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Synthesis and structure of *catena*-poly[3-[(hydrazin-2-ium-1-yl)carbonyl]pyridin-1-ium [aquadi-μ_3-chlorido-di-μ_2-chlorido-dichloridodicadmium(II)] monohydrate]

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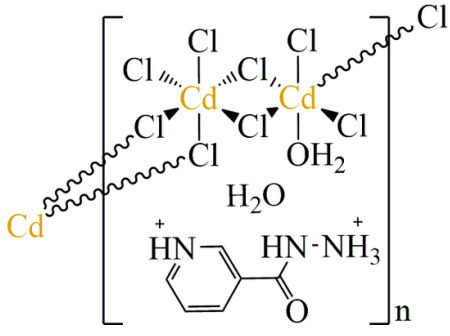
The crystal structure of the title compound, $\{(C_6H_9N_3O)[Cd_2Cl_6(H_2O)]\cdot H_2O\}_n$, is built up from edge-sharing $CdCl_5(H_2O)$ and $CdCl_6$ octahedra, which alternate about inversion centres to form infinite anionic double chains propagating along the *b*-axis direction. The organic dications and water molecules of crystallization occupy the interchain spaces, linking neighbouring $\{[Cd_2Cl_6(H_2O)]^{2-}\}_n$ chains through an extensive network of N—H···Cl, O—H···Cl and O—H···O hydrogen bonds. The packing is further supported by weak π–π and C—H···π interactions between adjacent cations.

1. Chemical context

Organic–inorganic cadmium(II) chloride compounds provide a useful setting for investigating how metal–halide coordination and hydrogen bonding contribute to crystal assembly. In these materials, the inorganic and organic components participate in complementary structural roles: cadmium–chloride connectivity defines the inorganic units, while interactions involving the organic cations can contribute to their organization in the crystal.



The present study focuses on a hybrid compound obtained using pyridine-3-carbohydrazide, also known as nicotinohydrazide, as the organic precursor. This molecule contains a pyridine ring and a hydrazide group, providing several sites for protonation and intermolecular interactions. The reaction of cadmium(II) chloride with pyridine-3-carbohydrazide in an acidified aqueous solution afforded the title compound, $(C_6H_9N_3O)[Cd_2Cl_6(H_2O)]H_2O$ (**I**) and we now report its crystal structure.

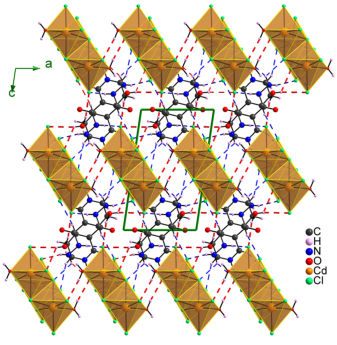


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Table 1
Selected bond lengths (Å).

Cd1—O2	2.340 (2)	Cd2—Cl2	2.5329 (8)
Cd1—Cl6	2.5441 (9)	Cd2—Cl4	2.6196 (8)
Cd1—Cl4	2.5840 (8)	Cd2—Cl3	2.6301 (8)
Cd1—Cl1^{i}	2.6260 (8)	Cd2—Cl3^{ii}	2.6472 (8)
Cd1—Cl5^{i}	2.6904 (8)	Cd2—Cl1	2.6641 (8)
Cd1—Cl5	2.7012 (8)	Cd2—Cl5	2.7524 (8)

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

2. Structural commentary

Compound (**I**) crystallizes in the triclinic space group $P\overline{1}$: the asymmetric unit consists of one 3-[(hydrazin-2-ium-1-y)-carbonyl]pyridin-1-ium dication, one water molecule of crystallization (O3), two crystallographically independent Cd^{II} centres, six chloride ions (Cl1–Cl6) and one coordinated water molecule (O2). The coordination geometry around Cd1 in the asymmetric unit is established by one terminal chloride ion (Cl6), one coordinated water molecule (O2) and two bridging chloride ligands (Cl4 and Cl5). The Cd2 centre is coordinated by the same pair of chloride ions (Cl4 and Cl5) along with three terminal chloride ligands (Cl1, Cl2, and Cl3) (Fig. 1).

