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Bis(μ-3,5-dinitrosalicylato)hexaimidazoledicadmium(II) dihydrate

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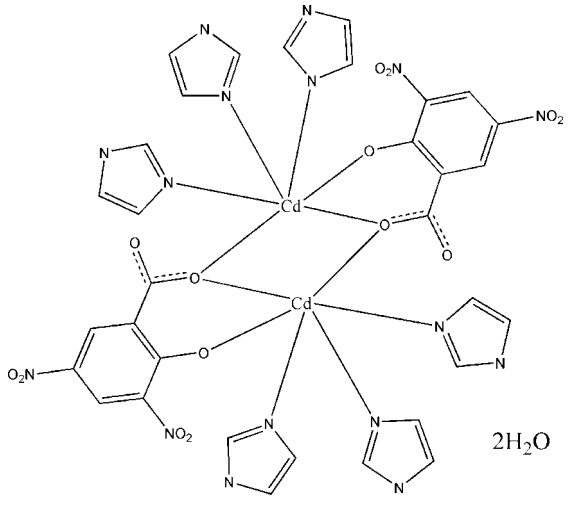
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.026; wR factor = 0.063; data-to-parameter ratio = 14.1.

The title dinuclear complex, $[Cd_2(C_7H_3N_2O_7)_2(C_3H_4N_2)_6]\cdot 2H_2O$, lies about an inversion centre. Each Cd^{II} atom is coordinated by three O atoms from two 3,5-dinitrosalicylate ligands and the N atoms of three imidazole ligands. Three ligand O atoms and one N atom lie in the equatorial plane with the two other imidazole ligands axial in a distorted octahedral coordination environment. The intramolecular Cd···Cd separation is 3.906 (4) Å. In the crystal structure, a supramolecular network forms through extensive intermolecular hydrogen-bonding interactions. One imidazole ring is disordered over two orientations in ratio of approximately 0.8:0.2.

Related literature

For related structures of 3,5-dinitrosalicylate complexes, see: Othman *et al.* (2003), Su & Xu (2005) and Tian *et al.* (2005).



Experimental

Crystal data

$[Cd_2(C_7H_3N_2O_7)_2(C_3H_4N_2)_6]\cdot 2H_2O$
M_r = 1121.54
Triclinic, $P\overline{1}$
a = 9.6267 (3) Å
b = 10.5305 (3) Å
c = 11.9560 (4) Å
α = 63.967 (2)°
β = 73.013 (2)°
γ = 79.712 (2)°
V = 1039.75 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.768, T_{max} = 0.825
17831 measured reflections
4797 independent reflections
4363 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.063
S = 1.04
4797 reflections
341 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O4^{i}	0.817 (16)	2.156 (16)	2.970 (3)	174 (3)
N6—H6···O3^{ii}	0.86	1.95	2.805 (4)	176
N4—H4···O1W^{iii}	0.86	2.09	2.932 (3)	165
N2—H2···O6^{iv}	0.86	2.51	3.132 (3)	130
N2—H2···O1W^{iv}	0.86	2.18	2.915 (3)	143
O1W—H2W···O1	0.839 (16)	1.987 (16)	2.825 (2)	179 (3)

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

Data collection: *APEXII* (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: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2305).

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supplementary materials

Acta Cryst. (2007). E**63**, m1596 [**doi:10.1107/S1600536807021460**]

Bis(μ-3,5-dinitrosalicylato)hexaimidazoledicadmium(II) dihydrate

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Comment

Whereas a large number of metal derivatives of benzoic acid have been reported, there are few examples of metal derivatives of 3,5-dinitrosalicylic acid, and examples of crystal structure reports are limited to the silver (Othman *et al.*, 2003), copper (Su & Xu, 2005) and tin (Tian *et al.*, 2005) derivatives only. We report here a dinuclear cadmium(II) complex formed by the reaction of cadmium nitrate, 3,5-dinitrosalicylic acid and imidazole in an aqueous solution.

