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Tetraaquabis(nicotinamide-κN)-cadmium(II) bis(4-formylbenzoate)

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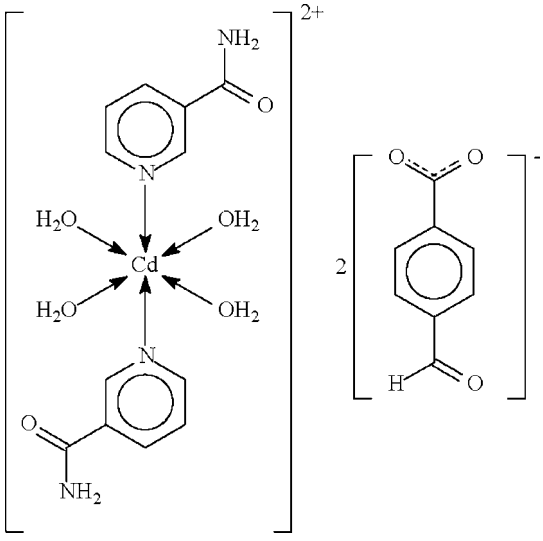
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.048; wR factor = 0.151; data-to-parameter ratio = 13.4.

The Cd^{II} ion in the title compound, $[Cd(C_6H_6N_2O)_2(H_2O)_4](C_8H_5O_3)_2$, lies on a crystallographic inversion centre in a slightly distorted octahedral environment. In the crystal structure, cations and anions interact through intermolecular hydrogen bonds to form a three-dimensional network. The amide group of the cation and the formyl group of the anion are each disordered over two sites, the approximate ratio of occupancies being 0.59:0.41 for both groups.

Related literature

For literature on metal 4-formylbenzoates, see, for example: Deng *et al.* (2006*a*,*b*).



Experimental

Crystal data

$[Cd(C_6H_6N_2O)_2(H_2O)_4](C_8H_5O_3)_2$
M_r = 726.96
Monoclinic, $P2_1/c$
a = 14.922 (1) Å
b = 7.0382 (4) Å
c = 14.030 (1) Å
β = 98.634 (2)°
V = 1456.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.82 mm^{-1}
T = 295 (2) K
0.35 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.680, T_{max} = 0.866
13559 measured reflections
3332 independent reflections
2816 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.151
S = 1.14
3332 reflections
249 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O2	0.85 (1)	1.88 (2)	2.715 (6)	168 (6)
O1w—H1w2···O3^{i}	0.85 (1)	1.98 (1)	2.828 (6)	172 (6)
O2w—H2w1···O3^{ii}	0.85 (1)	2.02 (1)	2.871 (6)	178 (7)
O2w—H2w2···O3^{iii}	0.85 (1)	1.93 (1)	2.782 (6)	174 (7)
N1—H1n1···O4^{iv}	0.86	2.03	2.86 (2)	163
N1′—H1n3···O4′^{iv}	0.86	2.10	2.95 (4)	173

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

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: LH2474).

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supplementary materials

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Tetraaquabis(nicotinamide-*κN*)cadmium(II) bis(4-formylbenzoate)

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Comment

Cadmium bis(4-formylbenzoate) forms a hydrated 1:2 adduct with imidazole; in the crystal structure, two molecules are linked by two Cd—$O_{carboxyl}$ interactions into a dinuclear species. The formylbenzoate anion functions in a chelating mode (Deng *et al.*, 2006*a*). With the larger benzimidazole ligand, a 1:1 aqua adduct is formed, and one carboxylate anion is bidentate whereas the other is monodentate in the seven-coordinate structure (Deng *et al.*, 2006*b*). Replacing the *N*-heterocycle by nicotinamide furnishes the title compound as a salt whose cation has two nicotinamide ligands binding to the tetraaquacadmium group; the carboxylate group is displaced from the coordination sphere and it exists as a free anion (Fig. 1). Hydrogen bonds link the cation and anion into a three-dimensional network.

