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Di-μ-nitrato-$\kappa^3O,O':O'';\kappa^3O:O',O''$-bis[bis(3-nitrobenzohydrazide-κ^2N',O)cadmium(II)] dinitrate

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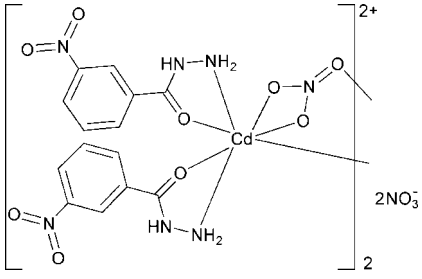
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.064; data-to-parameter ratio = 16.2.

The title compound, $[Cd_2(NO_3)_2(C_7H_7N_3O_3)_2](NO_3)_2$, contains centrosymmetric dimeric cations in which two nitrate anions each serve as a bidentate ligand to one Cd atom and a bridge to the other. The other anion in the asymmetric unit (half the formula unit) is uncoordinated. The ligands form an atypical seven-coordinated augmented trigonal prism around the Cd^{II} atom, with a displacement from the centre of the polyhedron in the direction of the uncoordinated nitrate anion. The crystal structure displays numerous N—H···O hydrogen bonds.

Related literature

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



Experimental

Crystal data

$[Cd_2(NO_3)_2(C_7H_7N_3O_3)_2](NO_3)_2$
M_r = 598.73
Monoclinic, $P2_1/c$
a = 7.9218 (16) Å
b = 7.6237 (15) Å
c = 34.325 (7) Å
β = 93.67 (3)°
V = 2068.7 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 293 (2) K
0.38 × 0.35 × 0.10 mm

Data collection

Kuma KM-4 rea-detector diffractometer
Absorption correction: numerical (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.672, T_{max} = 0.871
26291 measured reflections
5111 independent reflections
3275 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.064
S = 0.94
5111 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O11*A*	2.287 (2)	Cd1—O1*A*	2.399 (2)
Cd1—O11*B*	2.301 (2)	Cd1—O2*A*	2.778 (2)
Cd1—N12*A*	2.262 (2)	Cd1—O3*A*^{i}	2.848 (2)
Cd1—N12*B*	2.268 (2)		
N12*A*—Cd1—N12*B*	133.23 (9)	N12*B*—Cd1—O11*A*	151.16 (8)
N12*A*—Cd1—O11*A*	72.73 (8)	N12*B*—Cd1—O1*A*	99.40 (8)
N12*A*—Cd1—O11*B*	138.33 (8)	O11*A*—Cd1—O11*B*	79.41 (7)
N12*A*—Cd1—O1*A*	87.82 (8)	O11*A*—Cd1—O1*A*	93.12 (8)
N12*B*—Cd1—O11*B*	72.07 (8)	O11*B*—Cd1—O1*A*	124.58 (8)

Symmetry code: (i) $-x, -y+2, -z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11*A*—H11*A*···O1*B*^{ii}	0.88	1.98	2.833 (3)	164.5
N12*A*—H21*A*···O2*B*^{iii}	0.89	2.12	2.963 (3)	157.8
N12*A*—H22*A*···O3*A*^{iv}	0.89	2.25	2.931 (3)	133.3
N11*B*—H11*B*···O1*B*^{v}	0.88	2.11	2.872 (3)	144.3
N12*B*—H21*B*···O1*A*^{i}	0.90	2.33	3.093 (3)	142.2
N12*B*—H21*B*···O2*B*^{v}	0.90	2.42	3.143 (3)	137.5
N12*B*—H22*B*···O2*B*^{vi}	0.85	2.30	3.124 (3)	163.6

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; 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* (Version 1.9.0_c; Westrip, 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2040).