As illustrated in Fig. 1, in the asymmetric unit of (I) each Cd^{II} centre is coordinated by three O atoms from two 3,5-dinitrosalicylate ligands, three N atoms from three imidazole ligands, and displaying a distorted octahedral geometry. The complex lies about an inversion centre to form a dinuclear complex with a Cd···Cd separation of 3.906 (4) Å. Individual molecules are further extended into a supramolecular network through intermolecular hydrogen bonds (Table 1) involving both the complex and the water solvate.

Experimental

The title complex was prepared by the addition of a stoichiometric amount of cadmium nitrate (20 mmol) and imidazole (20 mmol) to a hot aqueous solution (25 ml) of 3,5-dinitrosalicylic acid (30 mmol). The pH was then adjusted to 7.0 to 8.0 with NaOH (30 mmol). The resulting solution was filtered, and colorless crystals were obtained at room temperature on slow evaporation of the solvent over several days.

Refinement

Atoms C14, N6, C15 and C16 of one of the imidazole rings are disordered over two positions such that the two disordered rings are inclined at 75.5 (8)° to one another. The occupancy factor of the major disorder component refined to 0.792 (6). Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, N—H = 0.86 Å and with U_{iso}(H) = 1.2 U_{eq}(C, N). Water H atoms were tentatively located in a difference Fourier map and were refined with distance restraints of O–H = 0.85 Å and H···H = 1.39 Å, each within a standard deviation of 0.01 Å; and U_{iso}(H) = 1.2 U_{eq}(O).

Figures

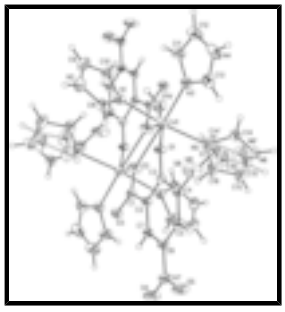


Fig. 1. The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are related to the labelled atoms by the symmetry operator $(2 - x, 2 - y, 1 - z)$.

Bis(μ-3,5-dinitrosalicylato)hexaimidazoledicadmium(II) dihydrate

Crystal data

$[Cd_2(C_7H_3N_2O_7)_2(C_3H_4N_2)_6]\cdot 2H_2O$	$Z = 1$
$M_r = 1121.54$	$F_{000} = 560$
Triclinic, $P\overline{1}$	$D_x = 1.791$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.6267$ (3) Å	Cell parameters from 4650 reflections
$b = 10.5305$ (3) Å	$\theta = 1.7$–28.0º
$c = 11.9560$ (4) Å	$\mu = 1.11$ mm^{-1}
$\alpha = 63.967$ (2)º	$T = 293$ (2) K
$\beta = 73.013$ (2)º	Block, colorless
$\gamma = 79.712$ (2)º	0.25 × 0.20 × 0.18 mm
$V = 1039.75$ (6) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	4797 independent reflections
Radiation source: fine-focus sealed tube	4363 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
$T = 293(2)$ K	$\theta_{max} = 27.6$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.768$, $T_{max} = 0.825$	$k = -13 \rightarrow 13$
17831 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of

	independent and constrained refinement
$wR(F^2) = 0.063$	$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.3686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.002$
4797 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
341 parameters	$\Delta\rho_{min} = -0.67$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	1.0356 (2)	1.0810 (2)	0.66201 (19)	0.0293 (4)	
C2	0.9348 (2)	1.0536 (2)	0.79176 (19)	0.0268 (4)	
C3	0.8365 (2)	0.9396 (2)	0.85829 (18)	0.0263 (4)	
C4	0.7447 (2)	0.9367 (2)	0.9779 (2)	0.0301 (4)	
C5	0.7498 (2)	1.0257 (2)	1.0315 (2)	0.0333 (5)	
H5	0.6902	1.0151	1.1116	0.040*	
C6	0.8463 (2)	1.1323 (2)	0.9633 (2)	0.0329 (5)	
C7	0.9366 (2)	1.1464 (2)	0.8448 (2)	0.0310 (4)	
H7	0.9996	1.2197	0.8002	0.037*	
C8	1.0851 (3)	0.6339 (3)	0.7404 (2)	0.0432 (6)	
H8	1.0668	0.6728	0.8001	0.052*	
C9	1.1692 (3)	0.4916 (3)	0.6460 (3)	0.0635 (8)	
H9	1.2188	0.4171	0.6260	0.076*	
C10	1.0809 (3)	0.5935 (3)	0.5818 (3)	0.0552 (7)	
H10	1.0582	0.6012	0.5085	0.066*	
C11	0.7147 (3)	0.5666 (3)	0.6729 (3)	0.0649 (9)	
H11	0.7910	0.5560	0.6082	0.078*	
C12	0.6127 (4)	0.4720 (4)	0.7488 (4)	0.0761 (10)	
H12	0.6052	0.3862	0.7468	0.091*	
C13	0.5730 (3)	0.6516 (3)	0.7986 (2)	0.0496 (6)	
H13	0.5295	0.7110	0.8397	0.060*	
N5	0.6563 (2)	1.0255 (2)	0.5937 (2)	0.0453 (5)	
C14	0.5098 (3)	1.0074 (3)	0.6268 (3)	0.0427 (9)	0.792 (6)

