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Crystal structure of bis(1,3-diaminopropane-κ^2N,N')bis[2-(4-nitrophenyl)acetato-κO]cadmium

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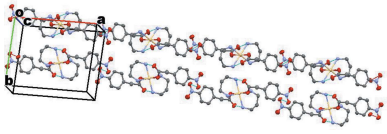
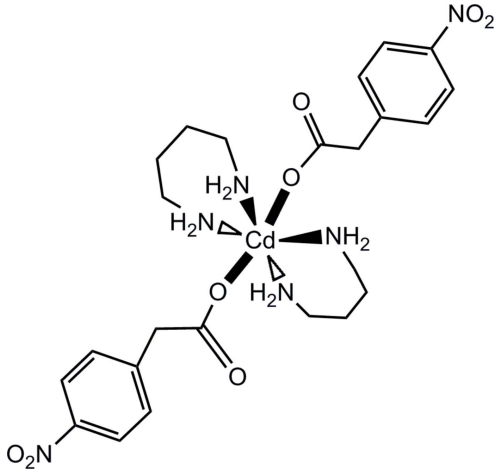
In the structure of the title compound, $[Cd(C_8H_6NO_4)_2(C_3H_{10}N_2)_2]$, the Cd^{II} atom is located on a center of symmetry with one independent Cd—O distance of 2.3547 (17) Å and two Cd—N distances of 2.3265 (18) and 2.3449 (19) Å. The Cd^{II} atom has an overall octahedral coordination environment. Several types of hydrogen-bonding interactions are evident. Both intra- and intermolecular interactions occur between the amino groups and the O atoms of the acetate group. These N—H···O hydrogen bonds lead to a layered structure extending parallel to the *bc* plane. In addition, weak intermolecular C—H···O interactions involving the nitro groups exist, leading to the formation of a three-dimensional network structure.

1. Chemical context

The motivation for this study is based on the desire to expand the crystal engineering aspect of 1,3-diamino propane and carboxylate ligands and enhance their applications in host–guest chemistry (Sundberg *et al.*, 2001). It is known that the 1,3-diaminopropane ligand behaves as a strong chelator and forms a stable six-membered ring in its metal complexes as well as being a good hydrogen-bond donor due to the existence of the amino groups (Sundberg *et al.*, 2001). In contrast, the 2-(4-nitrophenyl)acetate ligand has the potential to act as a linker and can also act as a good hydrogen-bond acceptor due to the four oxygen atoms it contains. Combination of these ligands in a single system has the potential to construct hydrogen-bond-directed supramolecular networks. Herein, we report the synthesis and structure of the title compound, $[Cd(C_8H_6NO_4)_2(C_3H_{10}N_2)_2]$, which displays such a hydrogen-bond-directed structure.





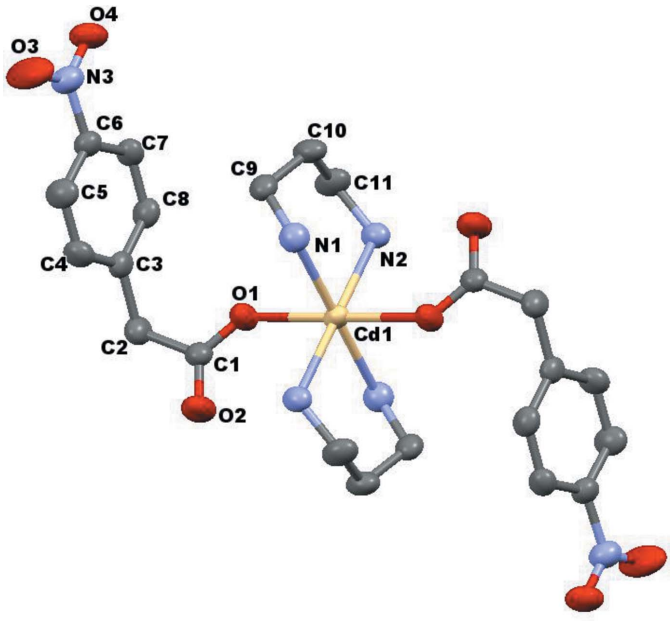


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. Non-labelled atoms are generated by the symmetry code $-x+1, -y+1, -z+2$.