When crystal symmetry generates the complete structure, the Cd^{II} centres display distinct coordination environments (Table 1) and degrees of distortion. Cd1 is coordinated by one water oxygen atom and five chloride ligands within a distorted $CdCl_5O$ octahedron, with Cd—Cl distances ranging from 2.340 (2) to 2.7012 (8) Å. In contrast, Cd2 is coordinated exclusively by chloride ligands to form a more regular $CdCl_6$ octahedron, with Cd—Cl distances spanning 2.5329 (8) to 2.7524 (8) Å. Bond-length distortion parameters ($\Delta d = 2.20 \times 10^{-3}$ and 0.60×10^{-3}), quadratic elongation values (<λ> = 1.0022 and 1.0006) and bond-angle variances (σ^2 = 27.73 and 22.18°^{2}), for Cd1 and Cd2, respectively, confirm that the Cd1 octahedron exhibits noticeably higher distortion than Cd2. Bond-valence-sum (BVS) calculations yield values of 2.30 for Cd1 and 2.31 for Cd2, which are somewhat higher than the expected value (2.00) for Cd^{2+}. The asymmetry for Cd1 is reflected in a broader deviation of *cis*-angles from the ideal 90°. Conversely, Cd2, being coordinated solely by chloride ligands adopts a more regular octahedral geometry. This geometric disparity between the two metal sites carries functional structural significance: Cd1, bearing the coordinated water molecule, serves as the primary anchoring point between the inorganic $\{Cd_2Cl_6(H_2O)\}$ framework and the surrounding species by accepting and forming hydrogen bonds with both the water molecule of crystallisation and the organic cation. Meanwhile, Cd2 contributes primarily to the structural connectivity of the inorganic chain through its bridging chloride ligands (Fig. 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···Cl2^{iii}	0.93	2.99	3.607 (4)	126
C1—H1A···Cl3^{iv}	0.93	2.75	3.603 (3)	153
C2—H2···O1^{iii}	0.93	2.41	3.125 (5)	134
C5—H5···Cl4^{ii}	0.93	2.64	3.459 (3)	147
N1—H1···Cl3	0.86	2.30	3.163 (3)	177
N2—H2N···Cl6^{v}	0.91	2.36	3.235 (3)	160
N3—H3A···Cl2^{vi}	0.89	2.30	3.175 (3)	167
N3—H3B···Cl1^{vii}	0.89	2.32	3.143 (3)	153
N3—H3B···Cl5^{vi}	0.89	2.65	3.075 (3)	110
N3—H3C···O3^{v}	0.89	1.89	2.773 (4)	172
O2—H2A···O3	0.93	2.10	3.016 (3)	166
O2—H2B···Cl1^{viii}	0.93	2.39	3.318 (2)	174
O3—H3O···Cl4^{viii}	0.93	2.85	3.506 (3)	128
O3—H3O···Cl6^{viii}	0.93	2.72	3.392 (3)	129
O3—H3P···Cl6^{ix}	0.93	2.41	3.314 (2)	162

Symmetry codes: (ii) $-x+2, -y, -z+1$; (iii) $x-1, y, z$; (iv) $-x+1, -y, -z+1$; (v) $x-1, y-1, z-1$; (vi) $-x+2, -y, -z$; (vii) $-x+1, -y, -z$; (viii) $x+1, y, z$; (ix) $-x+3, -y+1, -z+2$.

