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1,1'-[1,1'-(Pyridinium-2,6-diyl)-diethylidene]diimino}diguanidinium pentachloridocadmate(II) monohydrate

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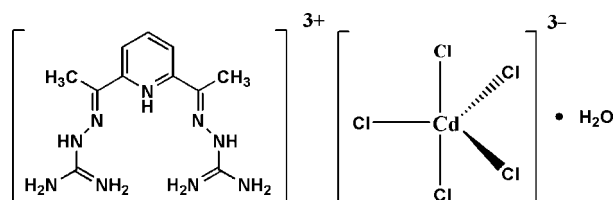
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.034; wR factor = 0.068; data-to-parameter ratio = 20.1.

In the title organic–inorganic hybrid salt, $(\text{C}_{11}\text{H}_{20}\text{N}_9)^+[\text{CdCl}_5]^{2-} \cdot \text{H}_2\text{O}$, the crystal structure is stabilized by intermolecular hydrogen bonds between the organic cation, the complex inorganic anion and the uncoordinated water molecule, forming a three-dimensional network.

Related literature

 For details of the synthesis, see: Valdes-Martinez *et al.* (2002).


Experimental

Crystal data

 $(\text{C}_{11}\text{H}_{20}\text{N}_9)[\text{CdCl}_5] \cdot \text{H}_2\text{O}$
 $M_r = 586.03$
 Monoclinic, $P2_1/n$
 $a = 10.638$ (2) Å
 $b = 13.700$ (3) Å
 $c = 14.839$ (3) Å
 $\beta = 90.90$ (3)°

 $V = 2162.3$ (8) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.65$ mm⁻¹
 $T = 298$ K
 $0.25 \times 0.20 \times 0.18$ mm

Data collection

 Rigaku Mercury2 diffractometer
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku, 2005)
 $T_{\min} = 0.681$, $T_{\max} = 0.745$

 22228 measured reflections
 4947 independent reflections
 4155 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.068$
 $S = 1.10$
 4947 reflections

 246 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.45$ e Å⁻³
 $\Delta\rho_{\min} = -0.38$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N1}-\text{H1} \cdots \text{O1W}$	0.86	2.42	3.194 (4)	151
$\text{N4}-\text{H4A} \cdots \text{Cl5}$	0.86	2.31	3.154 (3)	168
$\text{N5}-\text{H5A} \cdots \text{Cl1}$	0.86	2.49	3.256 (2)	149
$\text{N8}-\text{H8B} \cdots \text{O1W}$	0.86	2.03	2.854 (3)	160
$\text{O1W}-\text{H1WB} \cdots \text{Cl4}$	0.84	2.82	3.478 (3)	136
$\text{N3}-\text{H3} \cdots \text{Cl2}^{\text{i}}$	0.86	2.56	3.196 (2)	132
$\text{N5}-\text{H5B} \cdots \text{Cl2}^{\text{i}}$	0.86	2.75	3.394 (3)	133
$\text{N5}-\text{H5B} \cdots \text{Cl4}^{\text{i}}$	0.86	2.60	3.313 (3)	140
$\text{N7}-\text{H7} \cdots \text{Cl4}^{\text{ii}}$	0.86	2.56	3.367 (2)	156
$\text{N8}-\text{H8A} \cdots \text{Cl1}^{\text{iii}}$	0.86	2.40	3.247 (3)	168
$\text{N9}-\text{H9A} \cdots \text{Cl2}^{\text{iii}}$	0.86	2.41	3.227 (3)	160
$\text{N9}-\text{H9B} \cdots \text{Cl4}^{\text{ii}}$	0.86	2.67	3.450 (3)	152
$\text{O1W}-\text{H1WA} \cdots \text{Cl3}^{\text{iv}}$	0.85	2.67	3.266 (3)	129

 Symmetry codes: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 2, -y, -z + 1$; (iii) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$.

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: *ORTEP-III* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PRPKAPPA* (Ferguson, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2466).

