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Aqua(nitrato-κ^2O,O')bis(4-nitrobenzohydrazide-κ^2N^2,O)cadmium(II) nitrate

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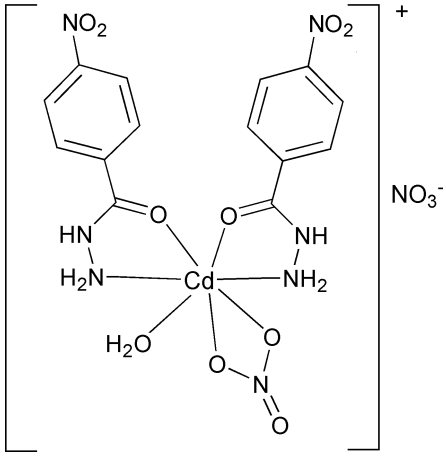
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.052; data-to-parameter ratio = 16.7.

In the title compound, $[Cd(NO_3)(C_7H_7N_3O_3)_2(H_2O)]NO_3$, the Cd atom is coordinated by two organic ligands, a water molecule and a nitrate anion. The coordination can be described as distorted pentagonal bipyramidal. Geometric parameters show that the nitrate anion is coordinated in the bidentate mode. Non-coordinated and bidentate chelating nitrates create hydrogen-bonding networks in the *a*- and *b*-axis directions, respectively. Parallel-oriented 4-nitrobenzohydrazides help to establish the packing.

Related literature

For geometrical studies of the coordination mode of the nitrate anion, see: Kleywegt *et al.* (1985) and Dowling *et al.*, (1996).



Experimental

Crystal data

$[Cd(NO_3)(C_7H_7N_3O_3)_2(H_2O)]NO_3$
M_r = 616.75
Triclinic, $P\overline{1}$
a = 5.6112 (5) Å
b = 13.1253 (12) Å
c = 14.8985 (13) Å
α = 101.314 (8)°
β = 96.944 (7)°
γ = 92.410 (7)°
V = 1065.60 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 293 (2) K
0.52 × 0.38 × 0.27 mm

Data collection

Kuma KM-4 diffractometer with CCD area-detector
Absorption correction: numerical (CrysAlis; Mayer, 2006)
T_{min} = 0.732, T_{max} = 0.871
15437 measured reflections
5431 independent reflections
4512 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.052
S = 0.97
5431 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O*W*1	2.2590 (14)	Cd1—N12*B*	2.3518 (16)
Cd1—O11*A*	2.3242 (13)	Cd1—O1*A*	2.3934 (13)
Cd1—O11*B*	2.3339 (12)	Cd1—O2*A*	2.5755 (15)
Cd1—N12*A*	2.3489 (17)		
O*W*1—Cd1—O1*A*	98.97 (5)	O11*B*—Cd1—O1*A*	81.00 (5)
O*W*1—Cd1—O2*A*	89.50 (6)	O11*B*—Cd1—O2*A*	81.90 (5)
O*W*1—Cd1—O11*A*	93.34 (5)	O11*B*—Cd1—N12*A*	100.01 (6)
O*W*1—Cd1—O11*B*	168.98 (5)	O11*B*—Cd1—N12*B*	71.62 (5)
O*W*1—Cd1—N12*A*	90.92 (6)	N12*A*—Cd1—O1*A*	83.53 (5)
O*W*1—Cd1—N12*B*	99.57 (5)	N12*A*—Cd1—O2*A*	133.98 (5)
O11*A*—Cd1—O1*A*	150.85 (5)	N12*A*—Cd1—N12*B*	149.50 (6)
O11*A*—Cd1—O2*A*	155.97 (5)	N12*B*—Cd1—O1*A*	122.36 (5)
O11*A*—Cd1—O11*B*	91.78 (5)	N12*B*—Cd1—O2*A*	75.09 (5)
O11*A*—Cd1—N12*A*	69.88 (5)	O1*A*—Cd1—O2*A*	51.06 (4)
O11*A*—Cd1—N12*B*	80.91 (5)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11*A*—H11*A*···O3*B*^{i}	0.86	2.03	2.886 (2)	171.2
N12*A*—H21*A*···O1*B*^{i}	0.87	2.42	2.977 (2)	122.2
N12*A*—H22*A*···O1*B*	0.86	2.60	3.209 (2)	128.8
N11*B*—H11*B*···O3*A*^{ii}	0.84	2.59	3.176 (2)	127.6
N12*B*—H22*B*···O11*B*^{iii}	0.86	2.40	3.212 (2)	156.9
O*W*1—H*W*1···O1*A*^{iii}	0.84	2.05	2.815 (2)	151.2
O*W*1—H*W*2···O2*B*	0.82	1.95	2.769 (2)	174.2

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

Data collection: *CrysAlis* (Mayer, 2006); cell refinement: *CrysAlis*; data reduction: *CrysAlis*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *publCIF* (Westrip, 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2039).