Within the organic cation, the small dihedral angle (~4.2°) between the mean planes of the pyridine ring and the hydrazide group presumably reflects extended π-conjugation, where the lone pair on the amide N2 atom and the carbonyl π-system (C6═O1) overlap efficiently with the aromatic π-system of the pyridine ring. Delocalization of electron density across the C4—C6(═O)—N2 linkage restricts rotation around the C4—C6 bond, imparting partial double-bond character typical of amide/hydrazide linkages. From a crystal-engineering standpoint, this planar arrangement promotes efficient π–π stacking interactions between adjacent cationic units and reinforces the hydrogen-bonding network by holding the participating functional groups in a rigid, coplanar orientation relative to the aromatic ring.

3. Supramolecular features

The crystal packing for (**I**) is consolidated by an extensive network of N—H···Cl, N—H···O, O—H···Cl, O—H···O, and C—H···Cl/O hydrogen bonds (Table 2), involving the

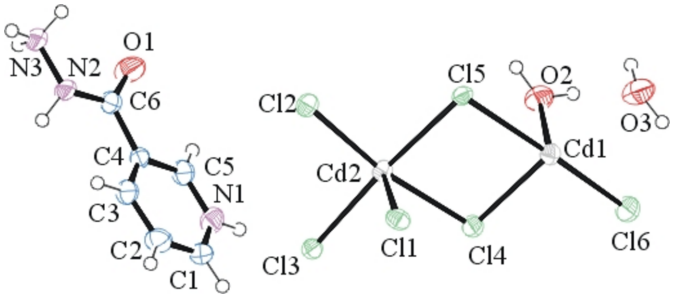

Figure 1
The asymmetric unit of (**I**) with displacement ellipsoids drawn at the 50% probability level.

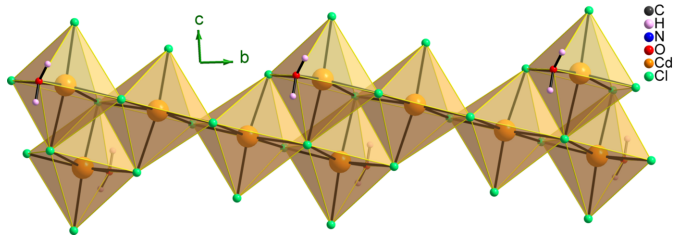

Figure 2
Polyhedral view of the anionic double chains extending along the *b*-axis direction.

organic dication, the metal-coordinated water molecule (O2), and the water molecule of crystallization (O3). The strongest interaction in the structure is the N3—H3*C*···O3 contact, which links the terminal –NH_3^+ group of the hydrazinium moiety to the water molecule of crystallization. The pyridinium N1—H1···Cl3 contact is also notably short and nearly linear (177°), while the remaining N—H···Cl interactions originating from the hydrazinium group (N2—H2*N*···Cl6, N3—H3*A*···Cl2, and N3—H3*B*···Cl1/Cl5) exhibit H···Cl distances ranging from 2.30 to 2.65 Å, effectively anchoring the organic cation to the chloride ligands of the anionic chains.

The coordinated water molecule serves a dual role in the network. As a hydrogen-bond donor, it forms an O2—H2*A*···O3 interaction to link with the water molecule of crystallization, as well as an O2—H2*B*···Cl1 interaction connecting it to a neighbouring chain. The water molecule of crystallization further bridges adjacent chains through bifurcated O3—H3*O*···(Cl4,Cl6) contacts. Weaker C—H···Cl and C—H···O interactions originating from the pyridine ring carbon atoms (C1, C2, and C5) complete the packing. Together, these cooperative hydrogen-bonding interactions connect the components of (**I**) into a three-dimensional supramolecular framework (Fig. 3).

4. Database survey

Related cadmium(II) chloride structures provide useful comparisons for the title compound in terms of metal coordination, inorganic connectivity and the arrangement of the charge-balancing organic cations.