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supplementary materials

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Di-μ-nitrato-$\kappa^3O,O':O'';\kappa^3O:O',O''$-bis[bis(3-nitrobenzohydrazide-κ^2N',O)cadmium(II)] dinitrate

S. Y. Chundak, L. Y. Lukachinec and M. Daszkiewicz

Comment

In the dimeric structure of bis((μ$_2$-nitrato-*O,O′,O″*)-*cis*-bis(*m*-nitrobenzoylhydrazino-*N,O*)cadmium(II)) bis(nitrate), two *cis* coordinated organic ligands and two bridging nitrate anions form atypical seven coordinated arrangement around the Cd-atom. Because the dimer lies on the inversion centre the asymmetric unit contains only half of the dimer. Therefore, two cadmium(II) ions and their coordination spheres are symmetrically dependent. By the same reason two bridging nitrate anions are also symmetrically dependent. Although bridging coordination mode of nitrate anion is clearly seen, it is worth noticing that this anion donates three oxygen atoms to the cadmium(II) and monodentate and bidentate coordination can be specified. In the former mode, the Cd—$O_{nitrate}$ bond lenghts difference, Co—O—N angles difference and Co—N—$O_{terminal}$ angle for one nitrate are 0.38 Å, 17.3° and 160.4° respectively and correlate well with the anisobidentate coordination mode (Kleywegt *et al.*, 1985; Dowling *et al.*, 1996). In the latter mode, respective parameters distinctly indicates monodentate coordination (0.93 Å, 45.9° and 139.3°).

Intriguingly, the Cd-atom is displaced from the centre of the coordination polyhedron (augmented trigonal prism) in the direction of one face (0.54 Å). However, it seems that this displacement is caused by free NO_3^- anion. In spite of the Cd···ONO_2 distance (3.184 Å) which is too long for a bond, indeed it is worth considering as a weak interaction. The position of the free nitrate anion is stabillized by several hydrogen bonding interactions both NH and NH_2 groups from organic ligand.

Experimental

1.8 g (1 mmol) of *m*-nitrobenzoylhydrazine was dissolved in 25 ml hot ethanol and mixed with 3 ml e thanolic solution of $Cd(NO_3)_2$ (3.1 g; 1 mmol). Colourless crystals were formed after 24 h, then filtered, washed with ethanol and dried on air.

Refinement

All the hydrogen atoms were visible in the difference maps and were refined 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 were determined from the difference maps and were not refined [U_{iso}(H) = 1.5U_{eq}(N,*O*)].

Figures

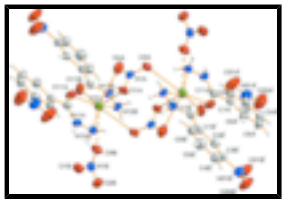


Fig. 1. Dimeric structure of the title compound with elipsoids drawn at the 50% probability level. [Symmetry code: (i) −*x*, −*y* + 2, −*z*.].

Di-μ-nitrato-κ^3*O*,*O*':*O*'';κ^3*O*:*O*',*O*''-bis[bis(3-nitrobenzohydrazide- κ^2*N*',*O*)cadmium(II)] dinitrate

Crystal data

$[Cd_2(NO_3)_2(C_7H_7N_3O_3)_2](NO_3)_2$	F_{000} = 1192
M_r = 598.73	D_x = 1.922 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3275 reflections
a = 7.9218 (16) Å	θ = 3.2–28.3º
b = 7.6237 (15) Å	μ = 1.14 mm^{-1}
c = 34.325 (7) Å	*T* = 293 (2) K
β = 93.67 (3)º	Plate, colourless
V = 2068.7 (7) Å^3	0.38 × 0.35 × 0.10 mm
Z = 4	