2. Structural commentary

As shown in Fig. 1, the Cd^{II} atom is located on a center of symmetry. Therefore the asymmetric unit consist of half of the molecule. The Cd^{II} atom is octahedrally coordinated by four N atoms from two diamino propane ligands and two O atoms of monodentate acetate groups from two nitrophenyl-acetate ligands. The diamino propane ligand shows a chelating coordination behavior and displays a chair conformation in the equatorial direction. This kind of coordination mode was also found in other similar complexes (Roberts *et al.*, 2015; Sundberg & Uggla, 1997 Sundberg *et al.*, 2001;), although the ligand has also been used as a linker of two metal atoms (Sheng *et al.*, 2014). The nitro group is slightly twisted out of the aromatic plane, with a dihedral angle of 3.6 (3)° between the two least-squares planes. A weak intramolecular hydrogen bond of the type N—H···O involving one of the amino N atoms of the diaminopropane ligand and the non-coordinating carboxylate O atom of the nitrophenylacetate ligand is evident in the structure at a distance of 3.029 (3) Å (Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2	0.90	2.23	3.029 (3)	147
N2—H2B···O2^{i}	0.90	2.34	3.173 (3)	155
N1—H1A···O2^{ii}	0.90	2.29	3.149 (3)	160
C5—H5···O4^{iii}	0.93	2.50	3.253 (3)	139
C7—H7···O3^{iv}	0.93	2.57	3.346 (3)	141
C10—H10B···O3^{v}	0.97	2.69	3.629 (3)	163

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+2, y-\frac{1}{2}, -z+\frac{5}{2}$; (iv) $-x+2, y+\frac{1}{2}, -z+\frac{5}{2}$; (v) $x-1, y, z-1$.

3. Supramolecular features

Somewhat weaker intermolecular N—H···O interactions involving the same types of donor and acceptor groups occur between neighboring molecules (Table 1) and lead to a layered arrangement of the molecules parallel to the *bc* plane (Fig. 2). It should be noted that one of the hydrogen atoms (H1*B*) of the amino group N1 has no acceptor group in its vicinity; the shortest donor···acceptor distance of N1—H1*B*···O2 = 3.868 Å seems to be too long for a significant interaction. Several other weak intermolecular hydrogen-bonding interactions of the C—H···O type also exist in the structure involving the O atoms of nitro groups and neighboring C—H groups.

