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Bis[1,3-bis(1*H*-benzimidazol-2-yl)-benzene-κN^3]bis(nitrato-$\kappa^2 O,O'$)-cadmium(II) dihydrate

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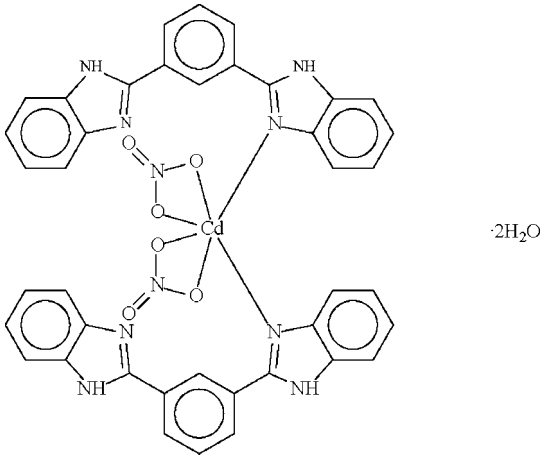
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.111; data-to-parameter ratio = 17.4.

In the title complex, $[Cd(NO_3)_2(C_{20}H_{14}N_4)_2]\cdot 2H_2O$, the Cd^{II} ion, which lies on a crystallographic twofold axis, is bis-chelated by two nitrate ligands and is coordinated by one tertiary N atom from each of two 1,3-bis(1*H*-benzimidazol-2-ylmethyl)benzene ligands in a distorted octahedral geometry. In the crystal structure, complex molecules and solvent water molecules are connected *via* hydrogen bonds to form a three-dimensional network.

Related literature

For the structure of the related adduct of 1,3-bis-(benzimidazol-2-ylmethyl)benzene with zinc terephthalate, see Meng, Liu & Ng (2007), and for the zinc succinate adduct, see Meng, Dong & Ng (2007). For the synthesis of 1,3-bis-(benzimidazol-2-ylmethyl)benzene, see Chawla & Gill (1997).



Experimental

Crystal data

$[Cd(NO_3)_2(C_{20}H_{14}N_4)_2]\cdot 2H_2O$
M_r = 893.16
Orthorhombic, *Pbcn*
a = 14.359 (1) Å
b = 16.809 (1) Å
c = 16.780 (1) Å
V = 4049.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.60 mm^{-1}
T = 293 (2) K
0.49 × 0.36 × 0.25 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.735, T_{max} = 0.863
33964 measured reflections
4651 independent reflections
3699 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.111
S = 1.01
4651 reflections
267 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*n*···O4	0.86	1.88	2.720 (3)	167
N3—H3*n*···O1^{i}	0.86	2.04	2.895 (3)	175
O4—H1*w*···O2^{ii}	0.83	2.13	2.931 (3)	163
O4—H2*w*···N4^{iii}	0.83	2.02	2.837 (3)	169

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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: LH2532).

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supplementary materials

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Bis[1,3-bis(1*H*-benzimidazol-2-yl)benzene-κN^3]bis(nitrato-$\kappa^2 O,O'$)cadmium(II) dihydrate

F.-Y. Meng, Y.-M. Zhang and S. W. Ng

Comment

We have reported the zinc terephthalate and zinc succinate adducts of 1,3-bis(benzimidazol-2-ylmethyl)benzene, an *N*-heterocycle that is capable of binding through two nitrogen sites (Meng, Dong & Ng, 2007; Meng, Liu & Ng, 2007). In the title cadmium nitrate adduct, the two ligands bind in a unidentate manner as the two nitrate groups are chelated to the metal (see Fig. 1). The Lewis-basic amino sites of the molecule engage in hydrogen bonding interactions with the lattice water molecule to furnish a three-dimensional network structure.

Experimental

1,3-Bis(benzimidazol-2-ylmethyl)benzene was prepared according to a reported procedure (Chawla & Gill, 1997). Cadmium nitrate tetrahydrate (0.08 g, 0.25 mmol), 1,3-bis(benzimidazol-2-ylmethyl)benzene (0.15 g, 0.5 mmol), ethanol (2 ml) and water (15 ml) were placed in a 23-ml, Teflon-lined, stainless -steel Parr bomb. The bomb was heated at 433 K for 5 days and cooled to room temperature at 5 K h^{-1}. Colorless crystals were obtained in 10% yield. A somewhat large block was used in the diffraction measurements.

Refinement

All H-atoms were generated geometrically, and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C,*N*,*O*) [O–H 0.83, N–H 0.86 and C–H 0.93 Å].