Data collection

Kuma KM-4 with CCD area-detector diffractometer	5111 independent reflections
Radiation source: fine-focus sealed tube	3275 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.060
Detector resolution: 1024x1024 with blocks 2x2, 33.133pixel/mm pixels mm^{-1}	θ_{max} = 28.3º
T = 293(2) K	θ_{min} = 3.2º
ω scans	*h* = −10→7
Absorption correction: numerical (CrysAlis; Oxford Diffraction, 2006)	*k* = −10→10
T_{min} = 0.672, T_{max} = 0.871	*l* = −45→45
26291 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
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H-atom parameters constrained
$wR(F^2)$ = 0.064	$w = 1/[\sigma^2(F_o^2) + (0.0233P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{max} = 0.001$
5111 reflections	$\Delta\rho_{max} = 0.63$ e Å^{-3}
316 parameters	$\Delta\rho_{min} = -0.76$ 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	0.21123 (3)	0.91697 (3)	0.065750 (7)	0.03871 (9)
C1A	0.3993 (3)	1.3516 (4)	0.14429 (8)	0.0283 (7)
C11A	0.3681 (4)	1.2144 (4)	0.11357 (8)	0.0299 (7)
O11A	0.2649 (3)	1.0959 (3)	0.11856 (6)	0.0420 (5)
N11A	0.4532 (3)	1.2260 (3)	0.08142 (7)	0.0325 (6)
H11A	0.5254	1.3101	0.0774	0.049*
N12A	0.4232 (3)	1.0998 (3)	0.05130 (7)	0.0348 (6)
H21A	0.3816	1.1528	0.0296	0.052*
H22A	0.5221	1.0456	0.0503	0.052*
C2A	0.4693 (3)	1.5141 (4)	0.13664 (9)	0.0305 (7)
H2A	0.5050	1.5402	0.1120	0.037*
C3A	0.4847 (4)	1.6360 (4)	0.16640 (9)	0.0320 (7)
N31A	0.5536 (4)	1.8102 (4)	0.15805 (9)	0.0488 (7)
O31A	0.5797 (4)	1.8452 (3)	0.12432 (8)	0.0784 (9)
O32A	0.5794 (4)	1.9129 (3)	0.18495 (8)	0.0781 (8)
C4A	0.4352 (4)	1.6029 (4)	0.20352 (9)	0.0406 (8)
H4A	0.4474	1.6873	0.2231	0.049*
C5A	0.3668 (4)	1.4395 (4)	0.21075 (9)	0.0431 (8)
H5A	0.3332	1.4133	0.2356	0.052*
C6A	0.3481 (3)	1.3157 (4)	0.18157 (8)	0.0351 (8)
H6A	0.3009	1.2072	0.1868	0.042*
C1B	−0.0259 (3)	0.4933 (4)	0.13333 (8)	0.0280 (7)
C11B	0.0584 (3)	0.6052 (4)	0.10467 (8)	0.0292 (7)
O11B	0.1456 (3)	0.7319 (3)	0.11554 (6)	0.0422 (6)
N11B	0.0386 (3)	0.5559 (3)	0.06711 (7)	0.0345 (6)
H11B	−0.0480	0.4930	0.0575	0.052*