H14	0.4703	0.9193	0.6660	0.051*	0.792 (6)
N6	0.4312 (4)	1.1290 (5)	0.5968 (5)	0.0439 (10)	0.792 (6)
H6	0.3383	1.1403	0.6070	0.053*	0.792 (6)
C15	0.5259 (5)	1.2320 (5)	0.5468 (9)	0.087 (2)	0.792 (6)
H15	0.5036	1.3291	0.5175	0.104*	0.792 (6)
C16	0.6577 (4)	1.1664 (4)	0.5481 (6)	0.0833 (19)	0.792 (6)
H16	0.7424	1.2138	0.5201	0.100*	0.792 (6)
C14'	0.6515 (15)	1.1041 (17)	0.4670 (12)	0.058 (5)	0.208 (6)
H14'	0.7160	1.1048	0.3917	0.070*	0.208 (6)
N6'	0.5244 (17)	1.1799 (19)	0.4856 (13)	0.077 (5)	0.208 (6)
H6'	0.4813	1.2355	0.4262	0.092*	0.208 (6)
C15'	0.477 (2)	1.156 (3)	0.607 (2)	0.057 (7)	0.208 (6)
H15'	0.3909	1.1931	0.6457	0.069*	0.208 (6)
C16'	0.5808 (16)	1.0657 (17)	0.6632 (13)	0.060 (5)	0.208 (6)
H16'	0.5879	1.0413	0.7462	0.072*	0.208 (6)
Cd1	0.850613 (15)	0.865319 (15)	0.612784 (14)	0.02985 (6)	
N1	1.0288 (2)	0.6853 (2)	0.6410 (2)	0.0396 (4)	
N2	1.1718 (3)	0.5189 (3)	0.7456 (2)	0.0532 (6)	
H2	1.2208	0.4706	0.8023	0.064*	
N3	0.6910 (2)	0.6798 (2)	0.70391 (19)	0.0419 (5)	
N4	0.5238 (3)	0.5281 (3)	0.8282 (2)	0.0636 (7)	
H4	0.4485	0.4905	0.8874	0.076*	
N7	0.8480 (2)	1.2320 (2)	1.0149 (2)	0.0438 (5)	
N8	0.6355 (2)	0.8313 (2)	1.04896 (19)	0.0384 (4)	
O1	0.83206 (16)	0.84395 (15)	0.82153 (13)	0.0322 (3)	
O2	1.01862 (18)	1.01829 (18)	0.59849 (14)	0.0429 (4)	
O3	1.13005 (17)	1.16861 (17)	0.61858 (16)	0.0406 (4)	
O4	0.9334 (2)	1.3270 (2)	0.9547 (2)	0.0656 (6)	
O5	0.7639 (2)	1.2197 (2)	1.1182 (2)	0.0639 (6)	
O6	0.6302 (2)	0.7591 (2)	1.16355 (17)	0.0640 (6)	
O7	0.55420 (19)	0.8200 (2)	0.99275 (19)	0.0528 (5)	
O1W	0.7629 (2)	0.56782 (18)	1.00690 (16)	0.0445 (4)	
H2W	0.783 (3)	0.6497 (18)	0.951 (2)	0.053*	
H1W	0.812 (3)	0.506 (2)	0.987 (3)	0.053*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0279 (9)	0.0333 (10)	0.0255 (10)	−0.0051 (8)	−0.0032 (8)	−0.0117 (8)
C2	0.0284 (9)	0.0278 (10)	0.0236 (9)	−0.0023 (8)	−0.0036 (8)	−0.0114 (8)
C3	0.0292 (9)	0.0254 (9)	0.0231 (9)	−0.0031 (7)	−0.0045 (8)	−0.0093 (7)
C4	0.0327 (10)	0.0272 (10)	0.0275 (10)	−0.0066 (8)	−0.0011 (8)	−0.0107 (8)
C5	0.0355 (11)	0.0363 (11)	0.0268 (10)	−0.0041 (9)	0.0009 (8)	−0.0164 (9)
C6	0.0394 (11)	0.0319 (11)	0.0325 (11)	−0.0048 (9)	−0.0038 (9)	−0.0198 (9)
C7	0.0318 (10)	0.0313 (10)	0.0307 (11)	−0.0071 (8)	−0.0024 (8)	−0.0147 (8)
C8	0.0435 (13)	0.0465 (14)	0.0406 (13)	−0.0047 (10)	−0.0084 (10)	−0.0191 (11)
C9	0.0635 (18)	0.0553 (17)	0.076 (2)	0.0171 (14)	−0.0181 (16)	−0.0375 (16)
C10	0.0565 (16)	0.0647 (18)	0.0589 (17)	0.0114 (13)	−0.0189 (13)	−0.0407 (15)