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supplementary materials

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Aqua(nitrato-κ^2O,O')bis(4-nitrobenzohydrazide-κ^2N^2,O)cadmium(II) nitrate

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Comment

In the title compound, cadmium is coordinated by two *p*-nitrobenzoylhydrazine molecules, a water molecules and a bidentate chelating nitrate. These ligands create atypical seven coordination sphere around the Cd atom and the geometry around Cd can be described as a pentagonal bipyramid. The Cd—$O_{nitrate}$ bond lenghts difference, Co—O—N angles difference and Co—N—$O_{terminal}$ are 0.18 Å, 7.9° and 173° respectively, and correlate well with the bidentate mode of the nitrate group (Kleywegt *et al.*, 1985; Dowling *et al.*, 1996). Noncoordinated and bidentate chelating nitrates create hydrogen bonding network in *a* and *b* directions, respectively. Interestingly, both oxygen atoms from the $–NO_2$ groups do not participate in hydrogen bonding network. But two parallel-oriented organic ligands help to establish the packing.

Experimental

1.8 g (1 mmol) of *p*-nitrobenzoylhydrazine was dissolved in 50 ml hot ethanol and mixed with 3 ml e thanolic solution of $Cd(NO_3)_2$ (3.1 g; 1 mmol). Pale yellow crystals were formed after 24 h, then filtered, washed with ethanol and dried in the air.

Refinement

All the hydrogen atoms were visible in the difference maps and were included in the refienements with isotropic displacement parameters correlated with the anisotropic displacement parameters of the atoms to which they were bonded [C—H 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The positions of hydrogen atoms from hydrazine group and water molecules were determined from the difference maps and were not refined [$U_{iso}(H) = 1.5U_{eq}(N, O)$].

Figures

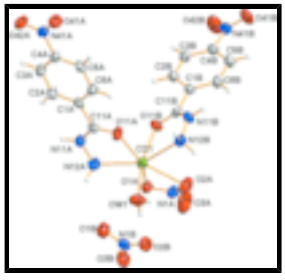


Fig. 1. Molecular diagram of the title compound; displacement ellipsoids are drawn at 50% probability level.

Aqua(nitrato-κ^2O,O')bis(4-nitrobenzohydrazide-κ^2N^2,O)cadmium(II) nitrate

Crystal data

$[Cd(NO_3)(C_7H_7N_3O_3)_2(H_2O)]NO_3$ $Z = 2$

M_r = 616.75	F_{000} = 616
Triclinic, $P\bar{1}$	D_x = 1.922 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 5.6112 (5) Å	Cell parameters from 4512 reflections
b = 13.1253 (12) Å	θ = 3.8–28.7º
c = 14.8985 (13) Å	μ = 1.11 mm^{-1}
α = 101.314 (8)º	T = 293 (2) K
β = 96.944 (7)º	Prism, pale yellow
γ = 92.410 (7)º	0.52 × 0.38 × 0.27 mm
V = 1065.60 (16) Å^3	

Data collection

Kuma KM-4 with CCD area-detector diffractometer	5431 independent reflections
Radiation source: fine-focus sealed tube	4512 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
Detector resolution: 1024x1024 with blocks 2x2, 33.133pixel/mm pixels mm^{-1}	θ_{max} = 28.7º
T = 293(2) K	θ_{min} = 3.8º
ω scans	h = −7→5
Absorption correction: numerical (CrysAlis; Mayer, 2006)	k = −17→17
T_{min} = 0.732, T_{max} = 0.871	l = −20→19
15437 measured reflections	

