29	−3.2 (8)
N2—C6—C7—C12	−179.7 (5)	C24—C25—C30—C29	177.8 (5)
N3—C6—C7—C12	1.6 (5)	C26—C25—C30—C31	178.0 (5)
N2—C6—C7—C8	2.2 (10)	C24—C25—C30—C31	−1.1 (6)
N3—C6—C7—C8	−176.4 (5)	C24—N7—C31—C30	3.5 (5)
C12—C7—C8—C9	0.3 (8)	C32—N7—C31—C30	−174.1 (4)
C6—C7—C8—C9	178.2 (5)	C29—C30—C31—N7	179.9 (5)
C7—C8—C9—C10	−0.7 (9)	C25—C30—C31—N7	−1.4 (6)
C8—C9—C10—C11	1.0 (10)	C24—N7—C32—C33	−176.9 (5)
C9—C10—C11—C12	−1.0 (9)	C31—N7—C32—C33	0.4 (7)
C8—C7—C12—C11	−0.3 (8)	C24—N7—C32—C36	0.2 (7)
C6—C7—C12—C11	−178.6 (5)	C31—N7—C32—C36	177.5 (4)
C8—C7—C12—C13	178.5 (5)	C36—C32—C33—C34	−1.8 (8)
C6—C7—C12—C13	0.2 (6)	N7—C32—C33—C34	175.5 (5)
C10—C11—C12—C7	0.6 (9)	C32—C33—C34—C35	−0.8 (9)
C10—C11—C12—C13	−178.0 (5)	C36—N8—C35—C34	0.8 (9)
C14—N3—C13—C12	−174.5 (4)	Cd1^{i}—N8—C35—C34	−163.1 (4)
C6—N3—C13—C12	2.9 (5)	C33—C34—C35—N8	1.4 (9)
C7—C12—C13—N3	−1.8 (6)	C35—N8—C36—C32	−3.6 (8)
C11—C12—C13—N3	176.9 (5)	Cd1^{i}—N8—C36—C32	162.7 (4)
C6—N3—C14—C15	−179.3 (5)	C33—C32—C36—N8	4.1 (7)
C13—N3—C14—C15	−2.3 (7)	N7—C32—C36—N8	−173.2 (4)
C6—N3—C14—C18	−2.0 (7)		

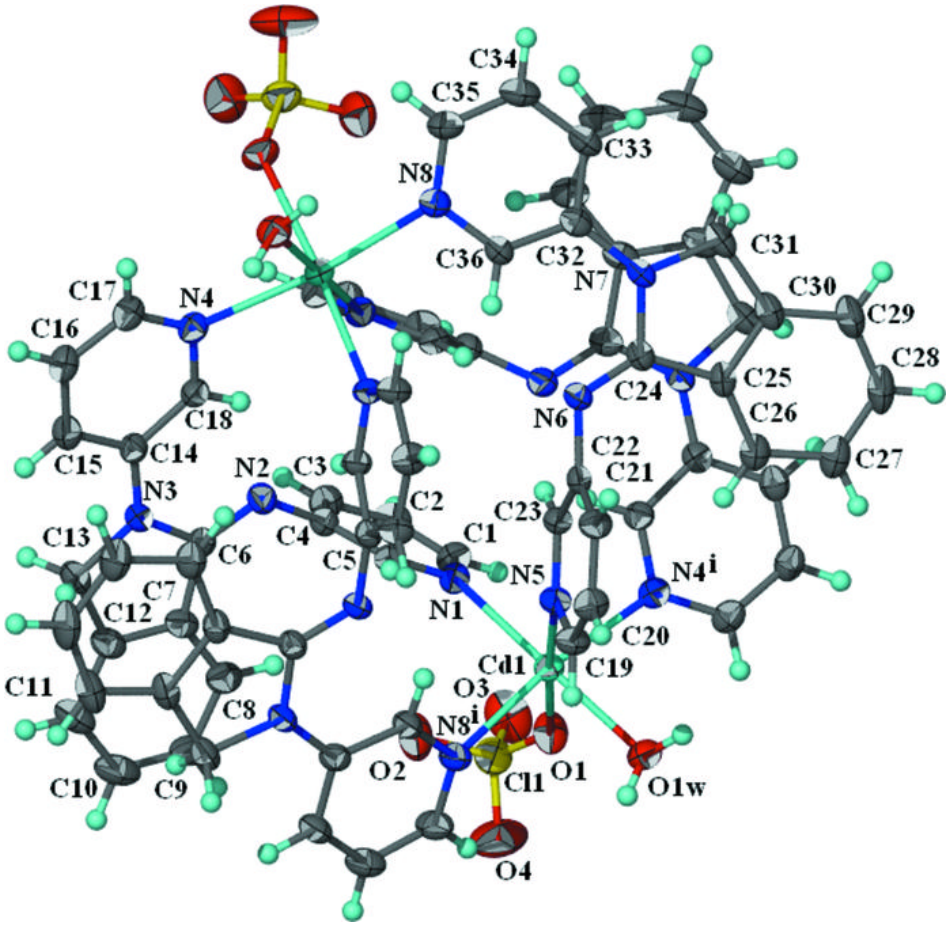
Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O3^{ii}	0.85	2.11	2.945 (6)	167
O1w—H1w2···O9	0.85	1.83	2.665 (7)	167
O9—H9o···O5	0.85	2.32	2.959 (9)	132

Symmetry codes: (ii) −*x*+3/2, *y*+1/2, *z*.

Fig. 1


C34
C35
C33
N8
C36
C32
N7
C31
C30
C29
C28
C17
N4
C16
C18
C24
C25
C26
N6
C22
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C15
C14
N2
C3
C21
N3
C2
C23
C13
C4
C1
C6
C5
N5
N4i
C7
C12
N1
C20
Cd1
C19
C11
O3
C8
N8i
O2
Cl1
O1
O1w
C10
C9
O4