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Bis(acetato-κO)triaquacadmium 2-amino-4,6-dimethylpyrimidine tetrasolvate dihydrate

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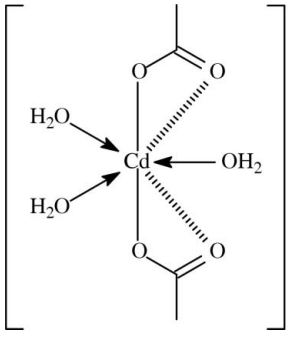
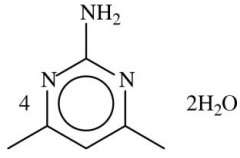
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.052; wR factor = 0.145; data-to-parameter ratio = 18.4.

The Cd atom (site symmetry 2) in the title compound, $[Cd(C_2H_3O_2)_2(H_2O)_3]\cdot 4C_6H_9N_3\cdot 2H_2O$, adopts a trigonal–bipyramidal coordination geometry but it tends towards a distorted pentagonal bipyramid owing to two long [2.674 (2) Å] Cd$\cdots$O$_{COO}$ interactions from the asymmetrically coordinated acetate anions. The neutral metal complex, uncoordinated water molecules and *N*-heterocycles engage in O—H$\cdots$O, O—H$\cdots$N, N—H$\cdots$O and N—H$\cdots$N hydrogen-bonding interactions, forming a three-dimensional network.

Related literature

For chemically related materials arising from cadmium acetate which contain cadmium coordinated by *N*-donor ligands, see: Wang *et al.* (2004); Ye *et al.* (2000); Sergienko *et al.* (1980). For details of the preparation, see: Xue *et al.* (1993).





Experimental

Crystal data

$[Cd(C_2H_3O_2)_2(H_2O)_3]\cdot 4C_6H_9N_3\cdot 2H_2O$
M_r = 813.22
Monoclinic, $P2/c$
a = 19.287 (1) Å
b = 6.7697 (4) Å
c = 14.2238 (4) Å
β = 91.444 (1)°
V = 1856.56 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 295 (2) K
0.40 × 0.20 × 0.16 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.567, T_{max} = 0.903
13020 measured reflections
4386 independent reflections
3794 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.145
S = 1.11
4386 reflections
238 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O1	2.198 (2)	Cd1—O2*w*	2.583 (5)
Cd1—O2	2.674 (2)	C1—O1	1.274 (5)
Cd1—O1*w*	2.260 (3)	C1—O2	1.214 (5)

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1*w*—H1*w*1$\cdots$N1	0.85	1.96	2.808 (3)	171
O1*w*—H1*w*2$\cdots$O3*w*	0.85	1.86	2.706 (4)	170
O2*w*—H2*w*1$\cdots$O2^{i}	0.86	2.34	3.165 (5)	162
O3*w*—H3*w*1$\cdots$O1^{ii}	0.85	1.89	2.728 (4)	167
O3*w*—H3*w*2$\cdots$O2^{iii}	0.85	1.95	2.776 (4)	164
N3—H3n1$\cdots$N4	0.86	2.20	3.055 (4)	176
N3—H3n2$\cdots$O3*w*	0.86	2.17	3.009 (4)	167
N6—H6n1$\cdots$N5^{iv}	0.86	2.47	3.324 (4)	177
N6—H6n2$\cdots$N2	0.86	2.44	3.302 (4)	175

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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: HB2393).

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supplementary materials

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Bis(acetato-*κO*)triaquacadmium 2-amino-4,6-dimethylpyrimidine tetrasolvate dihydrate

H. Fang and S. W. Ng

Comment

Cadmium acetate forms adducts with nitrogen-donor ligands and among the known crystal structures of such materials are the bis(4-aminophenyl)methane (Wang *et al.*, 2004), 2,2'-bipyridine (Ye *et al.*, 2000) and diethylnicotinamide (Sergienko *et al.*, 1980) adducts.

The title compound, (I), the product of the reaction of cadmium acetate with 2-amino-4,6-pyrimidine, has the *N*-heterocycle engaging instead in an outer-sphere type of coordination (*i.e.* interacting indirectly through hydrogen bonds). Compound (I) consists of a triaquadiacetatocadmium molecule (Cd site symmetry 2) along with an uncoordinated water molecule and two *N*-heterocycles (Fig. 1). The cadmium atom is five-coordinate, but the geometry is distorted towards a pentagonal bipyramid owing to two long Cd···O interactions (Table 1). Hydrogen bonds link the three entities into a three-dimensional network motif (Table 2).