C11	0.0561 (16)	0.0559 (17)	0.083 (2)	−0.0225 (14)	0.0106 (15)	−0.0395 (16)
C12	0.074 (2)	0.0573 (19)	0.095 (3)	−0.0318 (17)	−0.0073 (19)	−0.0274 (18)
C13	0.0445 (13)	0.0635 (17)	0.0393 (14)	−0.0131 (12)	−0.0044 (11)	−0.0195 (12)
N5	0.0478 (12)	0.0412 (11)	0.0470 (12)	0.0005 (9)	−0.0138 (10)	−0.0180 (10)
C14	0.0361 (15)	0.0462 (18)	0.0457 (18)	−0.0083 (13)	−0.0067 (13)	−0.0187 (14)
N6	0.027 (2)	0.0531 (19)	0.055 (2)	−0.0005 (17)	−0.0075 (17)	−0.0273 (16)
C15	0.042 (2)	0.043 (2)	0.146 (6)	−0.0050 (19)	0.000 (3)	−0.028 (3)
C16	0.0330 (18)	0.043 (2)	0.145 (5)	−0.0088 (15)	−0.002 (2)	−0.021 (2)
C14'	0.049 (7)	0.080 (10)	0.026 (6)	0.009 (7)	−0.003 (5)	−0.012 (6)
N6'	0.086 (11)	0.080 (11)	0.053 (8)	0.042 (8)	−0.046 (8)	−0.015 (7)
C15'	0.026 (10)	0.09 (2)	0.062 (11)	0.026 (11)	−0.017 (9)	−0.044 (12)
C16'	0.061 (9)	0.081 (11)	0.037 (7)	0.024 (8)	−0.027 (6)	−0.023 (7)
Cd1	0.03198 (9)	0.03015 (9)	0.02494 (9)	−0.00745 (6)	−0.00006 (6)	−0.01130 (6)
N1	0.0387 (10)	0.0431 (11)	0.0430 (11)	0.0020 (8)	−0.0110 (9)	−0.0242 (9)
N2	0.0506 (13)	0.0531 (13)	0.0510 (14)	0.0052 (10)	−0.0191 (11)	−0.0159 (11)
N3	0.0392 (10)	0.0432 (11)	0.0396 (11)	−0.0135 (8)	0.0007 (8)	−0.0160 (9)
N4	0.0557 (14)	0.0729 (17)	0.0478 (14)	−0.0376 (13)	−0.0041 (11)	−0.0047 (12)
N7	0.0494 (11)	0.0457 (11)	0.0454 (12)	−0.0090 (9)	−0.0006 (9)	−0.0312 (10)
N8	0.0416 (10)	0.0346 (10)	0.0363 (10)	−0.0113 (8)	0.0081 (8)	−0.0198 (8)
O1	0.0429 (8)	0.0287 (7)	0.0248 (7)	−0.0106 (6)	0.0008 (6)	−0.0133 (6)
O2	0.0507 (9)	0.0558 (10)	0.0267 (8)	−0.0256 (8)	0.0062 (7)	−0.0223 (7)
O3	0.0363 (8)	0.0446 (9)	0.0399 (9)	−0.0175 (7)	0.0064 (7)	−0.0207 (7)
O4	0.0769 (13)	0.0598 (12)	0.0708 (14)	−0.0355 (11)	0.0163 (11)	−0.0460 (11)
O5	0.0726 (13)	0.0752 (14)	0.0578 (12)	−0.0262 (11)	0.0184 (10)	−0.0530 (11)
O6	0.0927 (15)	0.0553 (12)	0.0311 (9)	−0.0352 (11)	0.0056 (9)	−0.0078 (8)
O7	0.0407 (9)	0.0622 (12)	0.0589 (12)	−0.0179 (8)	−0.0027 (8)	−0.0282 (10)
O1W	0.0536 (10)	0.0340 (9)	0.0377 (9)	−0.0083 (8)	−0.0008 (8)	−0.0118 (7)