Experimental

Cadmium diacetate dihydrate (0.133 g, 0.5 mmol) was added to an aqueous solution of 4-formylbenzoic acid (0.15 g, 1 mmol) and nicotinamide (0.122 g, 1 mmol). The pH value of the mixture was about 5. The solution was set aside for the growth of colorless prismatic crystals. CH&N elemental analysis. Calc. for $C_{28}H_{30}N_4O_{12}Cd$: C 46.26, H 4.16, N 7.71%. Found: C 46.24, H 4.11, N 7.76%.

Refinement

The amido and formyl parts are disordered over two positions; the occupancies refined to a 0.59 (1):0.41 ratio for both groups. The C6—O1 and C6—O1' bond distances were restrained to within 0.01 Å of each other, as were the C6—N1 and C6—N1' distances. The carbon- and nitrogen bound H atoms were generated geometrically (C—H 0.93, N—H 0.86 Å) and were included in the refinement in the riding-model approximation, with U(H) set to 1.2U_{eq}(C,*N*). The water H atoms were located in a difference Fourier map, and were refined with a distance restraint of O—H 0.85 (1) Å; their U_{iso}(H) values were freely refined. The final difference Fourier map had a large peak at about 1 Å from O3, but was otherwise diffuse.

Figures

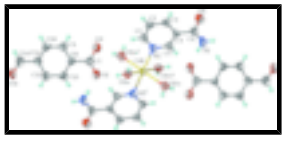


Fig. 1. Displacement ellipsoid plot of the formula unit of the salt, $[(C_6H_6N_2O)_2(H_2O)_4Cd]^{2+}$ $2[C_8H_5O_3]^-$; only the major disorder components is shown. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radius. Symmetry code: $i = 1 - x, 1 - y, 1 - z$.

Tetraaquabis(nicotinamide-κ*N*)cadmium(II) bis(4-formylbenzoate)

Crystal data

$[Cd(C_6H_6N_2O)_2(H_2O)_4](C_8H_5O_3)_2$ $F_{000} = 740$

M_r = 726.96	D_x = 1.657 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 10447 reflections
a = 14.922 (1) Å	θ = 3.1–27.5º
b = 7.0382 (4) Å	μ = 0.82 mm^{-1}
c = 14.030 (1) Å	T = 295 (2) K
β = 98.634 (2)º	Prism, colourless
V = 1456.8 (2) Å^3	0.35 × 0.24 × 0.18 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	3332 independent reflections
Radiation source: fine-focus sealed tube	2816 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 295(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −19→19
T_{min} = 0.680, T_{max} = 0.866	k = −9→8
13559 measured reflections	l = −17→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.151	$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 5.994P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.14	$(\Delta/\sigma)_{max}$ = 0.001
3332 reflections	$\Delta\rho_{max}$ = 1.08 e Å^{-3}
249 parameters	$\Delta\rho_{min}$ = −0.46 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	0.5000	0.5000	0.03018 (17)	
O1W	0.4608 (3)	0.7588 (6)	0.4012 (3)	0.0380 (8)	
H1W1	0.415 (2)	0.739 (9)	0.359 (3)	0.042 (16)*	
H1W2	0.498 (3)	0.835 (7)	0.381 (4)	0.046 (18)*	
O2W	0.5403 (3)	0.6836 (6)	0.6390 (3)	0.0429 (9)	