Figures

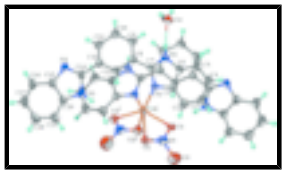


Fig. 1. **Figure 1**. The molecular structure with displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. [Symmery code (i): –*x*, *y*, 1/2 – *z*.]

Bis[1,3-bis(1*H*-benzimidazol-2-yl)benzene-κN^3]bis(nitrato- $\kappa^2 O,O'$)cadmium(II) dihydrate

Crystal data

$[Cd(NO_3)_2(C_{20}H_{14}N_4)_2]\cdot 2H_2O$	F_{000} = 1816
M_r = 893.16	D_x = 1.465 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 5514 reflections

a = 14.359 (1) Å	θ = 2.7–27.6º
b = 16.809 (1) Å	μ = 0.60 mm^{-1}
c = 16.780 (1) Å	T = 293 (2) K
V = 4049.8 (5) Å^3	Block, colorless
Z = 4	0.49 × 0.36 × 0.25 mm

Data collection

Bruker APEXII area-detector diffractometer	4651 independent reflections
Radiation source: fine-focus sealed tube	3699 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 291(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	h = −18→18
T_{min} = 0.735, T_{max} = 0.863	k = −21→21
33964 measured reflections	l = −21→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.111	$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 3.0327P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
4651 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
267 parameters	$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.0000	0.812267 (14)	0.2500	0.04011 (10)
O1	−0.06502 (14)	0.86543 (10)	0.36422 (11)	0.0525 (5)
O2	−0.11506 (18)	0.91958 (13)	0.25262 (11)	0.0589 (5)
O3	−0.1546 (3)	0.9858 (2)	0.3759 (2)	0.1299 (13)
O4	0.23158 (19)	0.46184 (12)	0.35459 (15)	0.0817 (8)
H1W	0.2820	0.4507	0.3332	0.098*
H2W	0.2029	0.4217	0.3686	0.098*
N1	0.10316 (14)	0.72662 (11)	0.30585 (11)	0.0385 (4)
N2	0.15475 (15)	0.60964 (12)	0.34838 (12)	0.0442 (5)
H2n	0.1704	0.5602	0.3479	0.053*
N3	0.09189 (15)	0.76740 (12)	−0.00421 (12)	0.0447 (5)
H3n	0.0810	0.7946	0.0382	0.054*