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supporting information

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1,1'-{[1,1'-(Pyridinium-2,6-diyl)diethylidyne]diimino}diguanidinium pentachloridocadm(II) monohydrate

Rui-jun Xu

S1. Comment

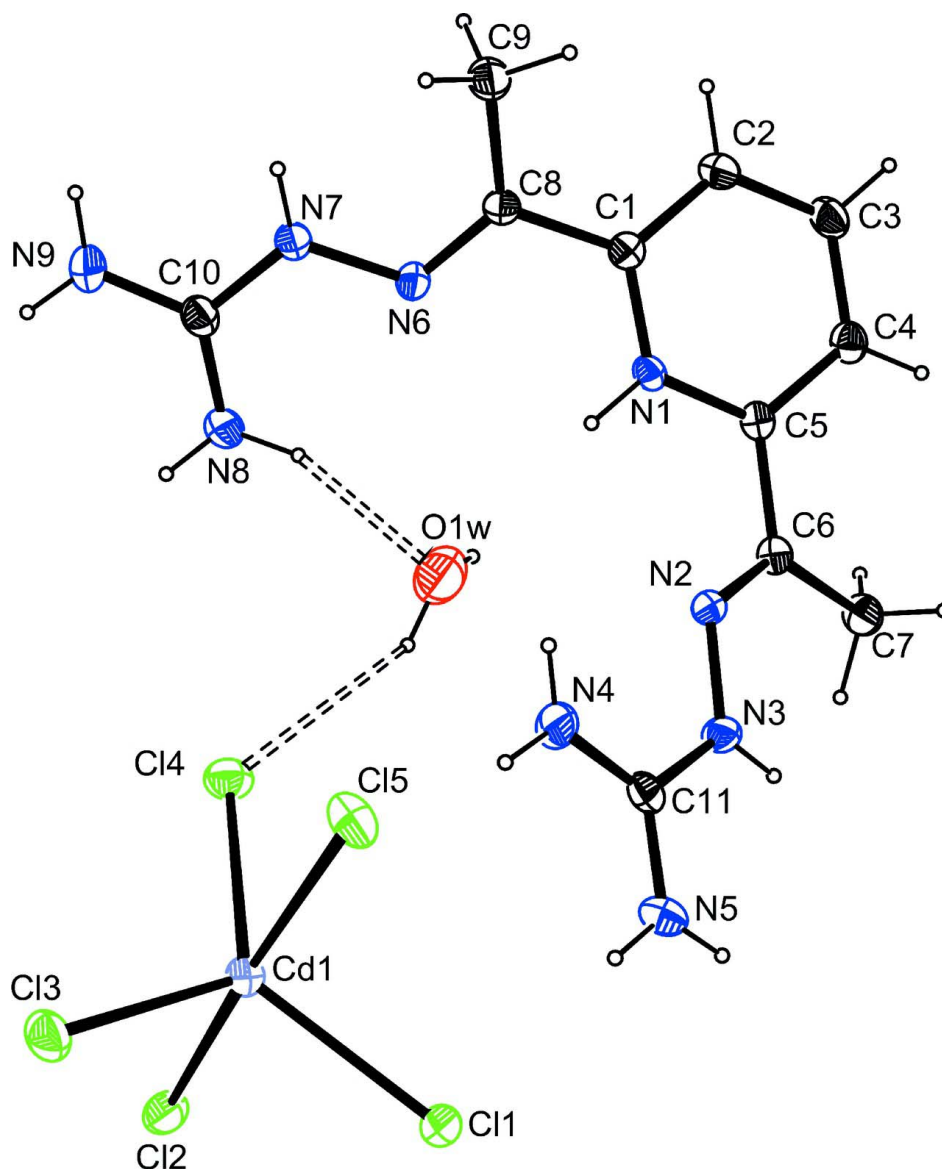
The asymmetric unit of the title compound (Fig 1) consists of pentachlorocadmium, a water molecule and H_3L , the latter resulting from protonation of the pyridyl nitrogen and the two guanyl N atoms. There are four intramolecular hydrogen bonds in the compound, *i.e.*, N4—H4···C15, N5—H5A···C11, N8—H8B···O1W and O1W—H1WB···C14 (table 1). The angle between the pyridine ring and the aminoguanidone moieties, N2—N3—C11—N4—N5 and N6—N7—C10—N8—N9, are 26.23 (2)° and 31.13 (1)° respectively. Additionally, there are also numerous hydrogen bonds among the terminal nitrogen atoms of the trication H_3L , the oxygen atom of the water molecule and the chloride atoms of pentachlorocadmium anion, leading to a complex three-dimensional network.