N12B	0.1088 (3)	0.6642 (3)	0.03862 (7)	0.0342 (6)
H21B	0.0277	0.6993	0.0207	0.051*
H22B	0.1590	0.5965	0.0233	0.051*
C2B	−0.0491 (3)	0.5612 (4)	0.16999 (9)	0.0345 (7)
H2B	−0.0152	0.6750	0.1764	0.041*
C3B	−0.1232 (4)	0.4572 (4)	0.19677 (9)	0.0383 (8)
N31B	−0.1504 (4)	0.5325 (5)	0.23589 (9)	0.0575 (9)
O31B	−0.1058 (4)	0.6833 (5)	0.24205 (8)	0.0936 (10)
O32B	−0.2169 (4)	0.4419 (4)	0.25973 (8)	0.0890 (10)
C4B	−0.1743 (4)	0.2890 (5)	0.18912 (10)	0.0467 (9)
H4B	−0.2244	0.2222	0.2079	0.056*
C5B	−0.1495 (4)	0.2211 (4)	0.15282 (10)	0.0461 (9)
H5B	−0.1831	0.1067	0.1469	0.055*
C6B	−0.0751 (4)	0.3213 (4)	0.12507 (9)	0.0365 (8)
H6B	−0.0578	0.2735	0.1007	0.044*
N1A	−0.1265 (3)	1.0524 (3)	0.03837 (8)	0.0355 (6)
O1A	0.0176 (3)	1.1213 (3)	0.03396 (6)	0.0446 (6)
O2A	−0.1387 (3)	0.9443 (3)	0.06509 (7)	0.0578 (7)
O3A	−0.2493 (3)	1.0939 (3)	0.01617 (6)	0.0458 (6)
N1B	0.6356 (3)	0.5968 (4)	0.03179 (7)	0.0369 (6)
O1B	0.6860 (3)	0.4722 (3)	0.05402 (6)	0.0470 (6)
O2B	0.7298 (3)	0.6450 (3)	0.00571 (6)	0.0483 (6)
O3B	0.4979 (3)	0.6670 (3)	0.03588 (7)	0.0605 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04042 (14)	0.03565 (13)	0.03968 (14)	−0.01622 (13)	−0.00052 (10)	0.00128 (13)
C1A	0.0280 (17)	0.0297 (16)	0.0271 (17)	−0.0040 (13)	0.0012 (13)	0.0007 (14)
C11A	0.0264 (17)	0.0321 (17)	0.0312 (17)	−0.0060 (14)	0.0024 (14)	0.0046 (15)
O11A	0.0475 (13)	0.0426 (13)	0.0373 (12)	−0.0235 (12)	0.0136 (10)	−0.0040 (11)
N11A	0.0346 (14)	0.0320 (14)	0.0317 (14)	−0.0172 (12)	0.0087 (12)	−0.0054 (12)
N12A	0.0315 (14)	0.0403 (15)	0.0331 (14)	−0.0098 (12)	0.0048 (11)	−0.0078 (13)
C2A	0.0310 (17)	0.0341 (17)	0.0268 (17)	−0.0051 (14)	0.0044 (13)	−0.0005 (14)
C3A	0.0350 (18)	0.0246 (16)	0.0360 (18)	−0.0058 (13)	0.0010 (15)	0.0018 (14)
N31A	0.064 (2)	0.0316 (17)	0.052 (2)	−0.0115 (15)	0.0120 (16)	−0.0047 (16)
O31A	0.136 (3)	0.0435 (15)	0.0596 (18)	−0.0336 (16)	0.0397 (18)	−0.0036 (14)
O32A	0.124 (2)	0.0463 (15)	0.0645 (17)	−0.0368 (17)	0.0137 (16)	−0.0237 (15)
C4A	0.047 (2)	0.040 (2)	0.0349 (18)	−0.0032 (17)	−0.0005 (15)	−0.0081 (17)
C5A	0.055 (2)	0.047 (2)	0.0272 (17)	−0.0048 (18)	0.0063 (15)	−0.0014 (17)
C6A	0.0384 (19)	0.0339 (18)	0.0333 (18)	−0.0077 (14)	0.0043 (15)	0.0025 (15)
C1B	0.0251 (16)	0.0306 (16)	0.0280 (17)	−0.0036 (13)	0.0000 (13)	−0.0003 (14)
C11B	0.0258 (16)	0.0279 (17)	0.0334 (17)	−0.0009 (14)	−0.0007 (13)	0.0023 (15)
O11B	0.0552 (14)	0.0336 (12)	0.0365 (12)	−0.0221 (11)	−0.0070 (10)	0.0011 (10)
N11B	0.0397 (15)	0.0324 (15)	0.0321 (14)	−0.0174 (12)	0.0086 (12)	−0.0052 (12)
N12B	0.0394 (15)	0.0357 (14)	0.0284 (14)	−0.0065 (12)	0.0096 (12)	−0.0019 (12)
C2B	0.0298 (17)	0.0353 (18)	0.0381 (18)	0.0000 (15)	−0.0008 (14)	−0.0034 (16)
C3B	0.0340 (19)	0.053 (2)	0.0281 (17)	0.0029 (16)	0.0049 (14)	−0.0035 (16)