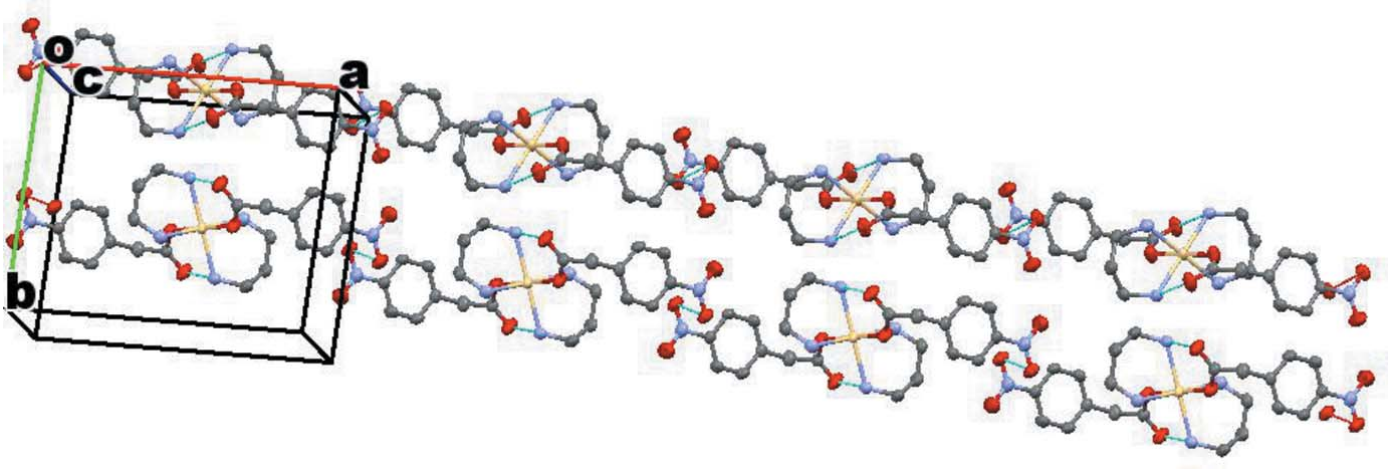


Figure 2
A packing diagram of the title compound. The light-blue dotted lines indicate intramolecular hydrogen-bonding interactions, as well as intralayer interactions involving the nitro groups of adjacent molecules. A weak N—H···O interlayer interaction also exists at 3.149 (3) Å, linking the layers (see Table 1 for details).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd(C_8H_6NO_4)_2(C_3H_{10}N_2)_2]$
M_r	620.94
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	14.6943 (5), 11.1227 (3), 8.3523 (3)
β (°)	105.778 (4)
V (Å^3)	1313.67 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.89
Crystal size (mm)	0.44 × 0.41 × 0.10
Data collection	
Diffractometer	Agilent Xcalibur Eos
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min}, T_{max}	0.923, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9750, 2400, 1911
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.056, 1.06
No. of reflections	2400
No. of parameters	170
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.26

Computer programs: *CrysAlis PRO* (Agilent, 2013), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL97* (Sheldrick, 2008)and *OLEX2* (Dolomanov *et al.*, 2009).

4. Synthesis and crystallization

0.2 mmol (36.7 mg) of anhydrous $CdCl_2$, 0.4 mmol (29.7 mg) of 1,3-diaminopropane, and 0.4 mmol (72.5 mg) of 4-nitrophenylacetic acid were added to 2 ml of methanol in a 5 ml beaker. The sample was covered with aluminum foil containing several small vent holes and left for a week to evaporate. The slow evaporation method was used to crystallize a colorless mononuclear species and crystals were gathered for X-ray crystallographic analysis.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed in calculated positions and allowed to ride during subsequent refinement, with $U_{iso}(H) = 1.2U_{eq}(C)$ and C—H distances of 0.93 Å for aromatic hydrogen atoms, $U_{iso}(H) = 1.2U_{eq}(C)$ and C—H distances of 0.97 Å for methylene hydrogen atoms, and $U_{iso}(H) = 1.2U_{eq}(N)$ and N—H distances of 0.90 Å for amino hydrogen atoms.

Acknowledgements

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References

Agilent (2013). *CrysAlis PRO*. Agilent Technologies, Yarton, England.
Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2015). *Acta Cryst.* A**71**, 59–75.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Roberts, T. J., Mehari, T. F., Assefa, Z., Hamby, T. & Sykora, R. E. (2015). *Acta Cryst.* E**71**, m240–m241.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheng, G. H., Cheng, X. S., You, Z. L. & Zhu, H. L. (2014). *Bull. Chem. Soc. Eth.* **28**, 315–319.
Sundberg, M. R., Kivekäs, R., Huovilainen, P. & Uggla, R. (2001). *Inorg. Chim. Acta*, **324**, 212–217.
Sundberg, M. R. & Uggla, R. (1997). *Inorg. Chim. Acta*, **254**, 259–265.

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO* (Agilent, 2013); data reduction: *CrysAlis PRO* (Agilent, 2013); program(s) used to solve structure: *OLEX2.solve* (Bourhis *et al.*, 2015); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Bis(1,3-diaminopropane-κ^2N,N')bis[2-(4-nitrophenyl)acetato-κO]cadmium

Crystal data

$[Cd(C_8H_6NO_4)_2(C_3H_{10}N_2)_2]$
M_r = 620.94
Monoclinic, $P2_1/c$
a = 14.6943 (5) Å
b = 11.1227 (3) Å
c = 8.3523 (3) Å
β = 105.778 (4)°
V = 1313.67 (7) Å^3
Z = 2
$F(000)$ = 636
D_x = 1.570 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3294 reflections
θ = 2.3–27.1°
μ = 0.89 mm^{-1}
T = 293 K
Plate, colourless
0.44 × 0.41 × 0.10 mm

Data collection

Agilent Xcalibur Eos diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0514 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.923, T_{max} = 1.000
9750 measured reflections
2400 independent reflections
1911 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.4°, θ_{min} = 2.3°
h = −17→17
k = −12→13
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.056
S = 1.06
2400 reflections
170 parameters
0 restraints
Primary atom site location: iterative
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0178P)^2 + 0.5991P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}

$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^{2}\lambda^{3}$/sin(2θ)]$^{-1/4}$
Extinction coefficient: 0.0012 (2)