S2. Experimental

The ligand L was prepared according to reported method (Valdes-Martinez *et al.* 2002). The title compound was prepared by refluxing an 30 ml EtOH–HCl mixture solution (v:v = 3:1) containing an equimolar amount of L (1.096 g, 4 mmol) and $CdCl_2$ for 1 h. The resulting solution was filtered and stood still until crystals formed.

S3. Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.96 Å (methyl) or 0.93 Å (aromatic) and N—H = 0.86 Å with $U_{iso}(H) = 1.2U_{eq}(C_{aromatic} \text{ or } N)$ and $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$. H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H = 0.85 (1)Å and H···H = 1.39 (2)Å) with $U_{iso}(H) = 1.5U_{eq}(O)$. In the last stage of structure refinement, they were treated as riding on their parent O atom.

**Figure 1**

Molecular structure of the title compound, with the atom labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. H bonds are shown as dashed lines.

1,1'-[1,1'-(Pyridinium-2,6-diyl)diethylidyne]diimino}diguanidinium pentachloridocadm(II) monohydrate

Crystal data

(C₁₁H₂₀N₉)[CdCl₅]·H₂O

M_r = 586.03

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2₁ *yn*

a = 10.638 (2) Å

b = 13.700 (3) Å

c = 14.839 (3) Å

β = 90.90 (3)°

V = 2162.3 (8) Å³

Z = 4

F(000) = 1168

D_x = 1.800 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 19919 reflections

θ = 3.1–27.6°

μ = 1.65 mm⁻¹

T = 298 K

Prism, colourless

0.25 × 0.20 × 0.18 mm

Data collection

Rigaku Mercury2 (2× 2 bin mode)
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm⁻¹
CCD_Profile_fitting scans
Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2005)
 $T_{\min} = 0.681$, $T_{\max} = 0.745$

22228 measured reflections
4947 independent reflections
4155 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$
 $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.1^\circ$
 $h = -13 \rightarrow 13$
 $k = -17 \rightarrow 17$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.068$
 $S = 1.10$
4947 reflections
246 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0222P)^2 + 1.3165P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.032$
 $\Delta\rho_{\max} = 0.45 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.38 \text{ e } \text{Å}^{-3}$

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. 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 (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.91113 (2)	0.240737 (14)	0.143910 (13)	0.03119 (7)
Cl1	0.88183 (8)	0.41966 (5)	0.11166 (5)	0.04173 (18)
Cl2	0.68199 (7)	0.21144 (5)	0.06726 (5)	0.03978 (18)
Cl3	1.02297 (8)	0.14273 (6)	0.03080 (5)	0.0464 (2)
Cl4	0.82906 (7)	0.15219 (6)	0.28367 (5)	0.04094 (18)
Cl5	1.11659 (7)	0.27884 (6)	0.23687 (5)	0.04219 (19)
N1	0.89827 (19)	0.31005 (15)	0.68390 (14)	0.0238 (5)
H1	0.8938	0.2862	0.6304	0.029*
N2	0.8635 (2)	0.43124 (15)	0.54498 (14)	0.0252 (5)
N3	0.8349 (2)	0.48151 (16)	0.46731 (14)	0.0302 (5)
H3	0.7842	0.5304	0.4672	0.036*
N4	0.9582 (3)	0.37103 (17)	0.39331 (16)	0.0428 (6)
H4A	0.9939	0.3508	0.3452	0.051*
H4B	0.9673	0.3390	0.4428	0.051*
N5	0.8730 (2)	0.50235 (18)	0.31717 (15)	0.0354 (6)
H5A	0.9073	0.4842	0.2678	0.042*