N4	0.12082 (18)	0.66241 (14)	−0.08129 (13)	0.0516 (5)
N5	−0.11018 (19)	0.91902 (15)	0.32757 (18)	0.0629 (7)
C1	0.12630 (16)	0.73325 (14)	0.38599 (14)	0.0394 (5)
C2	0.1238 (2)	0.79860 (17)	0.43769 (16)	0.0495 (6)
H2	0.1043	0.8485	0.4204	0.059*
C3	0.1513 (2)	0.78597 (19)	0.51496 (17)	0.0579 (7)
H3	0.1502	0.8284	0.5505	0.069*
C4	0.1808 (2)	0.7120 (2)	0.54192 (17)	0.0637 (8)
H4	0.1980	0.7060	0.5950	0.076*
C5	0.1852 (2)	0.64744 (19)	0.49195 (16)	0.0571 (7)
H5	0.2053	0.5980	0.5098	0.069*
C6	0.15785 (17)	0.65970 (15)	0.41296 (15)	0.0422 (5)
C7	0.12274 (16)	0.65194 (14)	0.28564 (14)	0.0381 (5)
C8	0.11145 (17)	0.61731 (14)	0.20567 (14)	0.0397 (5)
C9	0.09638 (18)	0.53648 (15)	0.19548 (16)	0.0465 (6)
H9	0.0941	0.5031	0.2396	0.056*
C10	0.0848 (2)	0.50543 (16)	0.11971 (17)	0.0520 (6)
H10	0.0746	0.4512	0.1133	0.062*
C11	0.08827 (19)	0.55436 (16)	0.05356 (16)	0.0494 (6)
H11	0.0806	0.5329	0.0029	0.059*
C12	0.10332 (17)	0.63595 (15)	0.06270 (15)	0.0418 (5)
C13	0.11557 (18)	0.66654 (15)	0.13896 (14)	0.0404 (5)
H13	0.1267	0.7207	0.1455	0.048*
C14	0.10567 (18)	0.68767 (14)	−0.00786 (15)	0.0428 (5)
C15	0.1167 (2)	0.73083 (17)	−0.12796 (16)	0.0507 (6)
C16	0.1305 (3)	0.7409 (2)	−0.21018 (18)	0.0707 (9)
H16	0.1434	0.6978	−0.2432	0.085*
C17	0.1241 (4)	0.8167 (2)	−0.23986 (19)	0.0782 (12)
H17	0.1330	0.8249	−0.2941	0.094*
C18	0.1049 (2)	0.8813 (2)	−0.1919 (2)	0.0689 (9)
H18	0.1010	0.9316	−0.2148	0.083*
C19	0.0915 (2)	0.87329 (18)	−0.11142 (18)	0.0587 (7)
H19	0.0784	0.9169	−0.0792	0.070*
C20	0.09844 (19)	0.79700 (16)	−0.08038 (15)	0.0461 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.05074 (17)	0.03035 (15)	0.03923 (16)	0.000	−0.00704 (10)	0.000
O1	0.0681 (12)	0.0402 (9)	0.0492 (10)	0.0111 (9)	−0.0009 (9)	0.0097 (8)
O2	0.0788 (15)	0.0489 (11)	0.0491 (11)	0.0134 (10)	−0.0123 (9)	0.0037 (8)
O3	0.155 (3)	0.110 (2)	0.126 (3)	0.045 (2)	0.046 (2)	0.003 (2)
O4	0.0975 (18)	0.0449 (11)	0.1028 (19)	0.0213 (11)	0.0434 (15)	0.0257 (12)
N1	0.0452 (11)	0.0350 (10)	0.0354 (10)	0.0008 (8)	−0.0050 (8)	0.0005 (8)
N2	0.0534 (12)	0.0371 (10)	0.0421 (11)	0.0076 (9)	0.0022 (9)	0.0071 (9)
N3	0.0537 (12)	0.0446 (11)	0.0359 (10)	0.0004 (10)	0.0009 (9)	−0.0019 (9)
N4	0.0656 (15)	0.0520 (13)	0.0373 (11)	0.0026 (11)	0.0037 (10)	−0.0036 (10)
N5	0.0662 (16)	0.0482 (13)	0.0744 (18)	−0.0002 (12)	0.0051 (13)	0.0069 (12)

C1	0.0377 (12)	0.0433 (13)	0.0373 (12)	−0.0023 (10)	−0.0029 (9)	0.0026 (10)
C2	0.0521 (15)	0.0494 (14)	0.0471 (14)	−0.0016 (12)	−0.0066 (12)	−0.0045 (11)
C3	0.0591 (17)	0.0701 (19)	0.0445 (15)	−0.0026 (15)	−0.0054 (13)	−0.0129 (14)
C4	0.0650 (19)	0.091 (2)	0.0356 (14)	−0.0044 (17)	−0.0078 (13)	0.0055 (15)
C5	0.0619 (17)	0.0670 (18)	0.0424 (14)	0.0025 (14)	−0.0019 (12)	0.0190 (13)
C6	0.0414 (13)	0.0466 (13)	0.0388 (12)	0.0005 (11)	0.0011 (10)	0.0068 (10)
C7	0.0394 (12)	0.0364 (12)	0.0385 (12)	0.0013 (9)	0.0023 (9)	0.0042 (10)
C8	0.0409 (12)	0.0367 (12)	0.0416 (13)	0.0033 (9)	0.0022 (10)	−0.0018 (10)
C9	0.0526 (14)	0.0371 (12)	0.0497 (14)	0.0020 (11)	0.0061 (12)	0.0029 (11)
C10	0.0632 (17)	0.0368 (13)	0.0560 (16)	−0.0061 (12)	0.0062 (13)	−0.0087 (11)
C11	0.0578 (15)	0.0448 (14)	0.0454 (14)	−0.0062 (12)	0.0049 (12)	−0.0093 (11)
C12	0.0424 (13)	0.0413 (13)	0.0417 (13)	0.0000 (10)	0.0048 (10)	−0.0042 (10)
C13	0.0459 (13)	0.0357 (11)	0.0396 (12)	0.0009 (10)	0.0026 (10)	−0.0014 (9)
C14	0.0440 (13)	0.0453 (13)	0.0392 (13)	−0.0012 (10)	0.0010 (10)	−0.0044 (10)
C15	0.0561 (16)	0.0561 (16)	0.0400 (13)	0.0003 (12)	0.0014 (11)	0.0005 (11)
C16	0.096 (3)	0.075 (2)	0.0408 (16)	0.0062 (19)	0.0077 (16)	−0.0025 (15)
C17	0.105 (3)	0.087 (3)	0.0428 (18)	0.002 (2)	0.0052 (17)	0.0148 (16)
C18	0.082 (2)	0.066 (2)	0.0584 (18)	−0.0030 (17)	−0.0055 (16)	0.0194 (16)
C19	0.0693 (19)	0.0529 (16)	0.0537 (16)	−0.0031 (14)	−0.0047 (14)	0.0043 (13)
C20	0.0451 (14)	0.0531 (15)	0.0399 (13)	−0.0019 (11)	−0.0019 (11)	0.0011 (11)