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 $F^2 > 2\sigma(F^2)$ 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	0.5000	0.5000	1.0000	0.03617 (10)
O1	0.62078 (12)	0.49421 (16)	0.8639 (2)	0.0497 (5)
C9	0.30006 (17)	0.5182 (2)	0.7208 (3)	0.0405 (6)
H9A	0.2571	0.5602	0.6291	0.049*
H9B	0.2751	0.5245	0.8167	0.049*
O2	0.57547 (14)	0.35381 (19)	0.6686 (2)	0.0639 (6)
C1	0.63446 (17)	0.4232 (2)	0.7568 (3)	0.0359 (6)
N2	0.44583 (14)	0.31282 (16)	0.8902 (2)	0.0387 (5)
H2A	0.4749	0.2947	0.8113	0.046*
H2B	0.4642	0.2579	0.9717	0.046*
C8	0.84336 (18)	0.5357 (2)	0.9702 (3)	0.0393 (6)
H8	0.8149	0.6073	0.9248	0.047*
C3	0.81242 (16)	0.4281 (2)	0.8897 (3)	0.0339 (5)
C7	0.91540 (18)	0.5390 (2)	1.1161 (3)	0.0386 (6)
H7	0.9355	0.6116	1.1690	0.046*
C6	0.95687 (16)	0.4323 (2)	1.1816 (3)	0.0354 (6)
C4	0.85551 (18)	0.3230 (2)	0.9607 (3)	0.0432 (6)
H4	0.8355	0.2500	0.9089	0.052*
C2	0.73382 (17)	0.4241 (3)	0.7300 (3)	0.0426 (6)
H2C	0.7414	0.3527	0.6682	0.051*
H2D	0.7394	0.4935	0.6628	0.051*
N3	1.03724 (15)	0.4348 (2)	1.3320 (3)	0.0465 (6)
C5	0.92748 (19)	0.3240 (2)	1.1067 (3)	0.0457 (7)
H5	0.9555	0.2526	1.1533	0.055*
C11	0.34305 (18)	0.2995 (2)	0.8167 (3)	0.0502 (7)
H11A	0.3109	0.3124	0.9025	0.060*
H11B	0.3297	0.2180	0.7757	0.060*
C10	0.30436 (19)	0.3869 (2)	0.6752 (3)	0.0482 (7)
H10A	0.3428	0.3806	0.5978	0.058*
H10B	0.2409	0.3613	0.6167	0.058*
O4	1.06568 (14)	0.53165 (17)	1.3946 (2)	0.0551 (5)
O3	1.07278 (16)	0.33928 (19)	1.3882 (3)	0.0844 (8)

N1	0.39369 (14)	0.57670 (19)	0.7594 (2)	0.0432 (5)
H1A	0.3865	0.6561	0.7727	0.052*
H1B	0.4183	0.5668	0.6727	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02686 (14)	0.03292 (15)	0.04385 (16)	−0.00022 (12)	0.00131 (10)	−0.00811 (12)
O1	0.0383 (10)	0.0604 (12)	0.0531 (11)	−0.0088 (9)	0.0174 (8)	−0.0232 (10)
C9	0.0345 (14)	0.0490 (16)	0.0338 (12)	0.0065 (12)	0.0017 (11)	0.0014 (11)
O2	0.0476 (12)	0.0746 (14)	0.0667 (13)	−0.0169 (11)	0.0109 (10)	−0.0331 (11)
C1	0.0340 (14)	0.0388 (14)	0.0310 (12)	0.0009 (12)	0.0024 (11)	−0.0012 (11)
N2	0.0410 (12)	0.0323 (11)	0.0375 (11)	0.0024 (10)	0.0017 (9)	−0.0008 (9)
C8	0.0380 (14)	0.0317 (13)	0.0472 (15)	0.0046 (11)	0.0097 (12)	0.0054 (11)
C3	0.0278 (12)	0.0433 (14)	0.0331 (12)	−0.0008 (12)	0.0126 (10)	0.0003 (11)
C7	0.0371 (14)	0.0296 (12)	0.0486 (15)	−0.0051 (11)	0.0107 (12)	−0.0057 (11)
C6	0.0300 (13)	0.0364 (14)	0.0388 (13)	−0.0041 (11)	0.0072 (11)	0.0001 (11)
C4	0.0467 (16)	0.0331 (14)	0.0469 (15)	−0.0065 (13)	0.0080 (13)	−0.0086 (12)
C2	0.0382 (15)	0.0568 (17)	0.0345 (13)	0.0017 (14)	0.0126 (11)	−0.0033 (12)
N3	0.0389 (13)	0.0500 (14)	0.0453 (13)	−0.0026 (12)	0.0023 (11)	0.0017 (11)
C5	0.0496 (17)	0.0301 (13)	0.0506 (16)	0.0023 (13)	0.0020 (13)	0.0055 (12)
C11	0.0450 (17)	0.0375 (14)	0.0589 (17)	−0.0096 (13)	−0.0015 (14)	−0.0011 (13)
C10	0.0440 (16)	0.0464 (16)	0.0428 (15)	−0.0008 (13)	−0.0077 (12)	−0.0060 (12)
O4	0.0533 (12)	0.0542 (12)	0.0502 (11)	−0.0163 (10)	0.0013 (9)	−0.0093 (9)
O3	0.0824 (17)	0.0538 (13)	0.0835 (16)	0.0104 (13)	−0.0346 (13)	0.0066 (12)
N1	0.0452 (13)	0.0394 (12)	0.0439 (12)	0.0007 (11)	0.0101 (10)	0.0025 (10)