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-atom parameters constrained
$wR(F^2)$ = 0.052	$w = 1/[\sigma^2(F_o^2) + (0.0267P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.97	$(\Delta/\sigma)_{max}$ = 0.002
5431 reflections	$\Delta\rho_{max}$ = 0.97 e Å^{-3}
325 parameters	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Cd1	0.59006 (2)	0.274165 (10)	0.565944 (9)	0.03011 (5)
C1A	0.5103 (3)	0.52629 (13)	0.81049 (12)	0.0261 (4)
C11A	0.5625 (3)	0.46464 (13)	0.71999 (13)	0.0290 (4)
O11A	0.4313 (2)	0.38598 (10)	0.68154 (10)	0.0407 (3)
N11A	0.7531 (3)	0.49594 (12)	0.68482 (11)	0.0348 (4)
H11A	0.8437	0.5527	0.7047	0.052*
N12A	0.8041 (3)	0.43772 (14)	0.59929 (12)	0.0460 (4)
H21A	0.9605	0.4373	0.6088	0.069*
H22A	0.7648	0.4700	0.5550	0.069*
C2A	0.6575 (3)	0.61149 (14)	0.86218 (13)	0.0330 (4)
H2A	0.7939	0.6339	0.8398	0.040*
C3A	0.6004 (3)	0.66265 (14)	0.94665 (13)	0.0326 (4)
H3A	0.6975	0.7193	0.9815	0.039*
C4A	0.3976 (3)	0.62799 (13)	0.97783 (12)	0.0268 (4)
N41A	0.3394 (3)	0.68027 (12)	1.06882 (11)	0.0333 (4)
O41A	0.1525 (3)	0.65143 (12)	1.09355 (10)	0.0501 (4)
O42A	0.4805 (3)	0.74886 (12)	1.11520 (10)	0.0508 (4)
C5A	0.2474 (3)	0.54486 (14)	0.92790 (13)	0.0323 (4)
H5A	0.1096	0.5238	0.9502	0.039*
C6A	0.3066 (3)	0.49366 (14)	0.84399 (13)	0.0318 (4)
H6A	0.2088	0.4369	0.8098	0.038*
C1B	0.8042 (3)	0.06198 (13)	0.76333 (12)	0.0260 (4)
C11B	0.6867 (3)	0.12651 (13)	0.70058 (11)	0.0249 (4)
O11B	0.8056 (2)	0.19365 (10)	0.67342 (9)	0.0330 (3)
N11B	0.4503 (3)	0.10695 (12)	0.67616 (11)	0.0299 (3)
H11B	0.3780	0.0572	0.6923	0.045*
N12B	0.3254 (3)	0.15387 (12)	0.60875 (11)	0.0308 (3)
H21B	0.2814	0.1053	0.5615	0.046*
H22B	0.2058	0.1828	0.6323	0.046*
C2B	1.0212 (3)	0.10100 (14)	0.81649 (13)	0.0302 (4)
H2B	1.0826	0.1678	0.8162	0.036*
C3B	1.1467 (3)	0.04045 (14)	0.87002 (13)	0.0332 (4)
H3B	1.2942	0.0651	0.9047	0.040*
C4B	1.0468 (3)	−0.05734 (14)	0.87046 (12)	0.0297 (4)
N41B	1.1799 (3)	−0.12260 (13)	0.92644 (11)	0.0364 (4)
O41B	1.0684 (3)	−0.19375 (12)	0.94828 (11)	0.0521 (4)
O42B	1.3962 (3)	−0.10346 (13)	0.94729 (13)	0.0647 (5)
C5B	0.8303 (3)	−0.09710 (15)	0.82013 (14)	0.0345 (4)
H5B	0.7669	−0.1630	0.8225	0.041*
C6B	0.7087 (3)	−0.03661 (14)	0.76572 (13)	0.0337 (4)