Geometric parameters (Å, °)

C1—O3	1.245 (2)	N5—C14	1.373 (4)
C1—O2	1.262 (3)	N5—C14'	1.382 (13)
C1—C2	1.503 (3)	N5—Cd1	2.276 (2)
C2—C7	1.384 (3)	C14—N6	1.323 (6)
C2—C3	1.447 (3)	C14—H14	0.9300
C3—O1	1.275 (2)	N6—C15	1.354 (6)
C3—C4	1.435 (3)	N6—H6	0.8600
C4—C5	1.362 (3)	C15—C16	1.333 (6)
C4—N8	1.459 (3)	C15—H15	0.9300
C5—C6	1.383 (3)	C16—H16	0.9300
C5—H5	0.9300	C14'—N6'	1.353 (19)
C6—C7	1.388 (3)	C14'—H14'	0.9300
C6—N7	1.437 (3)	N6'—C15'	1.31 (3)
C7—H7	0.9300	N6'—H6'	0.8600
C8—N1	1.305 (3)	C15'—C16'	1.37 (2)
C8—N2	1.331 (3)	C15'—H15'	0.9300
C8—H8	0.9300	C16'—H16'	0.9300
C9—C10	1.340 (4)	Cd1—N1	2.2949 (19)
C9—N2	1.348 (4)	Cd1—O2^{i}	2.3330 (14)