N31B	0.051 (2)	0.077 (3)	0.046 (2)	0.0013 (18)	0.0094 (16)	−0.0077 (19)
O31B	0.123 (3)	0.098 (2)	0.063 (2)	−0.031 (2)	0.0344 (17)	−0.0359 (19)
O32B	0.112 (2)	0.109 (3)	0.0502 (17)	−0.011 (2)	0.0390 (17)	0.0055 (18)
C4B	0.047 (2)	0.052 (2)	0.042 (2)	−0.0091 (18)	0.0073 (17)	0.0115 (19)
C5B	0.055 (2)	0.0328 (19)	0.051 (2)	−0.0122 (17)	0.0038 (18)	0.0057 (18)
C6B	0.0411 (19)	0.0340 (19)	0.0347 (19)	−0.0056 (15)	0.0046 (15)	−0.0031 (16)
N1A	0.0381 (17)	0.0395 (17)	0.0295 (15)	−0.0003 (13)	0.0081 (13)	−0.0109 (14)
O1A	0.0268 (12)	0.0586 (16)	0.0487 (14)	−0.0106 (11)	0.0053 (10)	−0.0038 (12)
O2A	0.0754 (18)	0.0577 (17)	0.0405 (14)	−0.0121 (14)	0.0046 (12)	0.0137 (13)
O3A	0.0289 (12)	0.0581 (15)	0.0502 (14)	0.0012 (12)	0.0011 (11)	0.0049 (13)
N1B	0.0352 (16)	0.0401 (17)	0.0349 (15)	−0.0143 (14)	−0.0018 (13)	−0.0052 (14)
O1B	0.0386 (14)	0.0502 (15)	0.0520 (15)	−0.0163 (11)	0.0007 (11)	0.0178 (12)
O2B	0.0522 (15)	0.0548 (15)	0.0391 (13)	−0.0167 (12)	0.0121 (11)	0.0088 (11)
O3B	0.0341 (14)	0.0755 (18)	0.0716 (18)	0.0063 (13)	0.0002 (13)	−0.0077 (15)

Geometric parameters (Å, °)

Cd1—O11A	2.287 (2)	C6A—H6A	0.9300
Cd1—O11B	2.301 (2)	C1B—C2B	1.384 (4)
Cd1—N12A	2.262 (2)	C1B—C6B	1.392 (4)
Cd1—N12B	2.268 (2)	C1B—C11B	1.492 (4)
Cd1—O1A	2.399 (2)	C11B—O11B	1.232 (3)
Cd1—O2A	2.778 (2)	C11B—N11B	1.342 (3)
Cd1—O3A^{i}	2.848 (2)	N11B—N12B	1.420 (3)
Cd1—O3B	3.184 (3)	N11B—H11B	0.8831
C1A—C2A	1.389 (4)	N12B—H21B	0.9017
C1A—C6A	1.394 (4)	N12B—H22B	0.8532
C1A—C11A	1.494 (4)	C2B—C3B	1.374 (4)
C11A—O11A	1.238 (3)	C2B—H2B	0.9300
C11A—N11A	1.333 (3)	C3B—C4B	1.365 (4)
N11A—N12A	1.421 (3)	C3B—N31B	1.489 (4)
N11A—H11A	0.8760	N31B—O32B	1.216 (4)
N12A—H21A	0.8908	N31B—O31B	1.217 (4)
N12A—H22A	0.8890	C4B—C5B	1.375 (4)
C2A—C3A	1.381 (4)	C4B—H4B	0.9300
C2A—H2A	0.9300	C5B—C6B	1.382 (4)
C3A—C4A	1.380 (4)	C5B—H5B	0.9300
C3A—N31A	1.471 (4)	C6B—H6B	0.9300
N31A—O32A	1.218 (3)	N1A—O3A	1.238 (3)
N31A—O31A	1.219 (3)	N1A—O2A	1.241 (3)
C4A—C5A	1.387 (4)	N1A—O1A	1.274 (3)
C4A—H4A	0.9300	N1B—O3B	1.232 (3)
C5A—C6A	1.377 (4)	N1B—O2B	1.256 (3)
C5A—H5A	0.9300	N1B—O1B	1.267 (3)
N12A—Cd1—N12B	133.23 (9)	C1A—C6A—H6A	119.7
N12A—Cd1—O11A	72.73 (8)	C2B—C1B—C6B	119.1 (3)
N12A—Cd1—O11B	138.33 (8)	C2B—C1B—C11B	118.4 (3)
N12A—Cd1—O1A	87.82 (8)	C6B—C1B—C11B	122.4 (3)
N12B—Cd1—O11B	72.07 (8)	O11B—C11B—N11B	122.6 (3)