H6B	0.5623	−0.0622	0.7306	0.040*
N1A	0.8415 (3)	0.12829 (13)	0.44641 (11)	0.0383 (4)
O1A	0.9180 (2)	0.22135 (10)	0.48264 (9)	0.0382 (3)
O2A	0.6359 (3)	0.09945 (13)	0.45746 (11)	0.0556 (4)
O3A	0.9691 (3)	0.06939 (14)	0.40305 (15)	0.0834 (7)
OW1	0.3449 (2)	0.32151 (12)	0.45157 (10)	0.0459 (4)
HW1	0.2073	0.2912	0.4406	0.069*
HW2	0.4094	0.3029	0.4051	0.069*
N1B	0.7706 (3)	0.32891 (13)	0.31690 (12)	0.0374 (4)
O1B	0.7783 (3)	0.40791 (12)	0.37923 (11)	0.0529 (4)
O2B	0.5936 (3)	0.26465 (13)	0.30181 (11)	0.0552 (4)
O3B	0.9381 (3)	0.31474 (12)	0.26942 (12)	0.0562 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03195 (8)	0.02853 (8)	0.03017 (8)	0.00387 (5)	0.00567 (5)	0.00542 (5)
C1A	0.0274 (9)	0.0229 (8)	0.0294 (9)	0.0037 (7)	0.0061 (7)	0.0068 (7)
C11A	0.0313 (10)	0.0229 (9)	0.0334 (10)	0.0017 (7)	0.0068 (8)	0.0056 (8)
O11A	0.0430 (8)	0.0320 (7)	0.0442 (8)	−0.0111 (6)	0.0201 (7)	−0.0050 (6)
N11A	0.0383 (9)	0.0304 (8)	0.0340 (9)	−0.0082 (7)	0.0136 (7)	−0.0006 (7)
N12A	0.0553 (11)	0.0431 (10)	0.0381 (10)	−0.0116 (8)	0.0232 (9)	−0.0023 (8)
C2A	0.0301 (10)	0.0301 (10)	0.0394 (11)	−0.0027 (8)	0.0119 (8)	0.0052 (8)
C3A	0.0305 (10)	0.0265 (9)	0.0373 (10)	−0.0048 (8)	0.0043 (8)	−0.0001 (8)
C4A	0.0286 (9)	0.0250 (9)	0.0275 (9)	0.0049 (7)	0.0051 (7)	0.0052 (7)
N41A	0.0385 (9)	0.0304 (8)	0.0312 (8)	0.0016 (7)	0.0072 (7)	0.0048 (7)
O41A	0.0526 (9)	0.0513 (9)	0.0458 (9)	−0.0077 (7)	0.0255 (7)	−0.0005 (7)
O42A	0.0523 (9)	0.0511 (9)	0.0396 (8)	−0.0104 (8)	0.0059 (7)	−0.0104 (7)
C5A	0.0291 (10)	0.0336 (10)	0.0346 (10)	−0.0044 (8)	0.0096 (8)	0.0061 (8)
C6A	0.0303 (10)	0.0304 (9)	0.0323 (10)	−0.0047 (8)	0.0041 (8)	0.0019 (8)
C1B	0.0275 (9)	0.0263 (9)	0.0238 (8)	0.0026 (7)	0.0041 (7)	0.0038 (7)
C11B	0.0254 (9)	0.0240 (8)	0.0235 (8)	0.0023 (7)	0.0030 (7)	0.0007 (7)
O11B	0.0265 (7)	0.0380 (7)	0.0370 (7)	−0.0032 (6)	0.0007 (6)	0.0168 (6)
N11B	0.0251 (8)	0.0310 (8)	0.0353 (8)	−0.0003 (6)	0.0023 (7)	0.0124 (7)
N12B	0.0247 (8)	0.0309 (8)	0.0351 (8)	0.0037 (6)	−0.0012 (7)	0.0055 (7)
C2B	0.0297 (10)	0.0258 (9)	0.0346 (10)	−0.0026 (7)	0.0012 (8)	0.0079 (8)
C3B	0.0294 (10)	0.0326 (10)	0.0348 (10)	−0.0035 (8)	−0.0050 (8)	0.0071 (8)
C4B	0.0320 (10)	0.0289 (9)	0.0298 (9)	0.0050 (8)	0.0030 (8)	0.0096 (8)
N41B	0.0368 (10)	0.0339 (9)	0.0380 (9)	0.0034 (7)	−0.0030 (8)	0.0106 (8)
O41B	0.0513 (10)	0.0496 (9)	0.0636 (10)	0.0014 (7)	0.0044 (8)	0.0336 (8)
O42B	0.0421 (10)	0.0599 (11)	0.0930 (14)	−0.0023 (8)	−0.0207 (9)	0.0366 (10)
C5B	0.0331 (10)	0.0282 (10)	0.0419 (11)	−0.0028 (8)	−0.0011 (9)	0.0111 (9)
C6B	0.0289 (10)	0.0308 (10)	0.0387 (11)	−0.0051 (8)	−0.0034 (8)	0.0070 (8)
N1A	0.0405 (10)	0.0376 (9)	0.0350 (9)	0.0023 (8)	0.0122 (8)	−0.0012 (8)
O1A	0.0403 (8)	0.0327 (7)	0.0396 (8)	−0.0032 (6)	0.0084 (6)	0.0014 (6)
O2A	0.0407 (9)	0.0597 (10)	0.0580 (10)	−0.0163 (7)	0.0172 (8)	−0.0108 (8)
O3A	0.0816 (14)	0.0546 (11)	0.1101 (16)	0.0039 (10)	0.0610 (13)	−0.0220 (11)
OW1	0.0313 (8)	0.0685 (10)	0.0401 (8)	0.0015 (7)	0.0009 (6)	0.0193 (7)