Geometric parameters (Å, °)

Cd1—N1^{i}	2.2682 (19)	C4—C5	1.373 (5)
Cd1—N1	2.2682 (19)	C4—H4	0.9300
Cd1—O1	2.3116 (19)	C5—C6	1.397 (4)
Cd1—O1^{i}	2.3116 (19)	C5—H5	0.9300
Cd1—O2^{i}	2.446 (2)	C7—C8	1.472 (3)
Cd1—O2	2.446 (2)	C8—C9	1.386 (3)
O1—N5	1.269 (3)	C8—C13	1.393 (3)
O2—N5	1.260 (3)	C9—C10	1.384 (4)
O3—N5	1.525 (4)	C9—H9	0.9300
O4—H1W	0.8298	C10—C11	1.382 (4)
O4—H2W	0.8250	C10—H10	0.9300
N1—C7	1.330 (3)	C11—C12	1.397 (3)
N1—C1	1.390 (3)	C11—H11	0.9300
N2—C7	1.351 (3)	C12—C13	1.390 (3)
N2—C6	1.373 (3)	C12—C14	1.469 (3)
N2—H2n	0.8600	C13—H13	0.9300
N3—C14	1.356 (3)	C15—C20	1.394 (4)
N3—C20	1.375 (3)	C15—C16	1.404 (4)
N3—H3n	0.8600	C16—C17	1.372 (5)
N4—C14	1.321 (3)	C16—H16	0.9300
N4—C15	1.393 (4)	C17—C18	1.379 (5)
C1—C6	1.392 (3)	C17—H17	0.9300
C1—C2	1.400 (4)	C18—C19	1.371 (4)
C2—C3	1.372 (4)	C18—H18	0.9300
C2—H2	0.9300	C19—C20	1.388 (4)

C3—C4	1.390 (4)	C19—H19	0.9300
C3—H3	0.9300		
$N1^{i}$—Cd1—N1	101.21 (10)	N2—C6—C1	106.1 (2)
$N1^{i}$—Cd1—O1	108.92 (7)	N2—C6—C5	131.9 (3)
N1—Cd1—O1	99.58 (7)	C1—C6—C5	122.0 (3)
$N1^{i}$—Cd1—$O1^{i}$	99.58 (7)	N1—C7—N2	111.7 (2)
N1—Cd1—$O1^{i}$	108.92 (7)	N1—C7—C8	125.6 (2)
O1—Cd1—$O1^{i}$	134.52 (9)	N2—C7—C8	122.7 (2)
$N1^{i}$—Cd1—$O2^{i}$	154.36 (7)	C9—C8—C13	119.3 (2)
N1—Cd1—$O2^{i}$	91.97 (8)	C9—C8—C7	121.2 (2)
O1—Cd1—$O2^{i}$	90.15 (7)	C13—C8—C7	119.5 (2)
$O1^{i}$—Cd1—$O2^{i}$	55.07 (6)	C8—C9—C10	120.1 (2)
$N1^{i}$—Cd1—O2	91.97 (8)	C8—C9—H9	120.0
N1—Cd1—O2	154.36 (7)	C10—C9—H9	120.0
O1—Cd1—O2	55.07 (6)	C11—C10—C9	120.6 (2)
$O1^{i}$—Cd1—O2	90.15 (7)	C11—C10—H10	119.7
$O2^{i}$—Cd1—O2	85.00 (12)	C9—C10—H10	119.7
N5—O1—Cd1	94.53 (17)	C10—C11—C12	120.1 (2)
N5—O2—Cd1	88.56 (16)	C10—C11—H11	119.9
H1W—O4—H2W	111.9	C12—C11—H11	119.9
C7—N1—C1	105.78 (19)	C13—C12—C11	118.9 (2)
C7—N1—Cd1	129.17 (15)	C13—C12—C14	121.3 (2)
C1—N1—Cd1	120.34 (15)	C11—C12—C14	119.7 (2)
C7—N2—C6	107.7 (2)	C12—C13—C8	121.0 (2)
C7—N2—H2n	126.2	C12—C13—H13	119.5
C6—N2—H2n	126.2	C8—C13—H13	119.5
C14—N3—C20	107.8 (2)	N4—C14—N3	112.6 (2)
C14—N3—H3n	126.1	N4—C14—C12	124.4 (2)
C20—N3—H3n	126.1	N3—C14—C12	123.0 (2)
C14—N4—C15	104.6 (2)	N4—C15—C20	110.2 (2)
O2—N5—O1	121.2 (3)	N4—C15—C16	130.2 (3)
O2—N5—O3	120.1 (3)	C20—C15—C16	119.6 (3)
O1—N5—O3	118.6 (3)	C17—C16—C15	117.3 (3)
N1—C1—C6	108.7 (2)	C17—C16—H16	121.3
N1—C1—C2	131.0 (2)	C15—C16—H16	121.3
C6—C1—C2	120.2 (2)	C16—C17—C18	122.2 (3)
C3—C2—C1	117.2 (3)	C16—C17—H17	118.9
C3—C2—H2	121.4	C18—C17—H17	118.9
C1—C2—H2	121.4	C19—C18—C17	121.7 (3)
C2—C3—C4	122.3 (3)	C19—C18—H18	119.2
C2—C3—H3	118.9	C17—C18—H18	119.2
C4—C3—H3	118.9	C18—C19—C20	116.8 (3)
C3—C4—C5	121.5 (3)	C18—C19—H19	121.6
C3—C4—H4	119.3	C20—C19—H19	121.6
C5—C4—H4	119.3	N3—C20—C19	132.7 (3)
C4—C5—C6	116.8 (3)	N3—C20—C15	104.9 (2)