Experimental

2-Amino-4,6-dimethylpyrimidine was synthesized according to a literature procedure (Xue *et al.*, 1993). This heterocycle (0.12 g, 1 mmol) was added to an aqueous solution (20 ml) of cadmium acetate dihydrate (0.27 g, 1 mmol). The solution was filtered and then set aside for the growth of crystals. Block-shaped crystals of (I) were harvested after a week.

Refinement

The cadmium atom, which lies on a twofold rotation axis, is disordered over two positions, the disorder refining to a 0.856 (2):0.144 (2) ratio. The vibration of the minor component was restrained to be nearly isotropic. The minor component is then covalently bonded to O2, and the distortion of geometry arises from the proximity of the O1 atom. The carbon- and nitrogen-bound H atoms were treated as riding; the methyl groups were rotated to fit the electron density. The H atoms of the water molecules were placed in chemically sensible positions on the basis of hydrogen bonding interactions, but they were not refined.

Figures

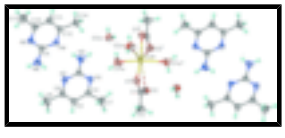


Fig. 1. The formula unit of (I). Displacement ellipsoids are shown at the 50% probability level (arbitrary spheres for the H atoms. Symmetry code (i): $1 + x$, $1 - y$, $1/2 + z$. The minor disorder component is not shown.

Bis(acetato-κ*O*)triaquacadmium dihydrate 2-amino-4,6-dimethylpyrimidine tetrasolvate dihydrate

Crystal data

$[Cd(C_2H_3O_2)_2(H_2O)_3]\cdot 4C_6H_9N_3\cdot 2H_2O$	$F_{000} = 848$
$M_r = 813.22$	$D_x = 1.455$ Mg m^{-3}
Monoclinic, $P2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yc	Cell parameters from 3660 reflections
$a = 19.287$ (1) Å	$\theta = 2.9$–27.5°
$b = 6.7697$ (4) Å	$\mu = 0.65$ mm^{-1}
$c = 14.2238$ (4) Å	$T = 295$ (2) K
$\beta = 91.444$ (1)°	Block, colorless
$V = 1856.56$ (16) Å^3	0.40 × 0.20 × 0.16 mm
$Z = 2$	