N12B—Cd1—O11A	151.16 (8)	O11B—C11B—C1B	121.0 (3)
N12B—Cd1—O1A	99.40 (8)	N11B—C11B—C1B	116.3 (3)
O11A—Cd1—O11B	79.41 (7)	C11B—O11B—Cd1	113.88 (18)
O11A—Cd1—O1A	93.12 (8)	C11B—N11B—N12B	118.2 (2)
O11B—Cd1—O1A	124.58 (8)	C11B—N11B—H11B	123.3
C2A—C1A—C6A	119.5 (3)	N12B—N11B—H11B	112.9
C2A—C1A—C11A	122.7 (3)	N11B—N12B—Cd1	110.89 (16)
C6A—C1A—C11A	117.8 (3)	N11B—N12B—H21B	110.5
O11A—C11A—N11A	122.5 (3)	Cd1—N12B—H21B	104.4
O11A—C11A—C1A	119.6 (3)	N11B—N12B—H22B	107.0
N11A—C11A—C1A	117.9 (3)	Cd1—N12B—H22B	126.8
C11A—O11A—Cd1	114.63 (18)	H21B—N12B—H22B	95.6
C11A—N11A—N12A	119.2 (2)	C3B—C2B—C1B	118.6 (3)
C11A—N11A—H11A	123.3	C3B—C2B—H2B	120.7
N12A—N11A—H11A	117.5	C1B—C2B—H2B	120.7
N11A—N12A—Cd1	110.48 (16)	C4B—C3B—C2B	123.2 (3)
N11A—N12A—H21A	109.7	C4B—C3B—N31B	118.5 (3)
Cd1—N12A—H21A	102.8	C2B—C3B—N31B	118.2 (3)
N11A—N12A—H22A	103.7	O32B—N31B—O31B	123.6 (4)
Cd1—N12A—H22A	113.0	O32B—N31B—C3B	118.8 (3)
H21A—N12A—H22A	117.3	O31B—N31B—C3B	117.7 (3)
C3A—C2A—C1A	118.5 (3)	C3B—C4B—C5B	118.0 (3)
C3A—C2A—H2A	120.7	C3B—C4B—H4B	121.0
C1A—C2A—H2A	120.7	C5B—C4B—H4B	121.0
C4A—C3A—C2A	122.9 (3)	C4B—C5B—C6B	120.6 (3)
C4A—C3A—N31A	118.4 (3)	C4B—C5B—H5B	119.7
C2A—C3A—N31A	118.7 (3)	C6B—C5B—H5B	119.7
O32A—N31A—O31A	123.3 (3)	C5B—C6B—C1B	120.4 (3)
O32A—N31A—C3A	118.6 (3)	C5B—C6B—H6B	119.8
O31A—N31A—C3A	118.1 (3)	C1B—C6B—H6B	119.8
C3A—C4A—C5A	117.8 (3)	O3A—N1A—O2A	122.0 (3)
C3A—C4A—H4A	121.1	O3A—N1A—O1A	119.8 (3)
C5A—C4A—H4A	121.1	O2A—N1A—O1A	118.3 (3)
C6A—C5A—C4A	120.7 (3)	N1A—O1A—Cd1	103.30 (18)
C6A—C5A—H5A	119.7	O3B—N1B—O2B	121.6 (3)
C4A—C5A—H5A	119.7	O3B—N1B—O1B	120.3 (3)
C5A—C6A—C1A	120.6 (3)	O2B—N1B—O1B	118.0 (3)
C5A—C6A—H6A	119.7		
C2A—C1A—C11A—O11A	−159.5 (3)	C6B—C1B—C11B—N11B	20.1 (4)
C6A—C1A—C11A—O11A	17.5 (4)	N11B—C11B—O11B—Cd1	15.5 (3)
C2A—C1A—C11A—N11A	20.1 (4)	C1B—C11B—O11B—Cd1	−167.0 (2)
C6A—C1A—C11A—N11A	−162.9 (3)	N12A—Cd1—O11B—C11B	−149.64 (19)
N11A—C11A—O11A—Cd1	−6.3 (4)	N12B—Cd1—O11B—C11B	−13.7 (2)
C1A—C11A—O11A—Cd1	173.26 (19)	O11A—Cd1—O11B—C11B	162.0 (2)
N12A—Cd1—O11A—C11A	6.32 (19)	O1A—Cd1—O11B—C11B	75.5 (2)
N12B—Cd1—O11A—C11A	163.6 (2)	O11B—C11B—N11B—N12B	−5.8 (4)
O11B—Cd1—O11A—C11A	155.0 (2)	C1B—C11B—N11B—N12B	176.6 (2)
O1A—Cd1—O11A—C11A	−80.4 (2)	C11B—N11B—N12B—Cd1	−7.1 (3)
O11A—C11A—N11A—N12A	1.1 (4)	N12A—Cd1—N12B—N11B	150.76 (16)