Relevant examples include the hydrated cadmium chloride polymer containing 1-chloromethyl-1,4-diazoniabicyclo[2.2.2]-octane cations reported by Xiao (2010), and the one-dimensional chloro-bridged cadmium(II) chains separated by dimethylhexadecylsulfonium cation layers described by Sokka *et al.* (2008). These compounds provide comparisons for the association of extended cadmium chloride units with organic cations. The title compound differs in containing a protonated nicotinohydrazide dication, together with both coordinated and non-coordinated water molecules, which participate in the interchain hydrogen-bonding network.

A contrasting mode of inorganic connectivity occurs in $[NH_2(CH_3)_2]_5Cd_3Cl_{11}$, reported by Trabelsi *et al.* (2022), in which the chains comprise face-sharing $CdCl_6$ octahedra. In the title compound, the inorganic double chains instead contain edge-sharing octahedra.

Further examples of extended cadmium halide architectures include the ladder-like, six-coordinate cadmium chloride polymer containing (*S*)-2-methylpiperazine-1,4-diium cations reported by Wu (2014), and the two *N*-methylethylenediammonium cadmium halide salts investigated by Thorn *et al.* (2005). The latter structures were discussed in terms of dimensional reduction and recombination of the hexagonal CdX_2 array.

The role of the organic component can also be considered alongside the influence of additional ligands on cadmium coordination. Huh *et al.* (2008), for example, reported cadmium coordination polymers with different topologies depending on the preparation method. Although those ligand-based coordination polymers are not direct analogues of the chlorido-bridged framework described here, they provide a complementary illustration of the structural variability accessible to cadmium(II).

5. Synthesis and crystallization

Single crystals of (**I**) were obtained by the reaction of pyridine-3-carbohydrazide with cadmium(II) dichloride in a 1:2 molar ratio. Pyridine-3-carbohydrazide (1 mmol) was dissolved in a small amount of ethanol and added to an aqueous solution of $CdCl_2$ (2 mmol) acidified with a few drops of concentrated hydrochloric acid to ensure complete protonation of both the pyridine and terminal hydrazide nitrogen atoms of the organic cation. The resulting solution was stirred for 30 minutes at room temperature until homogeneous, then filtered and left to crystallize by slow evaporation at room temperature. Colourless prismatic single crystals of (**I**) suitable for X-ray diffraction were obtained after two weeks (Fig. 4).

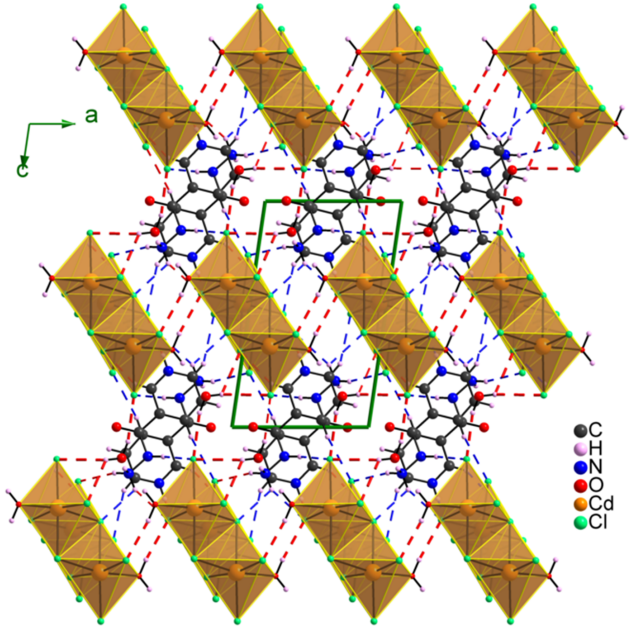

Figure 3
The packing in (**I**) viewed down the *a*-axis direction with dashed lines indicating hydrogen-bonding interactions.