H2W1	0.550 (4)	0.626 (8)	0.693 (2)	0.047 (17)*	
H2W2	0.503 (3)	0.771 (7)	0.649 (5)	0.053 (19)*	
O1	0.9598 (11)	0.607 (3)	0.579 (2)	0.059 (5)	0.589 (12)
N1	0.8621 (11)	0.553 (2)	0.6850 (11)	0.047 (3)	0.589 (12)
H1N1	0.9056	0.5424	0.7325	0.056*	0.589 (12)
H1N2	0.8068	0.5408	0.6945	0.056*	0.589 (12)
O1'	0.8628 (13)	0.638 (2)	0.6856 (12)	0.045 (4)	0.411 (12)
N1'	0.9589 (15)	0.547 (5)	0.587 (3)	0.048 (7)	0.411 (12)
H1N3	1.0032	0.5548	0.6338	0.057*	0.411 (12)
H1N4	0.9687	0.5133	0.5307	0.057*	0.411 (12)
O2	0.3258 (3)	0.6507 (8)	0.2597 (3)	0.0641 (14)	
O3	0.4294 (3)	0.5203 (6)	0.1818 (3)	0.0447 (9)	
O4	0.0030 (5)	0.6015 (14)	−0.1545 (5)	0.061 (3)	0.589 (12)
O4'	0.1012 (6)	0.5493 (16)	−0.2424 (6)	0.044 (3)	0.411 (12)
N2	0.6443 (3)	0.5390 (6)	0.4632 (3)	0.0329 (9)	
C1	0.6592 (3)	0.5775 (7)	0.3732 (4)	0.0348 (10)	
H1	0.6104	0.5721	0.3235	0.042*	
C2	0.7431 (4)	0.6246 (8)	0.3510 (3)	0.0376 (11)	
H2	0.7504	0.6553	0.2881	0.045*	
C3	0.8166 (3)	0.6255 (8)	0.4242 (4)	0.0352 (10)	
H3	0.8743	0.6539	0.4108	0.042*	
C4	0.8033 (3)	0.5835 (7)	0.5178 (3)	0.0303 (9)	
C5	0.7159 (3)	0.5422 (7)	0.5338 (3)	0.0320 (10)	
H5	0.7065	0.5154	0.5964	0.038*	
C6	0.8796 (3)	0.5866 (8)	0.6012 (4)	0.0388 (11)	
C7	0.3503 (4)	0.5841 (8)	0.1864 (3)	0.0361 (11)	
C8	0.2813 (3)	0.5820 (7)	0.0956 (3)	0.0314 (9)	
C9	0.3067 (4)	0.5421 (7)	0.0065 (4)	0.0361 (11)	
H9	0.3667	0.5124	0.0025	0.043*	
C10	0.2440 (4)	0.5460 (8)	−0.0759 (4)	0.0400 (12)	
H10	0.2625	0.5257	−0.1355	0.048*	
C11	0.1527 (3)	0.5804 (8)	−0.0705 (4)	0.0360 (10)	
C12	0.1262 (4)	0.6195 (8)	0.0193 (4)	0.0414 (12)	
H12	0.0656	0.6429	0.0240	0.050*	
C13	0.1909 (3)	0.6228 (8)	0.1008 (4)	0.0375 (11)	
H13	0.1737	0.6527	0.1601	0.045*	
C14	0.0842 (4)	0.5798 (9)	−0.1583 (4)	0.0465 (13)	
H14	0.1030	0.5625	−0.2179	0.056*	0.589 (12)
H14'	0.0243	0.6036	−0.1510	0.056*	0.411 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0234 (2)	0.0379 (3)	0.0283 (2)	−0.0023 (2)	0.00111 (16)	0.0026 (2)
O1W	0.039 (2)	0.040 (2)	0.0349 (18)	0.0032 (17)	0.0037 (15)	0.0051 (16)
O2W	0.046 (2)	0.041 (2)	0.039 (2)	0.0073 (18)	−0.0027 (17)	−0.0019 (17)
O1	0.029 (5)	0.090 (15)	0.061 (7)	−0.017 (6)	0.009 (5)	−0.013 (10)
N1	0.030 (4)	0.066 (9)	0.039 (5)	−0.013 (7)	−0.009 (4)	0.006 (6)