C9—H9	0.9300	Cd1—O1	2.3606 (15)
C10—N1	1.381 (3)	Cd1—N3	2.3647 (18)
C10—H10	0.9300	Cd1—O2	2.4015 (16)
C11—C12	1.348 (4)	N2—H2	0.8600
C11—N3	1.360 (4)	N4—H4	0.8600
C11—H11	0.9300	N7—O4	1.229 (3)
C12—N4	1.349 (5)	N7—O5	1.229 (3)
C12—H12	0.9300	N8—O7	1.220 (3)
C13—N3	1.317 (3)	N8—O6	1.231 (3)
C13—N4	1.327 (4)	O2—Cd1^{i}	2.3330 (14)
C13—H13	0.9300	O1W—H2W	0.839 (16)
N5—C16'	1.115 (15)	O1W—H1W	0.817 (16)
N5—C16	1.338 (4)		
O3—C1—O2	121.97 (18)	C16—C15—H15	126.9
O3—C1—C2	119.04 (19)	N6—C15—H15	126.9
O2—C1—C2	118.94 (17)	C15—C16—N5	113.4 (3)
C7—C2—C3	120.54 (18)	C15—C16—H16	123.3
C7—C2—C1	116.47 (17)	N5—C16—H16	123.3
C3—C2—C1	122.96 (18)	N6'—C14'—N5	98.6 (10)
O1—C3—C4	120.58 (17)	N6'—C14'—H14'	130.7
O1—C3—C2	125.47 (17)	N5—C14'—H14'	130.7
C4—C3—C2	113.87 (18)	C15'—N6'—C14'	110.3 (13)
C5—C4—C3	125.37 (18)	C15'—N6'—H6'	124.9
C5—C4—N8	116.31 (18)	C14'—N6'—H6'	124.9
C3—C4—N8	118.31 (18)	N6'—C15'—C16'	104.2 (15)
C4—C5—C6	117.91 (19)	N6'—C15'—H15'	127.9
C4—C5—H5	121.0	C16'—C15'—H15'	127.9
C6—C5—H5	121.0	N5—C16'—C15'	109.0 (14)
C5—C6—C7	120.9 (2)	N5—C16'—H16'	125.5
C5—C6—N7	118.89 (19)	C15'—C16'—H16'	125.5
C7—C6—N7	120.17 (19)	N5—Cd1—N1	173.81 (7)
C2—C7—C6	121.32 (19)	N5—Cd1—O2^{i}	94.73 (7)
C2—C7—H7	119.3	N1—Cd1—O2^{i}	89.21 (7)
C6—C7—H7	119.3	N5—Cd1—O1	90.80 (7)
N1—C8—N2	111.5 (2)	N1—Cd1—O1	89.17 (6)
N1—C8—H8	124.3	O2^{i}—Cd1—O1	140.55 (5)
N2—C8—H8	124.3	N5—Cd1—N3	89.69 (7)
C10—C9—N2	106.2 (3)	N1—Cd1—N3	84.13 (7)
C10—C9—H9	126.9	O2^{i}—Cd1—N3	130.33 (6)
N2—C9—H9	126.9	O1—Cd1—N3	88.64 (6)
C9—C10—N1	109.6 (3)	N5—Cd1—O2	96.54 (7)
C9—C10—H10	125.2	N1—Cd1—O2	89.33 (7)
N1—C10—H10	125.2	O2^{i}—Cd1—O2	68.82 (6)
C12—C11—N3	110.8 (3)	O1—Cd1—O2	71.75 (5)
C12—C11—H11	124.6	N3—Cd1—O2	159.44 (7)
N3—C11—H11	124.6	C8—N1—C10	104.9 (2)
C11—C12—N4	105.4 (3)	C8—N1—Cd1	121.98 (17)

C11—C12—H12	127.3	C10—N1—Cd1	132.17 (18)
N4—C12—H12	127.3	C8—N2—C9	107.9 (2)
N3—C13—N4	111.7 (3)	C8—N2—H2	126.1
N3—C13—H13	124.1	C9—N2—H2	126.1
N4—C13—H13	124.1	C13—N3—C11	104.3 (2)
C16'—N5—C16	69.1 (9)	C13—N3—Cd1	131.26 (19)
C16'—N5—C14	59.9 (9)	C11—N3—Cd1	124.20 (16)
C16—N5—C14	101.4 (2)	C13—N4—C12	107.8 (2)
C16'—N5—C14'	115.2 (9)	C13—N4—H4	126.1
C16—N5—C14'	62.3 (7)	C12—N4—H4	126.1
C14—N5—C14'	90.3 (6)	O4—N7—O5	121.9 (2)
C16'—N5—Cd1	131.7 (7)	O4—N7—C6	119.18 (19)
C16—N5—Cd1	127.5 (2)	O5—N7—C6	118.9 (2)
C14—N5—Cd1	131.09 (19)	O7—N8—O6	123.7 (2)
C14'—N5—Cd1	111.7 (6)	O7—N8—C4	118.77 (19)
N6—C14—N5	112.6 (3)	O6—N8—C4	117.5 (2)
N6—C14—H14	123.7	C3—O1—Cd1	129.08 (12)
N5—C14—H14	123.7	C1—O2—Cd1^{i}	107.47 (12)
C14—N6—C15	106.4 (4)	C1—O2—Cd1	138.66 (13)
C14—N6—H6	126.8	Cd1^{i}—O2—Cd1	111.18 (6)
C15—N6—H6	126.8	H2W—O1W—H1W	113 (2)
C16—C15—N6	106.2 (4)		