H5B	0.8276	0.5543	0.3182	0.042*
N6	0.9327 (2)	0.11265 (15)	0.66384 (14)	0.0275 (5)
N7	0.9631 (2)	0.01760 (16)	0.64548 (15)	0.0334 (5)
H7	1.0230	-0.0113	0.6745	0.040*
N8	0.8182 (2)	0.01826 (18)	0.52850 (16)	0.0396 (6)
H8A	0.7755	-0.0119	0.4875	0.048*
H8B	0.8094	0.0802	0.5353	0.048*
N9	0.9142 (3)	-0.12433 (18)	0.57366 (18)	0.0488 (7)
H9A	0.8735	-0.1574	0.5336	0.059*
H9B	0.9668	-0.1531	0.6094	0.059*
C1	0.9503 (2)	0.25487 (18)	0.74947 (17)	0.0248 (5)
C2	0.9574 (3)	0.2929 (2)	0.83576 (18)	0.0325 (6)
H2	0.9943	0.2568	0.8822	0.039*
C3	0.9094 (3)	0.3846 (2)	0.85289 (18)	0.0356 (7)
H3A	0.9125	0.4096	0.9112	0.043*
C4	0.8568 (3)	0.4394 (2)	0.78360 (17)	0.0306 (6)
H4	0.8246	0.5013	0.7949	0.037*
C5	0.8526 (2)	0.40094 (18)	0.69727 (17)	0.0234 (5)
C6	0.8104 (2)	0.45750 (18)	0.61734 (17)	0.0252 (6)
C7	0.7170 (3)	0.5381 (2)	0.62813 (19)	0.0353 (7)
H7A	0.7600	0.5968	0.6460	0.053*
H7B	0.6577	0.5204	0.6734	0.053*
H7C	0.6733	0.5488	0.5719	0.053*
C8	0.9938 (2)	0.15541 (18)	0.72746 (17)	0.0243 (5)
C9	1.1001 (3)	0.1131 (2)	0.7819 (2)	0.0387 (7)
H9C	1.0674	0.0701	0.8269	0.058*
H9D	1.1464	0.1649	0.8107	0.058*
H9E	1.1547	0.0773	0.7430	0.058*
C10	0.8962 (3)	-0.0298 (2)	0.58035 (18)	0.0315 (6)
C11	0.8901 (3)	0.4506 (2)	0.39114 (18)	0.0296 (6)
O1W	0.7726 (3)	0.22202 (18)	0.5047 (2)	0.0695 (8)
H1WA	0.7156	0.2329	0.5427	0.104*
H1WB	0.7448	0.2212	0.4511	0.104*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03641 (12)	0.02847 (12)	0.02866 (11)	0.00307 (9)	-0.00053 (8)	-0.00175 (8)
Cl1	0.0584 (5)	0.0293 (4)	0.0371 (4)	0.0015 (3)	-0.0135 (3)	-0.0001 (3)
Cl2	0.0407 (4)	0.0323 (4)	0.0460 (4)	-0.0014 (3)	-0.0088 (3)	0.0055 (3)
Cl3	0.0526 (5)	0.0486 (5)	0.0379 (4)	0.0167 (4)	-0.0043 (4)	-0.0125 (3)
Cl4	0.0444 (4)	0.0433 (4)	0.0351 (4)	-0.0054 (3)	-0.0023 (3)	0.0066 (3)
Cl5	0.0293 (4)	0.0566 (5)	0.0405 (4)	0.0036 (3)	-0.0015 (3)	-0.0156 (3)
N1	0.0263 (12)	0.0259 (11)	0.0192 (10)	-0.0011 (9)	0.0021 (9)	-0.0031 (8)
N2	0.0288 (12)	0.0231 (11)	0.0236 (11)	0.0011 (9)	0.0001 (9)	0.0007 (9)
N3	0.0350 (13)	0.0292 (12)	0.0264 (12)	0.0093 (10)	0.0007 (10)	0.0007 (9)
N4	0.0649 (18)	0.0338 (14)	0.0300 (13)	0.0124 (13)	0.0137 (12)	-0.0029 (10)
N5	0.0345 (14)	0.0473 (15)	0.0243 (12)	0.0015 (11)	0.0008 (10)	0.0007 (10)