Geometric parameters (Å, º)

Cd1—O1^{i}	2.3547 (17)	C3—C2	1.509 (3)
Cd1—O1	2.3547 (17)	C7—H7	0.9300
Cd1—N2^{i}	2.3265 (18)	C7—C6	1.377 (3)
Cd1—N2	2.3265 (18)	C6—N3	1.472 (3)
Cd1—N1^{i}	2.3449 (19)	C6—C5	1.373 (3)
Cd1—N1	2.3449 (19)	C4—H4	0.9300
O1—C1	1.250 (3)	C4—C5	1.379 (3)
C9—H9A	0.9700	C2—H2C	0.9700
C9—H9B	0.9700	C2—H2D	0.9700
C9—C10	1.515 (3)	N3—O4	1.220 (3)
C9—N1	1.476 (3)	N3—O3	1.220 (3)
O2—C1	1.242 (3)	C5—H5	0.9300
C1—C2	1.536 (3)	C11—H11A	0.9700
N2—H2A	0.9000	C11—H11B	0.9700
N2—H2B	0.9000	C11—C10	1.516 (3)
N2—C11	1.475 (3)	C10—H10A	0.9700
C8—H8	0.9300	C10—H10B	0.9700
C8—C3	1.387 (3)	N1—H1A	0.9000
C8—C7	1.380 (3)	N1—H1B	0.9000