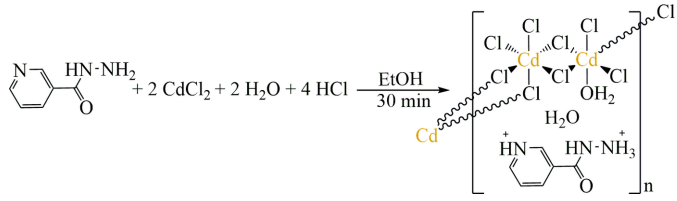

Figure 4
Scheme showing the formation of (**I**).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were initially located in a difference-Fourier map. Most H atoms were then placed in geometrically idealized positions and constrained to ride on their parent atoms at a C—H distance of 0.93 Å, at a N—H distance of 0.86 Å (N1), and at 0.89 Å for the ammonium group. The water molecules and NH_3 group were refined as idealized rotating moieties and the proton on N2 as a rotating unit after refining the N—H distance. U_{iso}(H) for aromatic protons and water molecules were fixed at $1.2U_{eq}$(parent atom) and at $1.5U_{eq}$(N) in the case of the ammonium group.

Acknowledgements

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supporting information

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Synthesis and structure of *catena*-poly[3-[(hydrazin-2-ium-1-yl)carbonyl]-pyridin-1-ium [aquadi-μ_3-chlorido-di-μ_2-chlorido-dichloridodicadmium(II)] monohydrate]

Sabrine Hermi, Werner Kaminsky and Cherif Ben Nasr

Computing details

***catena*-Poly[3-[(hydrazin-2-ium-1-yl)carbonyl]pyridin-1-ium [aquadi-μ_3-chlorido-di-μ_2-chlorido-dichloridodicadmium(II)] monohydrate]**

Crystal data

$(C_6H_9N_3O)[Cd_2Cl_6(H_2O)]\cdot H_2O$
$M_r = 612.69$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.0467$ (3) Å
$b = 10.3533$ (4) Å
$c = 11.7819$ (6) Å
$\alpha = 91.619$ (1)°
$\beta = 98.264$ (2)°
$\gamma = 92.892$ (1)°
$V = 849.01$ (7) Å^3
$Z = 2$
$F(000) = 584$
$D_x = 2.397$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6013 reflections
$\theta = 2$–20°
$\mu = 3.45$ mm^{-1}
$T = 294$ K
Prism, colorless
0.4 × 0.22 × 0.16 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Enraf–Nonius FR590
Horizonally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
CCD rotation images, thick slices scans
Absorption correction: multi-scan (HKL Scalepack; Otwiniwski & Minor, 1997)
$T_{min} = 0.636$, $T_{max} = 0.751$
7879 measured reflections
4136 independent reflections
3024 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.8°$
$h = -9\rightarrow9$
$k = -13\rightarrow13$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.074$
$S = 1$
4136 reflections
188 parameters
0 restraints
0 constraints
Primary atom site location: dual
Secondary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.47$ e Å^{-3}
$\Delta\rho_{min} = -0.94$ e Å^{-3}