N1B	0.0343 (9)	0.0400 (10)	0.0411 (10)	−0.0030 (8)	0.0015 (8)	0.0191 (8)
O1B	0.0530 (10)	0.0456 (9)	0.0582 (10)	−0.0054 (7)	0.0150 (8)	0.0026 (8)
O2B	0.0460 (9)	0.0629 (10)	0.0527 (10)	−0.0268 (8)	−0.0003 (8)	0.0131 (8)
O3B	0.0514 (10)	0.0489 (9)	0.0706 (11)	−0.0043 (7)	0.0279 (9)	0.0072 (8)

Geometric parameters (Å, °)

Cd1—OW1	2.2590 (14)	C1B—C2B	1.389 (2)
Cd1—O11A	2.3242 (13)	C1B—C11B	1.495 (2)
Cd1—O11B	2.3339 (12)	C11B—O11B	1.241 (2)
Cd1—N12A	2.3489 (17)	C11B—N11B	1.333 (2)
Cd1—N12B	2.3518 (16)	N11B—N12B	1.410 (2)
Cd1—O1A	2.3934 (13)	N11B—H11B	0.8442
Cd1—O2A	2.5755 (15)	N12B—H21B	0.8560
C1A—C6A	1.386 (2)	N12B—H22B	0.8629
C1A—C2A	1.399 (3)	C2B—C3B	1.387 (3)
C1A—C11A	1.499 (2)	C2B—H2B	0.9300
C11A—O11A	1.240 (2)	C3B—C4B	1.380 (3)
C11A—N11A	1.331 (2)	C3B—H3B	0.9300
N11A—N12A	1.419 (2)	C4B—C5B	1.372 (3)
N11A—H11A	0.8641	C4B—N41B	1.473 (2)
N12A—H21A	0.8728	N41B—O42B	1.219 (2)
N12A—H22A	0.8639	N41B—O41B	1.220 (2)
C2A—C3A	1.386 (3)	C5B—C6B	1.385 (3)
C2A—H2A	0.9300	C5B—H5B	0.9300
C3A—C4A	1.373 (2)	C6B—H6B	0.9300
C3A—H3A	0.9300	N1A—O3A	1.220 (2)
C4A—C5A	1.381 (3)	N1A—O2A	1.239 (2)
C4A—N41A	1.475 (2)	N1A—O1A	1.268 (2)
N41A—O42A	1.216 (2)	OW1—HW1	0.8358
N41A—O41A	1.222 (2)	OW1—HW2	0.8199
C5A—C6A	1.383 (3)	N1B—O3B	1.242 (2)
C5A—H5A	0.9300	N1B—O1B	1.244 (2)
C6A—H6A	0.9300	N1B—O2B	1.245 (2)
C1B—C6B	1.388 (2)		
OW1—Cd1—O1A	98.97 (5)	C4A—C5A—H5A	120.7
OW1—Cd1—O2A	89.50 (6)	C6A—C5A—H5A	120.7
OW1—Cd1—O11A	93.34 (5)	C5A—C6A—C1A	120.53 (17)
OW1—Cd1—O11B	168.98 (5)	C5A—C6A—H6A	119.7
OW1—Cd1—N12A	90.92 (6)	C1A—C6A—H6A	119.7
OW1—Cd1—N12B	99.57 (5)	C6B—C1B—C2B	120.07 (16)
O11A—Cd1—O1A	150.85 (5)	C6B—C1B—C11B	121.82 (16)
O11A—Cd1—O2A	155.97 (5)	C2B—C1B—C11B	118.03 (15)
O11A—Cd1—O11B	91.78 (5)	O11B—C11B—N11B	122.99 (16)
O11A—Cd1—N12A	69.88 (5)	O11B—C11B—C1B	121.07 (15)
O11A—Cd1—N12B	80.91 (5)	N11B—C11B—C1B	115.94 (15)
O11B—Cd1—O1A	81.00 (5)	C11B—O11B—Cd1	114.86 (11)
O11B—Cd1—O2A	81.90 (5)	C11B—N11B—N12B	120.89 (14)
O11B—Cd1—N12A	100.01 (6)	C11B—N11B—H11B	120.1