C3—C4	1.384 (3)		
O1—Cd1—O1^{i}	180.0	C6—C7—C8	118.6 (2)
N2—Cd1—O1	90.41 (7)	C6—C7—H7	120.7
N2—Cd1—O1^{i}	89.59 (7)	C7—C6—N3	119.3 (2)
N2^{i}—Cd1—O1^{i}	90.41 (7)	C5—C6—C7	121.6 (2)
N2^{i}—Cd1—O1	89.59 (7)	C5—C6—N3	119.0 (2)
N2—Cd1—N2^{i}	180.0	C3—C4—H4	119.2
N2—Cd1—N1^{i}	95.11 (7)	C5—C4—C3	121.6 (2)
N2^{i}—Cd1—N1	95.11 (7)	C5—C4—H4	119.2
N2^{i}—Cd1—N1^{i}	84.89 (7)	C1—C2—H2C	108.8
N2—Cd1—N1	84.89 (7)	C1—C2—H2D	108.8
N1—Cd1—O1^{i}	89.42 (7)	C3—C2—C1	113.60 (19)
N1^{i}—Cd1—O1^{i}	90.58 (7)	C3—C2—H2C	108.8
N1^{i}—Cd1—O1	89.42 (7)	C3—C2—H2D	108.8
N1—Cd1—O1	90.58 (7)	H2C—C2—H2D	107.7
N1—Cd1—N1^{i}	180.00 (7)	O4—N3—C6	119.0 (2)
C1—O1—Cd1	130.67 (16)	O4—N3—O3	122.9 (2)
H9A—C9—H9B	107.9	O3—N3—C6	118.2 (2)
C10—C9—H9A	109.1	C6—C5—C4	118.7 (2)
C10—C9—H9B	109.1	C6—C5—H5	120.7
N1—C9—H9A	109.1	C4—C5—H5	120.7
N1—C9—H9B	109.1	N2—C11—H11A	109.1
N1—C9—C10	112.3 (2)	N2—C11—H11B	109.1
O1—C1—C2	116.4 (2)	N2—C11—C10	112.6 (2)
O2—C1—O1	126.5 (2)	H11A—C11—H11B	107.8
O2—C1—C2	117.1 (2)	C10—C11—H11A	109.1
Cd1—N2—H2A	108.0	C10—C11—H11B	109.1
Cd1—N2—H2B	108.0	C9—C10—C11	117.0 (2)
H2A—N2—H2B	107.3	C9—C10—H10A	108.0
C11—N2—Cd1	117.10 (15)	C9—C10—H10B	108.0
C11—N2—H2A	108.0	C11—C10—H10A	108.0
C11—N2—H2B	108.0	C11—C10—H10B	108.0
C3—C8—H8	119.3	H10A—C10—H10B	107.3
C7—C8—H8	119.3	Cd1—N1—H1A	109.0
C7—C8—C3	121.5 (2)	Cd1—N1—H1B	109.0
C8—C3—C2	121.6 (2)	C9—N1—Cd1	113.02 (14)
C4—C3—C8	118.0 (2)	C9—N1—H1A	109.0
C4—C3—C2	120.4 (2)	C9—N1—H1B	109.0
C8—C7—H7	120.7	H1A—N1—H1B	107.8
Cd1—O1—C1—O2	17.7 (4)	C3—C8—C7—C6	0.1 (4)
Cd1—O1—C1—C2	−163.60 (16)	C3—C4—C5—C6	−0.4 (4)
Cd1—N2—C11—C10	58.8 (3)	C7—C8—C3—C4	0.5 (4)
O1^{i}—Cd1—N2—C11	46.37 (18)	C7—C8—C3—C2	−179.9 (2)
O1—Cd1—N2—C11	−133.63 (18)	C7—C6—N3—O4	−0.5 (4)
O1—Cd1—N1—C9	135.70 (16)	C7—C6—N3—O3	179.8 (3)
O1^{i}—Cd1—N1—C9	−44.30 (16)	C7—C6—C5—C4	1.0 (4)

O1—C1—C2—C3	43.5 (3)	C4—C3—C2—C1	95.2 (3)
O2—C1—C2—C3	−137.7 (2)	C2—C3—C4—C5	−180.0 (2)
N2^{i}—Cd1—O1—C1	−170.6 (2)	N3—C6—C5—C4	−176.5 (2)
N2—Cd1—O1—C1	9.4 (2)	C5—C6—N3—O4	177.1 (2)
N2—Cd1—N1—C9	45.35 (16)	C5—C6—N3—O3	−2.6 (4)
N2^{i}—Cd1—N1—C9	−134.65 (16)	C10—C9—N1—Cd1	−65.9 (2)
N2—C11—C10—C9	−71.0 (3)	N1^{i}—Cd1—O1—C1	104.5 (2)
C8—C3—C4—C5	−0.3 (4)	N1—Cd1—O1—C1	−75.5 (2)
C8—C3—C2—C1	−84.5 (3)	N1^{i}—Cd1—N2—C11	136.92 (18)
C8—C7—C6—N3	176.6 (2)	N1—Cd1—N2—C11	−43.08 (18)
C8—C7—C6—C5	−0.8 (4)	N1—C9—C10—C11	76.7 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2	0.90	2.23	3.029 (3)	147
N2—H2*B*···O2^{ii}	0.90	2.34	3.173 (3)	155
N1—H1*A*···O2^{iii}	0.90	2.29	3.149 (3)	160
C5—H5···O4^{iv}	0.93	2.50	3.253 (3)	139
C7—H7···O3^{v}	0.93	2.57	3.346 (3)	141
C10—H10*B*···O3^{vi}	0.97	2.69	3.629 (3)	163

Symmetry codes: (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*+1, *y*+1/2, −*z*+3/2; (iv) −*x*+2, *y*−1/2, −*z*+5/2; (v) −*x*+2, *y*+1/2, −*z*+5/2; (vi) *x*−1, *y*, *z*−1.