C1A—C11A—N11A—N12A	−178.5 (2)	O11A—Cd1—N12B—N11B	1.2 (3)
C11A—N11A—N12A—Cd1	4.7 (3)	O11B—Cd1—N12B—N11B	10.11 (16)
N12B—Cd1—N12A—N11A	−170.52 (15)	O1A—Cd1—N12B—N11B	−113.34 (17)
O11A—Cd1—N12A—N11A	−5.34 (16)	C6B—C1B—C2B—C3B	−1.3 (4)
O11B—Cd1—N12A—N11A	−55.6 (2)	C11B—C1B—C2B—C3B	−178.6 (3)
O1A—Cd1—N12A—N11A	88.61 (17)	C1B—C2B—C3B—C4B	0.5 (5)
C6A—C1A—C2A—C3A	−0.5 (4)	C1B—C2B—C3B—N31B	−178.9 (2)
C11A—C1A—C2A—C3A	176.5 (3)	C4B—C3B—N31B—O32B	0.1 (5)
C1A—C2A—C3A—C4A	0.7 (4)	C2B—C3B—N31B—O32B	179.5 (3)
C1A—C2A—C3A—N31A	−178.1 (3)	C4B—C3B—N31B—O31B	−179.2 (3)
C4A—C3A—N31A—O32A	6.8 (4)	C2B—C3B—N31B—O31B	0.3 (5)
C2A—C3A—N31A—O32A	−174.4 (3)	C2B—C3B—C4B—C5B	0.2 (5)
C4A—C3A—N31A—O31A	−172.1 (3)	N31B—C3B—C4B—C5B	179.6 (3)
C2A—C3A—N31A—O31A	6.7 (4)	C3B—C4B—C5B—C6B	−0.1 (5)
C2A—C3A—C4A—C5A	−0.2 (5)	C4B—C5B—C6B—C1B	−0.8 (5)
N31A—C3A—C4A—C5A	178.5 (3)	C2B—C1B—C6B—C5B	1.4 (4)
C3A—C4A—C5A—C6A	−0.5 (5)	C11B—C1B—C6B—C5B	178.6 (3)
C4A—C5A—C6A—C1A	0.7 (5)	O3A—N1A—O1A—Cd1	−158.5 (2)
C2A—C1A—C6A—C5A	−0.2 (4)	O2A—N1A—O1A—Cd1	21.3 (3)
C11A—C1A—C6A—C5A	−177.3 (3)	N12A—Cd1—O1A—N1A	−178.19 (17)
C2B—C1B—C11B—O11B	19.6 (4)	N12B—Cd1—O1A—N1A	48.31 (17)
C6B—C1B—C11B—O11B	−157.6 (3)	O11A—Cd1—O1A—N1A	−105.62 (16)
C2B—C1B—C11B—N11B	−162.8 (3)	O11B—Cd1—O1A—N1A	−26.34 (19)