N6	0.0329 (13)	0.0228 (11)	0.0269 (12)	0.0018 (9)	0.0009 (10)	-0.0020 (9)
N7	0.0373 (14)	0.0295 (12)	0.0332 (13)	0.0073 (10)	-0.0095 (11)	-0.0055 (10)
N8	0.0488 (16)	0.0329 (13)	0.0366 (14)	-0.0056 (12)	-0.0141 (12)	-0.0023 (11)
N9	0.0656 (19)	0.0311 (14)	0.0492 (16)	0.0037 (13)	-0.0145 (14)	-0.0112 (12)
C1	0.0216 (13)	0.0262 (13)	0.0265 (13)	-0.0032 (10)	0.0022 (10)	0.0007 (10)
C2	0.0357 (16)	0.0355 (15)	0.0263 (14)	-0.0001 (13)	-0.0041 (12)	0.0013 (12)
C3	0.0441 (18)	0.0384 (17)	0.0244 (14)	-0.0012 (13)	0.0018 (13)	-0.0063 (12)
C4	0.0327 (15)	0.0305 (15)	0.0288 (14)	0.0007 (12)	0.0063 (12)	-0.0044 (11)
C5	0.0201 (13)	0.0252 (13)	0.0250 (13)	-0.0026 (10)	0.0057 (10)	-0.0025 (10)
C6	0.0221 (13)	0.0263 (14)	0.0272 (14)	0.0003 (10)	0.0028 (11)	-0.0020 (10)
C7	0.0339 (16)	0.0368 (16)	0.0350 (16)	0.0122 (13)	-0.0005 (13)	-0.0068 (12)
C8	0.0237 (13)	0.0265 (14)	0.0228 (13)	-0.0003 (10)	0.0021 (11)	0.0014 (10)
C9	0.0335 (17)	0.0387 (17)	0.0436 (17)	0.0074 (13)	-0.0108 (14)	-0.0069 (13)
C10	0.0363 (16)	0.0318 (15)	0.0265 (14)	-0.0038 (12)	0.0028 (12)	-0.0032 (11)
C11	0.0303 (15)	0.0324 (15)	0.0260 (14)	-0.0064 (12)	-0.0016 (11)	-0.0056 (11)
O1W	0.0682 (18)	0.0488 (15)	0.091 (2)	0.0023 (13)	-0.0178 (16)	0.0015 (14)

Geometric parameters (Å, °)

Cd1—C13	2.4695 (9)	N8—H8B	0.8600
Cd1—C11	2.5160 (9)	N9—C10	1.313 (4)
Cd1—C14	2.5675 (9)	N9—H9A	0.8600
Cd1—C15	2.6188 (10)	N9—H9B	0.8600
Cd1—C12	2.7036 (10)	C1—C2	1.383 (4)
N1—C1	1.344 (3)	C1—C8	1.477 (3)
N1—C5	1.352 (3)	C2—C3	1.381 (4)
N1—H1	0.8600	C2—H2	0.9300
N2—C6	1.273 (3)	C3—C4	1.385 (4)
N2—N3	1.373 (3)	C3—H3A	0.9300
N3—C11	1.350 (3)	C4—C5	1.385 (3)
N3—H3	0.8600	C4—H4	0.9300
N4—C11	1.309 (4)	C5—C6	1.481 (3)
N4—H4A	0.8600	C6—C7	1.496 (4)
N4—H4B	0.8600	C7—H7A	0.9600
N5—C11	1.317 (3)	C7—H7B	0.9600
N5—H5A	0.8600	C7—H7C	0.9600
N5—H5B	0.8600	C8—C9	1.496 (4)
N6—C8	1.280 (3)	C9—H9C	0.9600
N6—N7	1.370 (3)	C9—H9D	0.9600
N7—C10	1.356 (3)	C9—H9E	0.9600
N7—H7	0.8600	O1W—H1WA	0.8473
N8—C10	1.301 (4)	O1W—H1WB	0.8446
N8—H8A	0.8600		
C13—Cd1—C11	117.39 (3)	C3—C2—H2	120.1
C13—Cd1—C14	117.76 (3)	C1—C2—H2	120.1
C11—Cd1—C14	124.84 (3)	C2—C3—C4	120.2 (3)
C13—Cd1—C15	93.40 (3)	C2—C3—H3A	119.9