O11B—Cd1—N12B	71.62 (5)	N12B—N11B—H11B	117.8
N12A—Cd1—O1A	83.53 (5)	N11B—N12B—Cd1	109.29 (10)
N12A—Cd1—O2A	133.98 (5)	N11B—N12B—H21B	106.6
N12A—Cd1—N12B	149.50 (6)	Cd1—N12B—H21B	108.0
N12B—Cd1—O1A	122.36 (5)	N11B—N12B—H22B	107.2
N12B—Cd1—O2A	75.09 (5)	Cd1—N12B—H22B	112.5
O1A—Cd1—O2A	51.06 (4)	H21B—N12B—H22B	113.0
C6A—C1A—C2A	119.63 (16)	C3B—C2B—C1B	120.11 (17)
C6A—C1A—C11A	116.70 (16)	C3B—C2B—H2B	119.9
C2A—C1A—C11A	123.66 (16)	C1B—C2B—H2B	119.9
O11A—C11A—N11A	122.42 (17)	C4B—C3B—C2B	118.22 (17)
O11A—C11A—C1A	119.54 (16)	C4B—C3B—H3B	120.9
N11A—C11A—C1A	118.03 (16)	C2B—C3B—H3B	120.9
C11A—O11A—Cd1	115.35 (12)	C5B—C4B—C3B	122.94 (17)
C11A—N11A—N12A	118.33 (15)	C5B—C4B—N41B	118.46 (16)
C11A—N11A—H11A	127.5	C3B—C4B—N41B	118.59 (16)
N12A—N11A—H11A	113.8	O42B—N41B—O41B	123.56 (17)
N11A—N12A—Cd1	109.97 (11)	O42B—N41B—C4B	118.14 (16)
N11A—N12A—H21A	101.8	O41B—N41B—C4B	118.29 (16)
Cd1—N12A—H21A	116.1	C4B—C5B—C6B	118.30 (17)
N11A—N12A—H22A	110.9	C4B—C5B—H5B	120.9
Cd1—N12A—H22A	109.0	C6B—C5B—H5B	120.9
H21A—N12A—H22A	108.9	C5B—C6B—C1B	120.33 (17)
C3A—C2A—C1A	120.16 (17)	C5B—C6B—H6B	119.8
C3A—C2A—H2A	119.9	C1B—C6B—H6B	119.8
C1A—C2A—H2A	119.9	O3A—N1A—O2A	121.62 (18)
C4A—C3A—C2A	118.62 (17)	O3A—N1A—O1A	120.49 (18)
C4A—C3A—H3A	120.7	O2A—N1A—O1A	117.88 (16)
C2A—C3A—H3A	120.7	N1A—O1A—Cd1	99.38 (11)
C3A—C4A—C5A	122.53 (17)	N1A—O2A—Cd1	91.41 (11)
C3A—C4A—N41A	118.90 (16)	Cd1—OW1—HW1	114.8
C5A—C4A—N41A	118.56 (16)	Cd1—OW1—HW2	104.6
O42A—N41A—O41A	123.75 (17)	HW1—OW1—HW2	106.1
O42A—N41A—C4A	118.31 (16)	O3B—N1B—O1B	120.05 (17)
O41A—N41A—C4A	117.94 (16)	O3B—N1B—O2B	120.16 (18)
C4A—C5A—C6A	118.51 (17)	O1B—N1B—O2B	119.78 (18)
C6A—C1A—C11A—O11A	−3.2 (3)	N12A—Cd1—O11B—C11B	150.92 (12)
C2A—C1A—C11A—O11A	175.24 (18)	N12B—Cd1—O11B—C11B	1.23 (12)
C6A—C1A—C11A—N11A	178.11 (17)	O1A—Cd1—O11B—C11B	−127.35 (13)
C2A—C1A—C11A—N11A	−3.4 (3)	O2A—Cd1—O11B—C11B	−75.68 (12)
N11A—C11A—O11A—Cd1	14.9 (2)	O11B—C11B—N11B—N12B	7.5 (3)
C1A—C11A—O11A—Cd1	−163.67 (12)	C1B—C11B—N11B—N12B	−172.32 (14)
OW1—Cd1—O11A—C11A	−106.43 (14)	C11B—N11B—N12B—Cd1	−5.45 (18)
O11B—Cd1—O11A—C11A	83.33 (14)	OW1—Cd1—N12B—N11B	175.23 (10)
N12A—Cd1—O11A—C11A	−16.68 (14)	O11A—Cd1—N12B—N11B	−92.89 (11)
N12B—Cd1—O11A—C11A	154.41 (14)	O11B—Cd1—N12B—N11B	2.05 (10)
O1A—Cd1—O11A—C11A	8.7 (2)	N12A—Cd1—N12B—N11B	−76.23 (16)
O2A—Cd1—O11A—C11A	157.28 (13)	O1A—Cd1—N12B—N11B	68.13 (12)
O11A—C11A—N11A—N12A	1.2 (3)	O2A—Cd1—N12B—N11B	88.32 (11)