C4—C5—H5	121.6	C19—C20—C15	122.4 (3)
C6—C5—H5	121.6		
$N1^{i}$—Cd1—O1—N5	−83.37 (16)	Cd1—N1—C7—N2	−153.49 (17)
N1—Cd1—O1—N5	171.20 (16)	C1—N1—C7—C8	−178.7 (2)
$O1^{i}$—Cd1—O1—N5	42.36 (14)	Cd1—N1—C7—C8	26.2 (3)
$O2^{i}$—Cd1—O1—N5	79.17 (16)	C6—N2—C7—N1	−1.1 (3)
O2—Cd1—O1—N5	−4.61 (16)	C6—N2—C7—C8	179.2 (2)
$N1^{i}$—Cd1—O2—N5	116.45 (17)	N1—C7—C8—C9	−153.4 (2)
N1—Cd1—O2—N5	−4.9 (3)	N2—C7—C8—C9	26.3 (4)
O1—Cd1—O2—N5	4.63 (16)	N1—C7—C8—C13	26.4 (4)
$O1^{i}$—Cd1—O2—N5	−143.95 (18)	N2—C7—C8—C13	−154.0 (2)
$O2^{i}$—Cd1—O2—N5	−89.06 (17)	C13—C8—C9—C10	−0.6 (4)
$N1^{i}$—Cd1—N1—C7	25.06 (18)	C7—C8—C9—C10	179.2 (2)
O1—Cd1—N1—C7	136.7 (2)	C8—C9—C10—C11	0.1 (4)
$O1^{i}$—Cd1—N1—C7	−79.3 (2)	C9—C10—C11—C12	−0.2 (4)
$O2^{i}$—Cd1—N1—C7	−132.8 (2)	C10—C11—C12—C13	0.6 (4)
O2—Cd1—N1—C7	144.7 (2)	C10—C11—C12—C14	−179.2 (3)
$N1^{i}$—Cd1—N1—C1	−126.94 (19)	C11—C12—C13—C8	−1.1 (4)
O1—Cd1—N1—C1	−15.31 (18)	C14—C12—C13—C8	178.7 (2)
$O1^{i}$—Cd1—N1—C1	128.74 (17)	C9—C8—C13—C12	1.0 (4)
$O2^{i}$—Cd1—N1—C1	75.18 (18)	C7—C8—C13—C12	−178.7 (2)
O2—Cd1—N1—C1	−7.3 (3)	C15—N4—C14—N3	0.2 (3)
Cd1—O2—N5—O1	−8.1 (3)	C15—N4—C14—C12	179.9 (3)
Cd1—O2—N5—O3	168.7 (3)	C20—N3—C14—N4	−0.1 (3)
Cd1—O1—N5—O2	8.6 (3)	C20—N3—C14—C12	−179.8 (2)
Cd1—O1—N5—O3	−168.2 (2)	C13—C12—C14—N4	160.1 (3)
C7—N1—C1—C6	−1.5 (3)	C11—C12—C14—N4	−20.1 (4)
Cd1—N1—C1—C6	156.26 (16)	C13—C12—C14—N3	−20.2 (4)
C7—N1—C1—C2	177.2 (3)	C11—C12—C14—N3	159.6 (3)
Cd1—N1—C1—C2	−25.0 (4)	C14—N4—C15—C20	−0.2 (3)
N1—C1—C2—C3	179.8 (3)	C14—N4—C15—C16	177.7 (3)
C6—C1—C2—C3	−1.5 (4)	N4—C15—C16—C17	−178.4 (4)
C1—C2—C3—C4	0.1 (5)	C20—C15—C16—C17	−0.7 (5)
C2—C3—C4—C5	0.9 (5)	C15—C16—C17—C18	0.0 (7)
C3—C4—C5—C6	−0.5 (5)	C16—C17—C18—C19	0.3 (7)
C7—N2—C6—C1	0.1 (3)	C17—C18—C19—C20	0.2 (5)
C7—N2—C6—C5	−179.9 (3)	C14—N3—C20—C19	−179.2 (3)
N1—C1—C6—N2	0.9 (3)	C14—N3—C20—C15	−0.1 (3)
C2—C1—C6—N2	−178.0 (2)	C18—C19—C20—N3	178.0 (3)
N1—C1—C6—C5	−179.1 (2)	C18—C19—C20—C15	−1.0 (5)
C2—C1—C6—C5	2.0 (4)	N4—C15—C20—N3	0.2 (3)
C4—C5—C6—N2	179.1 (3)	C16—C15—C20—N3	−178.0 (3)
C4—C5—C6—C1	−1.0 (4)	N4—C15—C20—C19	179.4 (3)
C1—N1—C7—N2	1.6 (3)	C16—C15—C20—C19	1.2 (5)