C11—Cd1—C15	90.34 (3)	C4—C3—H3A	119.9
C14—Cd1—C15	87.73 (3)	C3—C4—C5	119.1 (3)
C13—Cd1—C12	94.25 (3)	C3—C4—H4	120.4
C11—Cd1—C12	87.50 (3)	C5—C4—H4	120.4
C14—Cd1—C12	87.36 (3)	N1—C5—C4	118.7 (2)
C15—Cd1—C12	172.19 (2)	N1—C5—C6	118.0 (2)
C1—N1—C5	123.8 (2)	C4—C5—C6	123.1 (2)
C1—N1—H1	118.1	N2—C6—C5	113.2 (2)
C5—N1—H1	118.1	N2—C6—C7	127.1 (2)
C6—N2—N3	118.1 (2)	C5—C6—C7	119.6 (2)
C11—N3—N2	116.9 (2)	C6—C7—H7A	109.5
C11—N3—H3	121.6	C6—C7—H7B	109.5
N2—N3—H3	121.6	H7A—C7—H7B	109.5
C11—N4—H4A	120.0	C6—C7—H7C	109.5
C11—N4—H4B	120.0	H7A—C7—H7C	109.5
H4A—N4—H4B	120.0	H7B—C7—H7C	109.5
C11—N5—H5A	120.0	N6—C8—C1	115.3 (2)
C11—N5—H5B	120.0	N6—C8—C9	126.3 (2)
H5A—N5—H5B	120.0	C1—C8—C9	118.3 (2)
C8—N6—N7	117.6 (2)	C8—C9—H9C	109.5
C10—N7—N6	118.3 (2)	C8—C9—H9D	109.5
C10—N7—H7	120.9	H9C—C9—H9D	109.5
N6—N7—H7	120.9	C8—C9—H9E	109.5
C10—N8—H8A	120.0	H9C—C9—H9E	109.5
C10—N8—H8B	120.0	H9D—C9—H9E	109.5
H8A—N8—H8B	120.0	N8—C10—N9	123.1 (3)
C10—N9—H9A	120.0	N8—C10—N7	120.1 (3)
C10—N9—H9B	120.0	N9—C10—N7	116.8 (3)
H9A—N9—H9B	120.0	N4—C11—N5	122.5 (3)
N1—C1—C2	118.3 (2)	N4—C11—N3	119.3 (2)
N1—C1—C8	119.0 (2)	N5—C11—N3	118.2 (3)
C2—C1—C8	122.6 (2)	H1WA—O1W—H1WB	112.7
C3—C2—C1	119.9 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O1W	0.86	2.42	3.194 (4)	151
N4—H4A \cdots C15	0.86	2.31	3.154 (3)	168
N5—H5A \cdots C11	0.86	2.49	3.256 (2)	149
N8—H8B \cdots O1W	0.86	2.03	2.854 (3)	160
O1W—H1WB \cdots C14	0.84	2.82	3.478 (3)	136
N3—H3 \cdots C12 ⁱ	0.86	2.56	3.196 (2)	132
N5—H5B \cdots C12 ⁱ	0.86	2.75	3.394 (3)	133
N5—H5B \cdots C14 ⁱ	0.86	2.60	3.313 (3)	140
N7—H7 \cdots C14 ⁱⁱ	0.86	2.56	3.367 (2)	156
N8—H8A \cdots C11 ⁱⁱⁱ	0.86	2.40	3.247 (3)	168
N9—H9A \cdots C12 ⁱⁱⁱ	0.86	2.41	3.227 (3)	160

N9—H9B···C14 ⁱⁱ	0.86	2.67	3.450 (3)	152
O1W—H1WA···C13 ^{iv}	0.85	2.67	3.266 (3)	129

Symmetry codes: (i) $-x+3/2, y+1/2, -z+1/2$; (ii) $-x+2, -y, -z+1$; (iii) $-x+3/2, y-1/2, -z+1/2$; (iv) $x-1/2, -y+1/2, z+1/2$.