Data collection

Bruker APEX CCD diffractometer	4386 independent reflections
Radiation source: fine-focus sealed tube	3794 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.053$
$T = 295$(2) K	$\theta_{max} = 28.2^\circ$
φ and ω scans	$\theta_{min} = 1.1^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -24\rightarrow25$
$T_{min} = 0.567$, $T_{max} = 0.903$	$k = -8\rightarrow8$
13020 measured reflections	$l = -15\rightarrow18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.145$	$w = 1/[\sigma^2(F_o^2) + (0.0786P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} = 0.001$
4386 reflections	$\Delta\rho_{max} = 0.88$ e Å^{-3}
238 parameters	$\Delta\rho_{min} = -0.62$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.5000	0.83464 (7)	0.2500	0.03522 (16)	0.856 (2)
Cd1'	0.5000	0.6668 (5)	0.2500	0.0545 (12)	0.144 (2)
O1	0.44455 (12)	0.8964 (4)	0.37992 (17)	0.0488 (6)	
O2	0.45034 (12)	0.5760 (4)	0.37344 (17)	0.0508 (6)	
O1w	0.40361 (12)	0.7807 (6)	0.15998 (19)	0.0725 (10)	
H1w1	0.3597	0.7741	0.1660	0.087*	
H1w2	0.4116	0.7753	0.1013	0.087*	
O2w	0.5000	1.2162 (7)	0.2500	0.0726 (12)	
H2w1	0.4831	1.2922	0.2920	0.087*	
O3w	0.41291 (12)	0.7615 (4)	−0.02930 (18)	0.0499 (6)	
H3w1	0.4292	0.8643	−0.0557	0.060*	
H3w2	0.4306	0.6557	−0.0509	0.060*	
N1	0.25822 (12)	0.7573 (4)	0.15794 (19)	0.0381 (6)	
N2	0.15315 (13)	0.7540 (5)	0.06446 (19)	0.0413 (6)	
N3	0.25850 (14)	0.7558 (6)	−0.0040 (2)	0.0568 (9)	
H3N1	0.2369	0.7547	−0.0577	0.068*	
H3N2	0.3031	0.7570	−0.0013	0.068*	
N4	0.18959 (12)	0.7447 (4)	−0.19967 (18)	0.0374 (6)	
N5	0.09175 (13)	0.7455 (5)	−0.3069 (2)	0.0426 (6)	
N6	0.07806 (14)	0.7472 (6)	−0.1467 (2)	0.0537 (8)	
H6N1	0.0339	0.7478	−0.1565	0.064*	
H6N2	0.0949	0.7475	−0.0901	0.064*	
C1	0.43394 (16)	0.7257 (6)	0.4143 (2)	0.0433 (8)	
C2	0.4002 (2)	0.7178 (7)	0.5091 (3)	0.0613 (10)	
H2A	0.3568	0.6487	0.5032	0.092*	
H2B	0.3921	0.8498	0.5310	0.092*	
H2C	0.4302	0.6500	0.5532	0.092*	
C3	0.22286 (15)	0.7559 (5)	0.0748 (2)	0.0376 (7)	
C4	0.22067 (15)	0.7571 (5)	0.2354 (2)	0.0383 (7)	
C5	0.14889 (16)	0.7550 (6)	0.2313 (2)	0.0452 (8)	
H5	0.1230	0.7541	0.2856	0.054*	
C6	0.11762 (15)	0.7543 (6)	0.1434 (3)	0.0440 (8)	
C7	0.25937 (18)	0.7567 (6)	0.3288 (2)	0.0479 (8)	
H7A	0.2491	0.6374	0.3621	0.072*	
H7B	0.2453	0.8686	0.3651	0.072*	
H7C	0.3083	0.7639	0.3185	0.072*	
C8	0.03971 (17)	0.7526 (9)	0.1313 (3)	0.0714 (13)	
H8A	0.0273	0.7562	0.0655	0.107*	
H8B	0.0207	0.8660	0.1619	0.107*	
H8C	0.0215	0.6345	0.1588	0.107*	
C9	0.12098 (15)	0.7459 (5)	−0.2201 (2)	0.0359 (6)	
C10	0.13499 (17)	0.7441 (6)	−0.3780 (2)	0.0452 (8)	
C11	0.20641 (17)	0.7422 (6)	−0.3641 (2)	0.0453 (8)	
H11	0.2361	0.7409	−0.4145	0.054*	
C12	0.23172 (15)	0.7423 (5)	−0.2725 (2)	0.0389 (7)	