O1'	0.041 (6)	0.058 (10)	0.034 (6)	−0.011 (8)	0.003 (4)	0.006 (7)
N1'	0.026 (8)	0.058 (16)	0.053 (12)	0.000 (8)	−0.013 (7)	−0.008 (11)
O2	0.058 (3)	0.100 (4)	0.0311 (19)	0.025 (3)	−0.0045 (18)	−0.005 (2)
O3	0.045 (2)	0.044 (2)	0.044 (2)	0.0017 (17)	−0.0005 (16)	−0.0002 (17)
O4	0.034 (4)	0.107 (7)	0.039 (4)	−0.010 (4)	−0.010 (3)	−0.007 (4)
O4'	0.028 (4)	0.075 (7)	0.027 (4)	0.010 (4)	0.000 (3)	0.000 (4)
N2	0.0265 (19)	0.037 (2)	0.035 (2)	−0.0021 (16)	0.0027 (16)	0.0034 (17)
C1	0.035 (2)	0.035 (2)	0.033 (2)	0.003 (2)	0.0001 (19)	−0.002 (2)
C2	0.043 (3)	0.043 (3)	0.029 (2)	0.007 (2)	0.011 (2)	−0.001 (2)
C3	0.030 (2)	0.039 (3)	0.039 (3)	0.000 (2)	0.0111 (19)	0.001 (2)
C4	0.025 (2)	0.032 (2)	0.033 (2)	0.0003 (19)	0.0017 (17)	−0.0002 (19)
C5	0.029 (2)	0.037 (3)	0.030 (2)	0.0011 (19)	0.0039 (18)	0.0063 (19)
C6	0.028 (2)	0.043 (3)	0.043 (3)	−0.003 (2)	0.001 (2)	0.000 (2)
C7	0.040 (3)	0.040 (3)	0.028 (2)	−0.002 (2)	0.005 (2)	0.005 (2)
C8	0.036 (2)	0.027 (2)	0.031 (2)	−0.004 (2)	0.0028 (19)	0.0007 (19)
C9	0.035 (2)	0.040 (3)	0.034 (2)	−0.002 (2)	0.009 (2)	0.003 (2)
C10	0.044 (3)	0.043 (3)	0.033 (2)	0.000 (2)	0.009 (2)	−0.002 (2)
C11	0.035 (2)	0.032 (2)	0.040 (3)	−0.005 (2)	0.003 (2)	0.001 (2)
C12	0.033 (2)	0.046 (3)	0.045 (3)	0.001 (2)	0.003 (2)	−0.007 (2)
C13	0.040 (3)	0.038 (3)	0.035 (2)	0.001 (2)	0.010 (2)	−0.002 (2)
C14	0.043 (3)	0.050 (3)	0.045 (3)	−0.005 (3)	−0.001 (2)	−0.003 (3)

Geometric parameters (Å, °)

Cd1—N2	2.305 (4)	C1—C2	1.376 (7)
Cd1—N2^{i}	2.305 (4)	C1—H1	0.9300
Cd1—O1w^{i}	2.311 (4)	C2—C3	1.385 (7)
Cd1—O1*w*	2.311 (4)	C2—H2	0.9300
Cd1—O2*w*	2.342 (4)	C3—C4	1.389 (7)
Cd1—O2w^{i}	2.342 (4)	C3—H3	0.9300
O1W—H1W1	0.85 (1)	C4—C5	1.387 (6)
O1W—H1W2	0.85 (1)	C4—C6	1.505 (7)
O2W—H2W1	0.85 (1)	C5—H5	0.9300
O2W—H2W2	0.85 (1)	C7—C8	1.512 (7)
O1—C6	1.289 (15)	C8—C9	1.388 (7)
N1—C6	1.264 (16)	C8—C13	1.392 (7)
N1—H1N1	0.8600	C9—C10	1.373 (8)
N1—H1N2	0.8600	C9—H9	0.9300
O1'—C6	1.299 (15)	C10—C11	1.397 (7)
N1'—C6	1.259 (19)	C10—H10	0.9300
N1'—H1N3	0.8600	C11—C12	1.404 (7)
N1'—H1N4	0.8600	C11—C14	1.477 (7)
O2—C7	1.235 (6)	C12—C13	1.381 (7)
O3—C7	1.274 (7)	C12—H12	0.9300
O4—C14	1.231 (9)	C13—H13	0.9300
O4'—C14	1.263 (10)	C14—H14	0.9300
N2—C1	1.342 (6)	C14—H14'	0.9300
N2—C5	1.344 (6)		