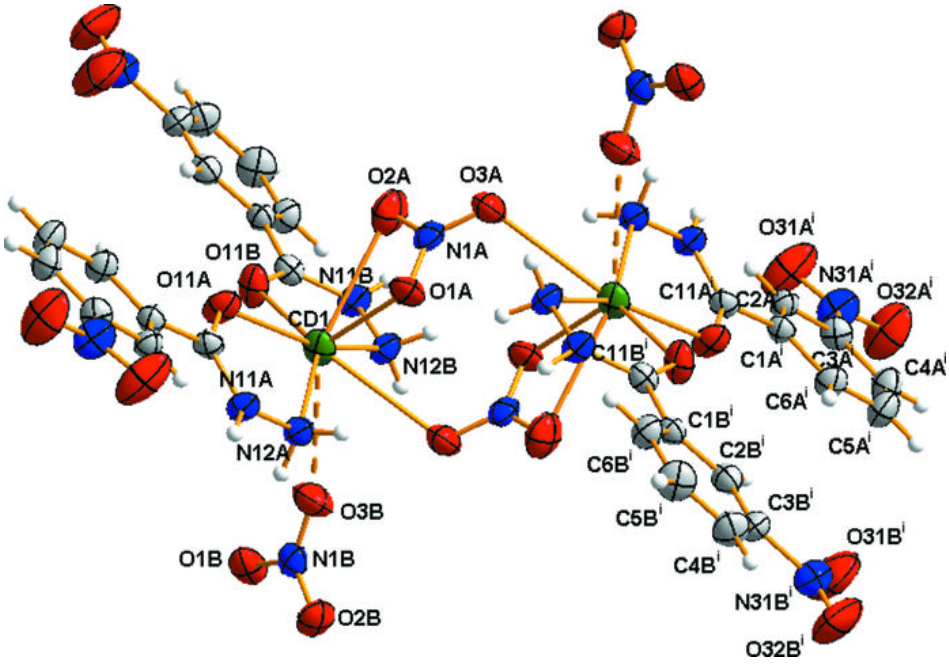
Symmetry codes: (i) −*x*, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11A—H11A···O1B^{ii}	0.88	1.98	2.833 (3)	164.5
N12A—H21A···O2B^{iii}	0.89	2.12	2.963 (3)	157.8
N12A—H22A···O3A^{iv}	0.89	2.25	2.931 (3)	133.3
N11B—H11B···O1B^{v}	0.88	2.11	2.872 (3)	144.3
N12B—H21B···O1A^{i}	0.90	2.33	3.093 (3)	142.2
N12B—H21B···O2B^{v}	0.90	2.42	3.143 (3)	137.5
N12B—H22B···O2B^{vi}	0.85	2.30	3.124 (3)	163.6

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

Fig. 1


O2A
O3A
N1A
O11B
O11A
N11B
O1A
CD1
N12B
N11A
N12A
O3B
O1B
N1B
O2B
C11A
C11B
O31A
N31A
O32A
C2A
C1A
C3A
C4A
C6A
C5A
C1B
C2B
C6B
C5B
C3B
C4B
O31B
N31B
O32B