Extinction correction: SHELXL2014/7 (Sheldrick 2015b), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0039 (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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3434 (5)	−0.0749 (3)	0.2235 (3)	0.0353 (8)
H1A	0.2772	−0.0431	0.2802	0.042*
C2	0.2516 (5)	−0.0989 (3)	0.1149 (3)	0.0387 (9)
H2	0.1223	−0.0831	0.0964	0.046*
C3	0.3522 (5)	−0.1468 (3)	0.0322 (3)	0.0332 (8)
H3	0.2903	−0.1644	−0.0422	0.04*
C4	0.5448 (4)	−0.1685 (3)	0.0601 (2)	0.0253 (8)
C5	0.6320 (5)	−0.1431 (3)	0.1705 (3)	0.0323 (8)
H5	0.7613	−0.1574	0.1917	0.039*
C6	0.6750 (5)	−0.2143 (3)	−0.0224 (3)	0.0302 (8)
Cd1	1.18772 (4)	0.47568 (2)	0.64271 (2)	0.02746 (9)
Cd2	0.94085 (3)	0.17160 (2)	0.45208 (2)	0.02557 (9)
Cl1	0.63248 (11)	0.31107 (8)	0.41047 (7)	0.02956 (19)
Cl2	0.93340 (12)	0.11583 (8)	0.24073 (7)	0.0322 (2)
Cl3	0.74760 (11)	−0.03952 (7)	0.49878 (6)	0.02474 (18)
Cl4	0.97927 (12)	0.26732 (8)	0.66285 (7)	0.02844 (19)
Cl5	1.13637 (11)	0.40097 (8)	0.41838 (6)	0.02431 (18)
Cl6	1.24792 (15)	0.52524 (9)	0.85800 (7)	0.0466 (3)
N1	0.5266 (4)	−0.0971 (3)	0.2478 (2)	0.0363 (7)
H1	0.5824	−0.0812	0.317	0.044*
N2	0.5851 (4)	−0.2486 (3)	−0.1291 (2)	0.0393 (8)
H2N	0.4715	−0.2954	−0.1302	0.047*
N3	0.7064 (4)	−0.2987 (3)	−0.2048 (2)	0.0406 (8)
H3A	0.811	−0.2462	−0.2023	0.061*
H3B	0.6435	−0.3042	−0.276	0.061*
H3C	0.7403	−0.377	−0.1833	0.061*
O1	0.8457 (4)	−0.2090 (3)	0.0009 (2)	0.0516 (7)
O2	1.4787 (3)	0.3735 (2)	0.65850 (17)	0.0412 (6)
H2A	1.5695	0.4112	0.7167	0.049*
H2B	1.5125	0.3556	0.5865	0.049*
O3	1.7748 (3)	0.4516 (2)	0.86321 (18)	0.0524 (7)
H3O	1.8889	0.4132	0.855	0.086 (16)*
H3P	1.7463	0.4699	0.9365	0.109 (19)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.040 (2)	0.036 (2)	0.032 (2)	−0.0058 (17)	0.0138 (16)	−0.0020 (16)
C2	0.025 (2)	0.051 (2)	0.039 (2)	0.0011 (18)	0.0030 (16)	0.0006 (18)
C3	0.0290 (19)	0.044 (2)	0.0239 (18)	−0.0026 (17)	−0.0028 (14)	−0.0035 (15)
C4	0.032 (2)	0.0251 (19)	0.0176 (16)	−0.0048 (15)	0.0027 (14)	0.0019 (14)
C5	0.0284 (19)	0.038 (2)	0.0281 (19)	−0.0008 (16)	−0.0026 (14)	−0.0011 (15)
C6	0.031 (2)	0.034 (2)	0.0242 (18)	−0.0037 (16)	0.0029 (14)	−0.0009 (15)
Cd1	0.02792 (16)	0.02836 (16)	0.02544 (15)	−0.00055 (11)	0.00264 (10)	−0.00052 (10)
Cd2	0.02781 (16)	0.02602 (16)	0.02268 (14)	0.00347 (11)	0.00252 (10)	−0.00026 (10)
Cl1	0.0210 (4)	0.0321 (5)	0.0357 (5)	0.0017 (3)	0.0039 (3)	0.0034 (4)
Cl2	0.0354 (5)	0.0388 (5)	0.0215 (4)	−0.0026 (4)	0.0028 (3)	−0.0015 (3)
Cl3	0.0220 (4)	0.0285 (4)	0.0235 (4)	0.0020 (3)	0.0023 (3)	−0.0002 (3)
Cl4	0.0318 (5)	0.0296 (5)	0.0234 (4)	−0.0020 (4)	0.0036 (3)	0.0009 (3)
Cl5	0.0225 (4)	0.0284 (4)	0.0229 (4)	0.0025 (3)	0.0065 (3)	−0.0017 (3)
Cl6	0.0544 (6)	0.0584 (7)	0.0248 (5)	−0.0168 (5)	0.0070 (4)	−0.0062 (4)
N1	0.042 (2)	0.0427 (19)	0.0221 (15)	−0.0013 (15)	−0.0005 (13)	−0.0004 (13)
N2	0.0292 (18)	0.060 (2)	0.0276 (16)	−0.0127 (15)	0.0091 (13)	−0.0179 (15)
N3	0.0349 (18)	0.054 (2)	0.0319 (17)	−0.0108 (15)	0.0104 (13)	−0.0161 (14)
O1	0.0274 (15)	0.090 (2)	0.0360 (15)	0.0011 (15)	0.0027 (11)	−0.0119 (14)
O2	0.0369 (15)	0.0472 (16)	0.0414 (15)	0.0086 (12)	0.0102 (12)	0.0012 (12)
O3	0.0485 (18)	0.067 (2)	0.0457 (18)	0.0081 (15)	0.0177 (13)	0.0003 (14)