C13	0.1036 (2)	0.7431 (9)	−0.4754 (3)	0.0721 (13)
H13A	0.0591	0.6794	−0.4748	0.108*
H13B	0.1335	0.6728	−0.5167	0.108*
H13C	0.0980	0.8766	−0.4972	0.108*
C14	0.30850 (16)	0.7406 (6)	−0.2523 (3)	0.0500 (9)
H14A	0.3287	0.8597	−0.2759	0.075*
H14B	0.3289	0.6286	−0.2824	0.075*
H14C	0.3170	0.7325	−0.1856	0.075*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02966 (19)	0.0508 (3)	0.0253 (2)	0.000	0.00195 (13)	0.000
Cd1'	0.0625 (18)	0.069 (3)	0.0324 (15)	0.000	0.0009 (11)	0.000
O1	0.0517 (12)	0.0571 (15)	0.0379 (13)	0.0050 (11)	0.0090 (10)	0.0006 (11)
O2	0.0545 (13)	0.0566 (16)	0.0419 (13)	−0.0019 (12)	0.0081 (11)	−0.0023 (12)
O1w	0.0333 (12)	0.148 (3)	0.0359 (15)	−0.0059 (14)	0.0006 (11)	−0.0090 (16)
O2w	0.087 (3)	0.078 (3)	0.055 (3)	0.000	0.027 (2)	0.000
O3w	0.0531 (13)	0.0574 (15)	0.0396 (14)	−0.0016 (11)	0.0077 (11)	0.0011 (11)
N1	0.0328 (12)	0.0482 (16)	0.0333 (14)	−0.0005 (10)	−0.0039 (11)	−0.0001 (11)
N2	0.0345 (12)	0.0579 (17)	0.0314 (14)	0.0002 (11)	−0.0023 (11)	−0.0005 (12)
N3	0.0355 (14)	0.104 (3)	0.0309 (15)	0.0007 (15)	0.0006 (12)	0.0001 (16)
N4	0.0347 (12)	0.0457 (15)	0.0318 (14)	0.0000 (10)	−0.0014 (11)	0.0003 (11)
N5	0.0349 (12)	0.0547 (18)	0.0380 (15)	−0.0006 (11)	−0.0030 (11)	0.0006 (12)
N6	0.0380 (14)	0.086 (2)	0.0374 (17)	−0.0002 (14)	0.0036 (13)	0.0009 (15)
C1	0.0323 (14)	0.067 (2)	0.0305 (16)	−0.0023 (14)	0.0029 (12)	0.0035 (15)
C2	0.061 (2)	0.086 (3)	0.037 (2)	−0.002 (2)	0.0163 (18)	0.0017 (19)
C3	0.0350 (14)	0.0467 (18)	0.0310 (16)	−0.0012 (12)	−0.0025 (12)	−0.0001 (13)
C4	0.0378 (15)	0.0460 (18)	0.0309 (16)	0.0001 (12)	−0.0018 (13)	0.0004 (13)
C5	0.0357 (15)	0.066 (2)	0.0342 (17)	−0.0004 (14)	0.0036 (14)	−0.0015 (15)
C6	0.0311 (14)	0.059 (2)	0.0412 (19)	0.0010 (13)	−0.0031 (13)	0.0003 (15)
C7	0.0461 (17)	0.065 (2)	0.0317 (17)	0.0006 (15)	−0.0072 (14)	−0.0021 (15)
C8	0.0298 (16)	0.135 (4)	0.050 (2)	−0.002 (2)	0.0001 (16)	0.001 (2)
C9	0.0352 (14)	0.0381 (16)	0.0344 (16)	−0.0014 (11)	−0.0004 (12)	−0.0009 (12)
C10	0.0423 (16)	0.057 (2)	0.0358 (18)	−0.0003 (14)	−0.0073 (14)	−0.0005 (15)
C11	0.0412 (16)	0.061 (2)	0.0333 (17)	0.0005 (14)	0.0031 (14)	−0.0018 (15)
C12	0.0340 (14)	0.0457 (18)	0.0367 (17)	−0.0013 (12)	−0.0008 (13)	−0.0005 (13)
C13	0.059 (2)	0.121 (4)	0.035 (2)	0.002 (2)	−0.0132 (18)	0.001 (2)
C14	0.0323 (14)	0.071 (3)	0.046 (2)	0.0003 (14)	0.0012 (14)	0.0011 (17)

Geometric parameters (Å, °)

Cd1—O1	2.198 (2)	N5—C9	1.345 (4)
Cd1—O1^{i}	2.198 (2)	N6—C9	1.348 (4)
Cd1—O2	2.674 (2)	N6—H6N1	0.8600
Cd1—O2^{i}	2.674 (2)	N6—H6N2	0.8600
Cd1—O1w	2.260 (3)	C1—C2	1.513 (5)
Cd1—O1w^{i}	2.260 (3)	C2—H2A	0.9600