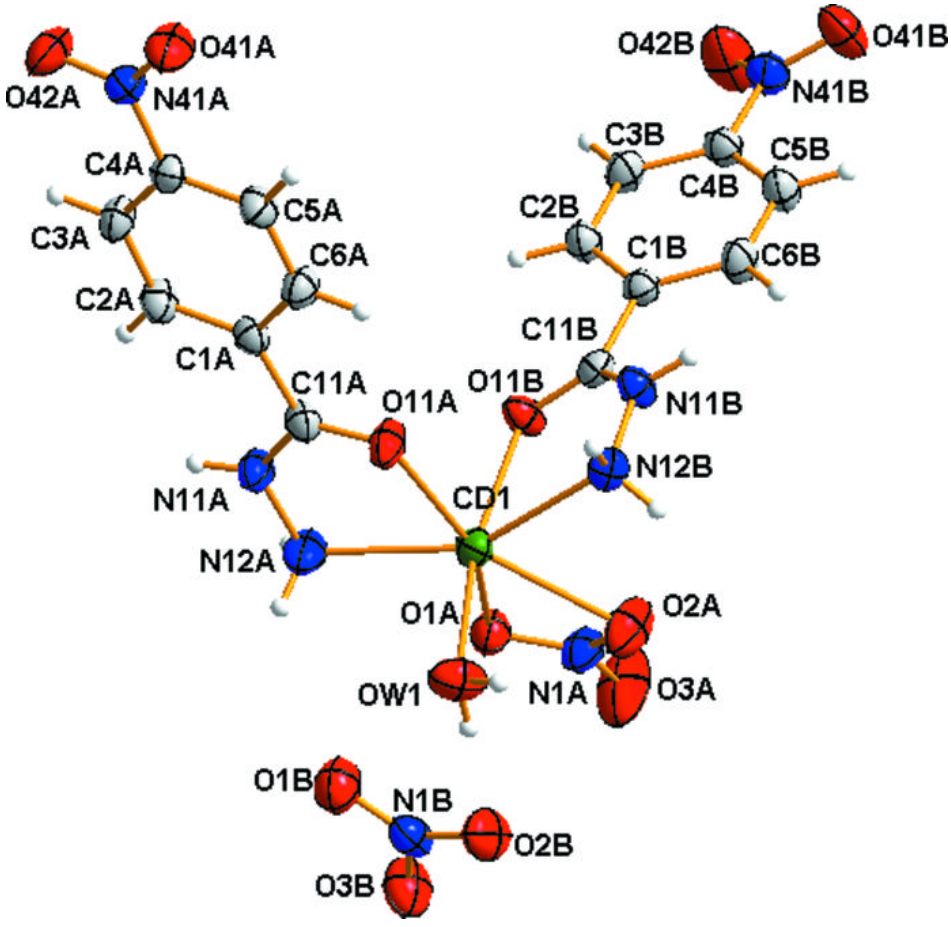
C1A—C11A—N11A—N12A	179.79 (16)	C6B—C1B—C2B—C3B	1.9 (3)
C11A—N11A—N12A—Cd1	−15.8 (2)	C11B—C1B—C2B—C3B	−174.74 (16)
OW1—Cd1—N12A—N11A	109.00 (13)	C1B—C2B—C3B—C4B	−1.6 (3)
O11A—Cd1—N12A—N11A	15.78 (12)	C2B—C3B—C4B—C5B	0.3 (3)
O11B—Cd1—N12A—N11A	−72.44 (13)	C2B—C3B—C4B—N41B	179.43 (16)
N12B—Cd1—N12A—N11A	−1.8 (2)	C5B—C4B—N41B—O42B	157.60 (19)
O1A—Cd1—N12A—N11A	−152.07 (14)	C3B—C4B—N41B—O42B	−21.6 (3)
O2A—Cd1—N12A—N11A	−160.80 (11)	C5B—C4B—N41B—O41B	−21.4 (3)
C6A—C1A—C2A—C3A	0.3 (3)	C3B—C4B—N41B—O41B	159.45 (18)
C11A—C1A—C2A—C3A	−178.11 (17)	C3B—C4B—C5B—C6B	0.8 (3)
C1A—C2A—C3A—C4A	−0.1 (3)	N41B—C4B—C5B—C6B	−178.35 (16)
C2A—C3A—C4A—C5A	−0.6 (3)	C4B—C5B—C6B—C1B	−0.5 (3)
C2A—C3A—C4A—N41A	178.35 (16)	C2B—C1B—C6B—C5B	−0.8 (3)
C3A—C4A—N41A—O42A	−3.8 (3)	C11B—C1B—C6B—C5B	175.71 (17)
C5A—C4A—N41A—O42A	175.18 (17)	O3A—N1A—O1A—Cd1	−173.76 (18)
C3A—C4A—N41A—O41A	176.75 (17)	O2A—N1A—O1A—Cd1	5.45 (19)
C5A—C4A—N41A—O41A	−4.3 (2)	OW1—Cd1—O1A—N1A	−85.00 (12)
C3A—C4A—C5A—C6A	1.1 (3)	O11A—Cd1—O1A—N1A	161.17 (11)
N41A—C4A—C5A—C6A	−177.84 (16)	O11B—Cd1—O1A—N1A	83.85 (11)
C4A—C5A—C6A—C1A	−0.9 (3)	N12A—Cd1—O1A—N1A	−174.90 (12)