Geometric parameters (Å, º)

C1—N1	1.315 (4)	Cd2—Cl2	2.5329 (8)
C1—C2	1.358 (4)	Cd2—Cl4	2.6196 (8)
C1—H1A	0.93	Cd2—Cl3	2.6301 (8)
C2—C3	1.380 (4)	Cd2—Cl3^{ii}	2.6472 (8)
C2—H2	0.93	Cd2—Cl1	2.6641 (8)
C3—C4	1.381 (4)	Cd2—Cl5	2.7524 (8)
C3—H3	0.93	Cl1—Cd1^{i}	2.6261 (8)
C4—C5	1.369 (4)	Cl3—Cd2^{ii}	2.6471 (8)
C4—C6	1.512 (4)	Cl5—Cd1^{i}	2.6904 (8)
C5—N1	1.347 (4)	N1—H1	0.86
C5—H5	0.93	N2—N3	1.425 (4)
C6—O1	1.193 (4)	N2—H2N	0.9131
C6—N2	1.353 (4)	N3—H3A	0.89
Cd1—O2	2.340 (2)	N3—H3B	0.89
Cd1—Cl6	2.5441 (9)	N3—H3C	0.89
Cd1—Cl4	2.5840 (8)	O2—H2A	0.93
Cd1—Cl1^{i}	2.6260 (8)	O2—H2B	0.93
Cd1—Cl5^{i}	2.6904 (8)	O3—H3O	0.9306
Cd1—Cl5	2.7012 (8)	O3—H3P	0.9308
N1—C1—C2	119.4 (3)	Cl4—Cd2—Cl3	93.90 (2)
N1—C1—H1A	120.3	Cl2—Cd2—Cl3^{ii}	90.03 (3)