N2—Cd1—N2^{i}	180.00 (5)	C5—C4—C6	119.8 (4)
N2—Cd1—O1W^{i}	93.85 (14)	C3—C4—C6	122.2 (4)
N2^{i}—Cd1—O1W^{i}	86.15 (14)	N2—C5—C4	123.2 (4)
N2—Cd1—O1W	86.15 (14)	N2—C5—H5	118.4
N2^{i}—Cd1—O1W	93.85 (14)	C4—C5—H5	118.4
O1W^{i}—Cd1—O1W	180.00 (15)	N1'—C6—N1	116 (2)
N2—Cd1—O2W	89.39 (15)	N1—C6—O1	125.1 (15)
N2^{i}—Cd1—O2W	90.61 (15)	N1'—C6—O1'	121 (2)
O1W^{i}—Cd1—O2W	85.69 (14)	O1—C6—O1'	120.1 (15)
O1W—Cd1—O2W	94.31 (14)	N1'—C6—C4	120 (2)
N2—Cd1—O2W^{i}	90.61 (15)	N1—C6—C4	118.9 (8)
N2^{i}—Cd1—O2W^{i}	89.39 (15)	O1—C6—C4	115.7 (13)
O1W^{i}—Cd1—O2W^{i}	94.31 (14)	O1'—C6—C4	119.0 (9)
O1W—Cd1—O2W^{i}	85.69 (14)	O2—C7—O3	124.6 (5)
O2W—Cd1—O2W^{i}	180.0	O2—C7—C8	117.1 (5)
Cd1—O1W—H1W1	113 (4)	O3—C7—C8	118.3 (4)
Cd1—O1W—H1W2	126 (4)	C9—C8—C13	119.0 (5)
H1W1—O1W—H1W2	111 (6)	C9—C8—C7	121.1 (4)
Cd1—O2W—H2W1	118 (5)	C13—C8—C7	119.8 (4)
Cd1—O2W—H2W2	116 (5)	C10—C9—C8	120.7 (5)
H2W1—O2W—H2W2	103 (6)	C10—C9—H9	119.6
C6—N1—H1N1	120.0	C8—C9—H9	119.6
C6—N1—H1N2	120.0	C9—C10—C11	120.3 (5)
H1N1—N1—H1N2	120.0	C9—C10—H10	119.8
C6—N1'—H1N3	120.0	C11—C10—H10	119.8
C6—N1'—H1N4	120.0	C10—C11—C12	119.4 (5)
H1N3—N1'—H1N4	120.0	C10—C11—C14	120.9 (5)
C1—N2—C5	117.7 (4)	C12—C11—C14	119.7 (5)
C1—N2—Cd1	121.8 (3)	C13—C12—C11	119.3 (5)
C5—N2—Cd1	120.2 (3)	C13—C12—H12	120.3
N2—C1—C2	123.1 (5)	C11—C12—H12	120.3
N2—C1—H1	118.4	C12—C13—C8	121.1 (5)
C2—C1—H1	118.4	C12—C13—H13	119.5
C1—C2—C3	118.7 (5)	C8—C13—H13	119.5
C1—C2—H2	120.7	O4—C14—C11	121.8 (6)
C3—C2—H2	120.7	O4'—C14—C11	124.6 (6)
C2—C3—C4	119.3 (4)	O4—C14—H14	119.1
C2—C3—H3	120.3	C11—C14—H14	119.1
C4—C3—H3	120.3	O4'—C14—H14'	117.7
C5—C4—C3	118.0 (4)	C11—C14—H14'	117.7
O1W^{i}—Cd1—N2—C1	137.5 (4)	C5—C4—C6—O1	173.3 (11)
O1W—Cd1—N2—C1	−42.5 (4)	C3—C4—C6—O1	−8.3 (13)
O2W—Cd1—N2—C1	−136.8 (4)	C5—C4—C6—O1'	−31.8 (11)
O2W^{i}—Cd1—N2—C1	43.2 (4)	C3—C4—C6—O1'	146.6 (9)
O1W^{i}—Cd1—N2—C5	−49.1 (4)	O2—C7—C8—C9	168.4 (5)
O1W—Cd1—N2—C5	130.9 (4)	O3—C7—C8—C9	−10.6 (7)