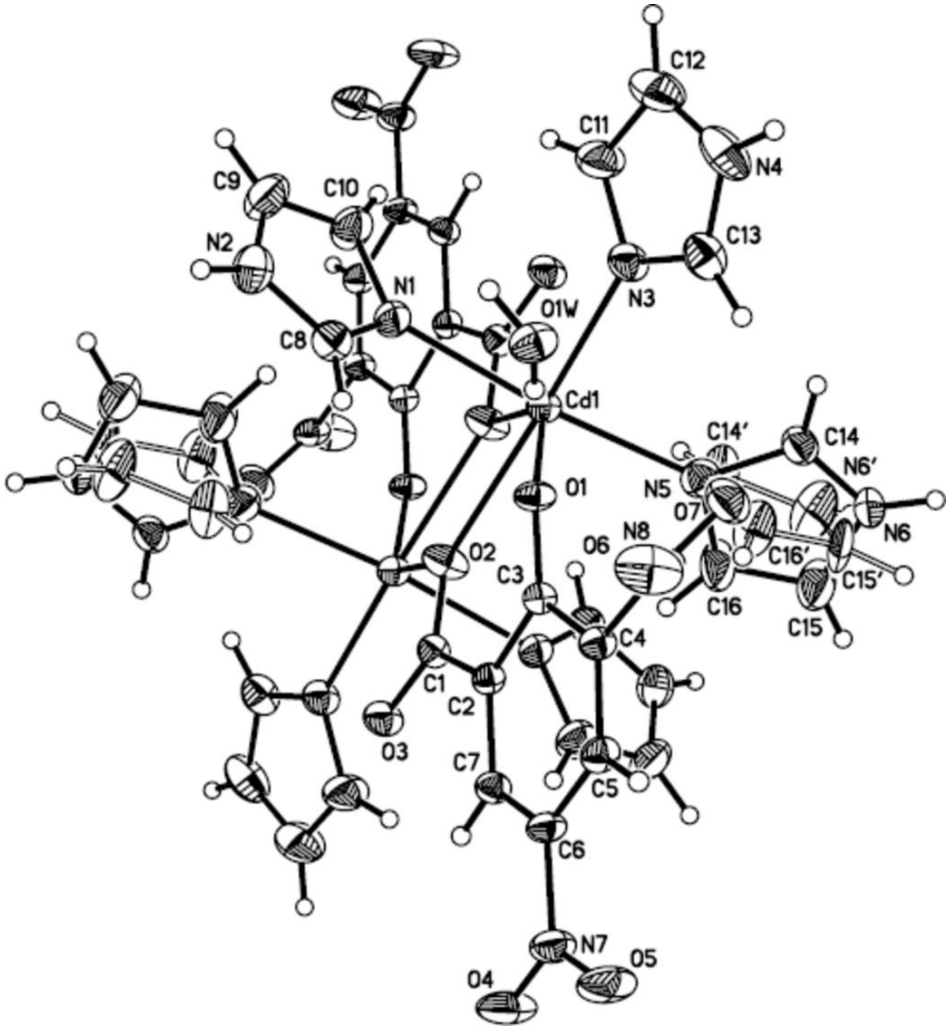
Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···O4^{ii}	0.817 (16)	2.156 (16)	2.970 (3)	174 (3)
N6—H6···O3^{iii}	0.86	1.95	2.805 (4)	176
N4—H4···O1W^{iv}	0.86	2.09	2.932 (3)	165
N2—H2···O6^{v}	0.86	2.51	3.132 (3)	130
N2—H2···O1W^{v}	0.86	2.18	2.915 (3)	143
O1W—H2W···O1	0.839 (16)	1.987 (16)	2.825 (2)	179 (3)

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

Fig. 1


C12
C11
N4
C9
C10
C13
N2
N1
O1W
N3
C8
Cd1
C14'
C14
N6'
O1
N5
O7
N8
N6
O6
O2
C3
C16'
C15'
C16
C15
C4
C1
C2
O3
C7
C5
C6
N7
O5
O4