Cd1—O2w	2.583 (5)	C2—H2B	0.9600
Cd1'—O2^{i}	2.113 (3)	C2—H2C	0.9600
Cd1'—O2	2.113 (3)	C4—C5	1.384 (4)
Cd1'—O1w^{i}	2.360 (3)	C4—C7	1.507 (4)
Cd1'—O1w	2.360 (3)	C5—C6	1.375 (5)
Cd1'—C1	2.719 (3)	C5—H5	0.9300
Cd1'—C1^{i}	2.719 (3)	C6—C8	1.508 (4)
C1—O1	1.274 (5)	C7—H7A	0.9600
C1—O2	1.214 (5)	C7—H7B	0.9600
O1w—H1w1	0.85	C7—H7C	0.9600
O1w—H1w2	0.85	C8—H8A	0.9600
O2w—H2w1	0.86	C8—H8B	0.9600
O3w—H3w1	0.85	C8—H8C	0.9600
O3w—H3w2	0.85	C10—C11	1.387 (5)
N1—C4	1.334 (4)	C10—C13	1.499 (5)
N1—C3	1.350 (4)	C11—C12	1.379 (5)
N2—C6	1.330 (4)	C11—H11	0.9300
N2—C3	1.349 (4)	C12—C14	1.502 (4)
N3—C3	1.330 (4)	C13—H13A	0.9600
N3—H3N1	0.8600	C13—H13B	0.9600
N3—H3N2	0.8600	C13—H13C	0.9600
N4—C12	1.332 (4)	C14—H14A	0.9600
N4—C9	1.348 (4)	C14—H14B	0.9600
N5—C10	1.326 (4)	C14—H14C	0.9600
Cd1'—Cd1—O1	100.96 (7)	H2B—C2—H2C	109.5
Cd1'—Cd1—O1^{i}	100.96 (7)	N3—C3—N2	116.3 (3)
O1—Cd1—O1^{i}	158.07 (15)	N3—C3—N1	118.6 (3)
Cd1'—Cd1—O1w^{i}	80.71 (11)	N2—C3—N1	125.2 (3)
O1—Cd1—O1w^{i}	88.00 (9)	N1—C4—C5	121.9 (3)
O1^{i}—Cd1—O1w^{i}	95.53 (9)	N1—C4—C7	117.4 (3)
O1—Cd1—O1w	95.53 (9)	C5—C4—C7	120.6 (3)
O1^{i}—Cd1—O1w	88.00 (9)	C6—C5—C4	117.0 (3)
O1w^{i}—Cd1—O1w	161.4 (2)	C6—C5—H5	121.5
O1—Cd1—O2w	79.04 (7)	C4—C5—H5	121.5
O1^{i}—Cd1—O2w	79.04 (7)	N2—C6—C5	123.0 (3)
O1w^{i}—Cd1—O2w	99.29 (11)	N2—C6—C8	115.9 (3)
O1w—Cd1—O2w	99.29 (11)	C5—C6—C8	121.1 (3)
O2^{i}—Cd1'—O2	146.2 (2)	C4—C7—H7A	109.5
O2^{i}—Cd1'—O1w^{i}	100.29 (9)	C4—C7—H7B	109.5
O2—Cd1'—O1w^{i}	90.67 (9)	H7A—C7—H7B	109.5
O2^{i}—Cd1'—O1w	90.67 (9)	C4—C7—H7C	109.5
O2—Cd1'—O1w	100.29 (9)	H7A—C7—H7C	109.5
O1w^{i}—Cd1'—O1w	141.9 (3)	H7B—C7—H7C	109.5
C1—O1—Cd1	103.7 (2)	C6—C8—H8A	109.5
C1—O2—Cd1'	106.5 (3)	C6—C8—H8B	109.5

Cd1—O1w—H1w1	139.0	H8A—C8—H8B	109.5
Cd1'—O1w—H1w1	134.2	C6—C8—H8C	109.5
Cd1—O1w—H1w2	113.3	H8A—C8—H8C	109.5
Cd1'—O1w—H1w2	111.0	H8B—C8—H8C	109.5
H1w1—O1w—H1w2	107.5	N5—C9—N4	125.8 (3)
Cd1—O2w—H2w1	126.8	N5—C9—N6	117.4 (3)
H3w1—O3w—H3w2	111.8	N4—C9—N6	116.9 (3)
C4—N1—C3	116.8 (3)	N5—C10—C11	122.2 (3)
C6—N2—C3	116.2 (3)	N5—C10—C13	117.2 (3)
C3—N3—H3N1	120.0	C11—C10—C13	120.6 (3)
C3—N3—H3N2	120.0	C12—C11—C10	117.5 (3)
H3N1—N3—H3N2	120.0	C12—C11—H11	121.3
C12—N4—C9	116.6 (3)	C10—C11—H11	121.3
C10—N5—C9	116.3 (3)	N4—C12—C11	121.7 (3)
C9—N6—H6N1	120.0	N4—C12—C14	118.0 (3)
C9—N6—H6N2	120.0	C11—C12—C14	120.3 (3)
H6N1—N6—H6N2	120.0	C10—C13—H13A	109.5
O2—C1—O1	121.8 (3)	C10—C13—H13B	109.5
O2—C1—C2	121.4 (4)	H13A—C13—H13B	109.5
O1—C1—C2	116.8 (3)	C10—C13—H13C	109.5
O2—C1—Cd1'	48.15 (19)	H13A—C13—H13C	109.5
O1—C1—Cd1'	73.72 (19)	H13B—C13—H13C	109.5
C2—C1—Cd1'	169.2 (3)	C12—C14—H14A	109.5
C1—C2—H2A	109.5	C12—C14—H14B	109.5
C1—C2—H2B	109.5	H14A—C14—H14B	109.5
H2A—C2—H2B	109.5	C12—C14—H14C	109.5
C1—C2—H2C	109.5	H14A—C14—H14C	109.5
H2A—C2—H2C	109.5	H14B—C14—H14C	109.5
$O1^{i}$—Cd1—O1—C1	−176.9 (2)	C7—C4—C5—C6	−179.6 (3)
$O1w^{i}$—Cd1—O1—C1	−77.0 (2)	C3—N2—C6—C5	−0.5 (6)
O1w—Cd1—O1—C1	84.7 (2)	C3—N2—C6—C8	179.9 (4)
O2w—Cd1—O1—C1	−176.9 (2)	C4—C5—C6—N2	0.5 (6)
$O2^{i}$—Cd1'—O2—C1	180.0 (2)	C4—C5—C6—C8	−179.8 (4)
$O1w^{i}$—Cd1'—O2—C1	70.2 (2)	C10—N5—C9—N4	−0.1 (5)
O1w—Cd1'—O2—C1	−73.1 (3)	C10—N5—C9—N6	180.0 (3)
Cd1'—O2—C1—O1	2.9 (4)	C12—N4—C9—N5	−0.2 (5)
Cd1'—O2—C1—C2	−176.8 (3)	C12—N4—C9—N6	179.7 (3)
Cd1—O1—C1—O2	−3.6 (4)	C9—N5—C10—C11	0.3 (5)
Cd1—O1—C1—C2	176.1 (2)	C9—N5—C10—C13	179.9 (4)
C6—N2—C3—N3	−179.9 (4)	N5—C10—C11—C12	−0.2 (6)
C6—N2—C3—N1	0.2 (5)	C13—C10—C11—C12	−179.7 (4)
C4—N1—C3—N3	−179.9 (3)	C9—N4—C12—C11	0.4 (5)
C4—N1—C3—N2	−0.1 (5)	C9—N4—C12—C14	−179.9 (3)
C3—N1—C4—C5	0.1 (5)	C10—C11—C12—N4	−0.2 (6)
C3—N1—C4—C7	179.4 (3)	C10—C11—C12—C14	−179.9 (3)
N1—C4—C5—C6	−0.3 (6)		