C2—C1—H1A	120.3	Cl4—Cd2—Cl3^{ii}	91.16 (3)
C1—C2—C3	119.4 (3)	Cl3—Cd2—Cl3^{ii}	86.19 (2)
C1—C2—H2	120.3	Cl2—Cd2—Cl1	92.09 (3)
C3—C2—H2	120.3	Cl4—Cd2—Cl1	86.54 (3)
C2—C3—C4	119.9 (3)	Cl3—Cd2—Cl1	94.78 (2)
C2—C3—H3	120.1	Cl3^{ii}—Cd2—Cl1	177.56 (2)
C4—C3—H3	120.1	Cl2—Cd2—Cl5	88.01 (3)
C5—C4—C3	118.9 (3)	Cl4—Cd2—Cl5	81.97 (2)
C5—C4—C6	115.3 (3)	Cl3—Cd2—Cl5	175.65 (2)
C3—C4—C6	125.7 (3)	Cl3^{ii}—Cd2—Cl5	95.23 (2)
N1—C5—C4	118.6 (3)	Cl1—Cd2—Cl5	83.64 (2)
N1—C5—H5	120.7	Cd1^{i}—Cl1—Cd2	96.91 (3)
C4—C5—H5	120.7	Cd2—Cl3—Cd2^{ii}	93.81 (2)
O1—C6—N2	122.0 (3)	Cd1—Cl4—Cd2	100.07 (3)
O1—C6—C4	122.7 (3)	Cd1^{i}—Cl5—Cd1	96.71 (2)
N2—C6—C4	114.9 (3)	Cd1^{i}—Cl5—Cd2	93.34 (2)
O2—Cd1—Cl6	89.20 (5)	Cd1—Cl5—Cd2	93.99 (2)
O2—Cd1—Cl4	95.25 (6)	C1—N1—C5	123.7 (3)
Cl6—Cd1—Cl4	93.24 (3)	C1—N1—H1	118.1
O2—Cd1—Cl1^{i}	89.02 (6)	C5—N1—H1	118.1
Cl6—Cd1—Cl1^{i}	94.91 (3)	C6—N2—N3	114.8 (3)
Cl4—Cd1—Cl1^{i}	170.85 (3)	C6—N2—H2N	114
O2—Cd1—Cl5^{i}	168.77 (5)	N3—N2—H2N	114.2
Cl6—Cd1—Cl5^{i}	101.05 (3)	N2—N3—H3A	109.5
Cl4—Cd1—Cl5^{i}	88.77 (3)	N2—N3—H3B	109.5
Cl1^{i}—Cd1—Cl5^{i}	85.60 (2)	H3A—N3—H3B	109.5
O2—Cd1—Cl5	86.74 (5)	N2—N3—H3C	109.5
Cl6—Cd1—Cl5	174.63 (3)	H3A—N3—H3C	109.5
Cl4—Cd1—Cl5	83.63 (3)	H3B—N3—H3C	109.5
Cl1^{i}—Cd1—Cl5	88.55 (3)	Cd1—O2—H2A	112.2
Cl5^{i}—Cd1—Cl5	83.29 (2)	Cd1—O2—H2B	110.9
Cl2—Cd2—Cl4	169.97 (3)	H2A—O2—H2B	120
Cl2—Cd2—Cl3	96.12 (3)	H3O—O3—H3P	119.3

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···Cl2^{iii}	0.93	2.99	3.607 (4)	126
C1—H1*A*···Cl3^{iv}	0.93	2.75	3.603 (3)	153
C2—H2···O1^{iii}	0.93	2.41	3.125 (5)	134
C5—H5···Cl4^{ii}	0.93	2.64	3.459 (3)	147
N1—H1···Cl3	0.86	2.30	3.163 (3)	177
N2—H2*N*···Cl6^{v}	0.91	2.36	3.235 (3)	160
N3—H3*A*···Cl2^{vi}	0.89	2.30	3.175 (3)	167
N3—H3*B*···Cl1^{vii}	0.89	2.32	3.143 (3)	153
N3—H3*B*···Cl5^{vi}	0.89	2.65	3.075 (3)	110

N3—H3*C*···O3^{v}	0.89	1.89	2.773 (4)	172
O2—H2*A*···O3	0.93	2.10	3.016 (3)	166
O2—H2*B*···Cl1^{viii}	0.93	2.39	3.318 (2)	174
O3—H3*O*···Cl4^{viii}	0.93	2.85	3.506 (3)	128
O3—H3*O*···Cl6^{viii}	0.93	2.72	3.392 (3)	129
O3—H3*P*···Cl6^{ix}	0.93	2.41	3.314 (2)	162

Symmetry codes: (ii) −*x*+2, −*y*, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, −*y*, −*z*+1; (v) *x*−1, *y*−1, *z*−1; (vi) −*x*+2, −*y*, −*z*; (vii) −*x*+1, −*y*, −*z*; (viii) *x*+1, *y*, *z*; (ix) −*x*+3, −*y*+1, −*z*+2.