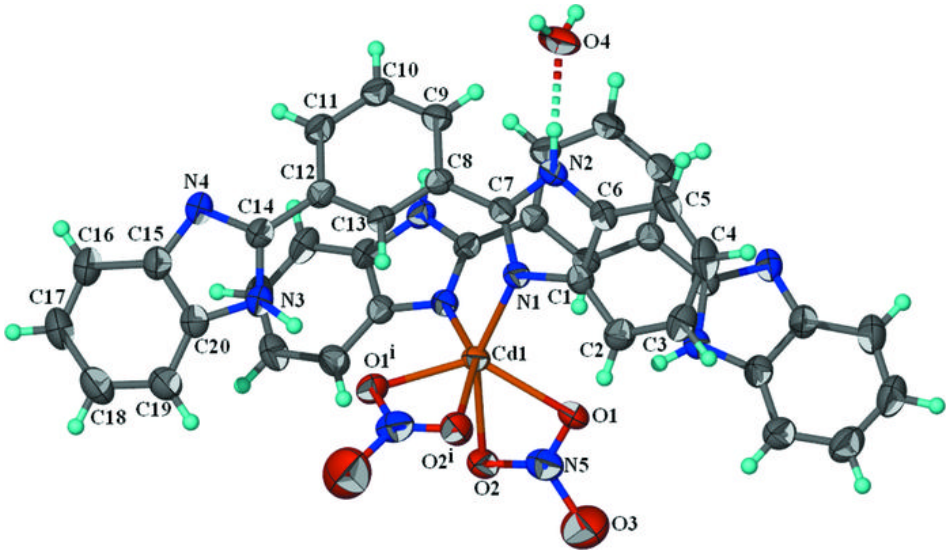
Symmetry codes: (i) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2n···O4	0.86	1.88	2.720 (3)	167
N3—H3n···O1^{i}	0.86	2.04	2.895 (3)	175
O4—H1W···O2^{ii}	0.83	2.13	2.931 (3)	163
O4—H2W···N4^{iii}	0.83	2.02	2.837 (3)	169

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

Fig. 1


O4
C10
C11
C9
C12
C8
C7
N2
C6
C5
N4
C14
C13
C16
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C17
N3
N1
C1
C20
O1i
Cd1
C2
C3
C18
C19
O1
O2i
N5
O2
O3