C2A—C1A—C6A—C5A	0.2 (3)	N12B—Cd1—O1A—N1A	22.41 (13)
C11A—C1A—C6A—C5A	178.74 (17)	O2A—Cd1—O1A—N1A	−2.98 (11)
C6B—C1B—C11B—O11B	−153.76 (18)	O3A—N1A—O2A—Cd1	174.2 (2)
C2B—C1B—C11B—O11B	22.8 (2)	O1A—N1A—O2A—Cd1	−5.00 (18)
C6B—C1B—C11B—N11B	26.0 (2)	OW1—Cd1—O2A—N1A	104.98 (12)
C2B—C1B—C11B—N11B	−157.42 (16)	O11A—Cd1—O2A—N1A	−157.92 (12)
N11B—C11B—O11B—Cd1	−4.9 (2)	O11B—Cd1—O2A—N1A	−81.93 (12)
C1B—C11B—O11B—Cd1	174.84 (11)	N12A—Cd1—O2A—N1A	14.19 (16)
OW1—Cd1—O11B—C11B	−36.6 (3)	N12B—Cd1—O2A—N1A	−154.98 (13)
O11A—Cd1—O11B—C11B	81.04 (12)	O1A—Cd1—O2A—N1A	3.01 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11A—H11A···O3B^{i}	0.86	2.03	2.886 (2)	171.2
N12A—H21A···O1B^{i}	0.87	2.42	2.977 (2)	122.2
N12A—H22A···O1B	0.86	2.60	3.209 (2)	128.8
N11B—H11B···O3A^{ii}	0.84	2.59	3.176 (2)	127.6
N12B—H22B···O11B^{iii}	0.86	2.40	3.212 (2)	156.9
OW1—HW1···O1A^{iii}	0.84	2.05	2.815 (2)	151.2
OW1—HW2···O2B	0.82	1.95	2.769 (2)	174.2

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

Fig. 1


O41A
O42A
N41A
C4A
C5A
C3A
C6A
C2A
C1A
C11A
O11A
N11A
N12A
CD1
O1A
OW1
O2A
N1A
O3A
O42B
O41B
N41B
C3B
C5B
C4B
C2B
C1B
C6B
C11B
O11B
N11B
N12B
O1B
N1B
O2B
O3B