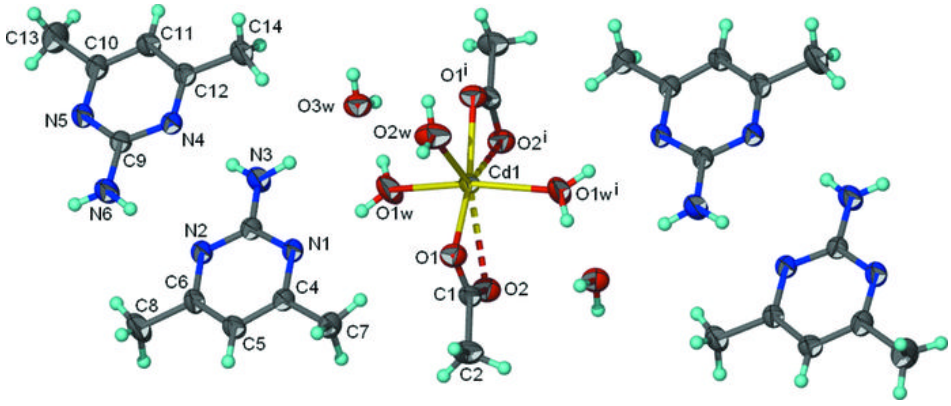
Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···N1	0.85	1.96	2.808 (3)	171
O1w—H1w2···O3w	0.85	1.86	2.706 (4)	170
O2w—H2w1···O2^{ii}	0.86	2.34	3.165 (5)	162
O3w—H3w1···O1^{iii}	0.85	1.89	2.728 (4)	167
O3w—H3w2···O2^{iv}	0.85	1.95	2.776 (4)	164
N3—H3n1···N4	0.86	2.20	3.055 (4)	176
N3—H3n2···O3w	0.86	2.17	3.009 (4)	167
N6—H6n1···N5^{v}	0.86	2.47	3.324 (4)	177
N6—H6n2···N2	0.86	2.44	3.302 (4)	175

Symmetry codes: (ii) x, y+1, z; (iii) x, −y+2, z−1/2; (iv) x, −y+1, z−1/2; (v) −x, y, −z−1/2.

Fig. 1


C13
C10
C11
C14
C12
N5
N4
C9
N6
N3
N2
N1
C6
C4
C8
C5
C7
O3w
O1i
O2w
O2i
Cd1
O1w
O1wi
O1
C1
O2
C2