O2W—Cd1—N2—C5	36.6 (4)	O2—C7—C8—C13	−10.9 (8)
O2W^{i}—Cd1—N2—C5	−143.4 (4)	O3—C7—C8—C13	170.1 (5)
C5—N2—C1—C2	−1.8 (8)	C13—C8—C9—C10	1.2 (8)
Cd1—N2—C1—C2	171.7 (4)	C7—C8—C9—C10	−178.1 (5)
N2—C1—C2—C3	2.5 (8)	C8—C9—C10—C11	−3.4 (8)
C1—C2—C3—C4	−1.5 (8)	C9—C10—C11—C12	2.9 (8)
C2—C3—C4—C5	0.0 (8)	C9—C10—C11—C14	−178.3 (5)
C2—C3—C4—C6	−178.5 (5)	C10—C11—C12—C13	−0.1 (8)
C1—N2—C5—C4	0.1 (7)	C14—C11—C12—C13	−179.0 (5)
Cd1—N2—C5—C4	−173.5 (4)	C11—C12—C13—C8	−2.1 (8)
C3—C4—C5—N2	0.7 (8)	C9—C8—C13—C12	1.6 (8)
C6—C4—C5—N2	179.2 (5)	C7—C8—C13—C12	−179.1 (5)
C5—C4—C6—N1'	151.4 (18)	C10—C11—C14—O4	176.8 (8)
C3—C4—C6—N1'	−30.1 (19)	C12—C11—C14—O4	−4.4 (11)
C5—C4—C6—N1	−0.7 (11)	C10—C11—C14—O4'	0.1 (11)
C3—C4—C6—N1	177.7 (9)	C12—C11—C14—O4'	178.9 (8)

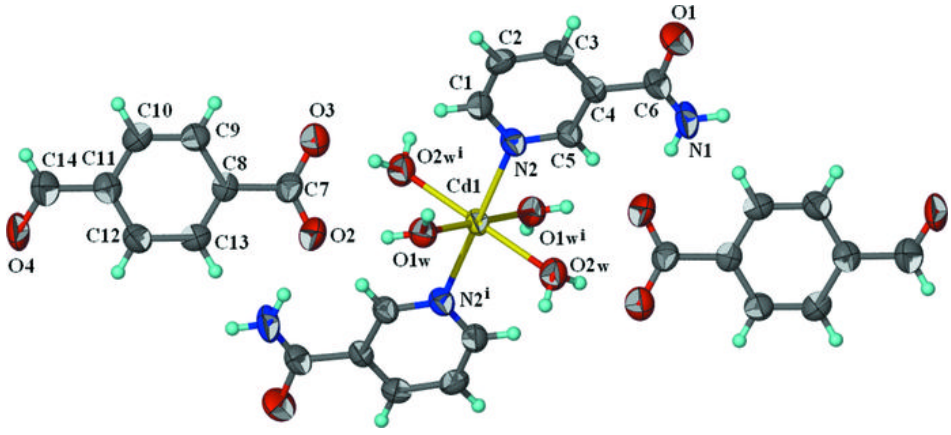
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O2	0.85 (1)	1.88 (2)	2.715 (6)	168 (6)
O1W—H1W2···O3^{ii}	0.85 (1)	1.98 (1)	2.828 (6)	172 (6)
O2W—H2W1···O3^{i}	0.85 (1)	2.02 (1)	2.871 (6)	178 (7)
O2W—H2W2···O3^{iii}	0.85 (1)	1.93 (1)	2.782 (6)	174 (7)
N1—H1N1···O4^{iv}	0.86	2.03	2.86 (2)	163
N1'—H1N3···O4'^{iv}	0.86	2.10	2.95 (4)	173

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

Fig. 1


O1
C2
C3
C1
C4
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N1
C5
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C10
C9
O3
C14
C11
C8
C7
C12
C13
O2
O4