Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(5,6:19,20-Dibenzo-1,4,11,14-tetraoxa-8,17-diazacycloeicosane-$\kappa^4N^8,O^{11},O^{14}$,-$N^{17}$)dinitrato-$\kappa^4O,O'$-cadmium(II)

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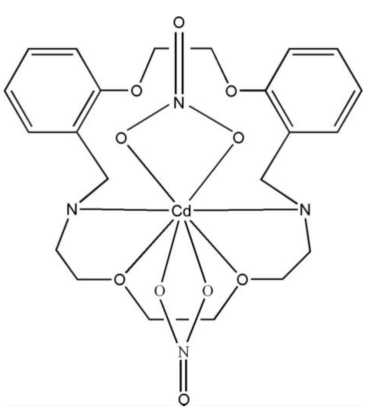
Received 16 October 2007; accepted 7 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.042; wR factor = 0.105; data-to-parameter ratio = 13.1.

In the title compound, $[Cd(NO_3)_2(C_{22}H_{30}N_2O_4)]$, the Cd^{II} atom is eight-coordinated by two amine N atoms and two O atoms from the 5,6:19,20-dibenzo-1,4,11,14-tetraoxa-8,17-diazacycloeicosane ligand and four O atoms from two nitrate groups. The coordination geometry about Cd is antiprismatic. One nitro O atom is disordered equally over two positions.

Related literature

For related literature, see: López-Deber *et al.* (2005); Vicente *et al.* (2003); Meyerstein (1990); Popović *et al.* (2006).



Experimental

Crystal data

$[Cd(NO_3)_2(C_{22}H_{30}N_2O_4)]$
M_r = 622.90
Monoclinic, $P2_1/c$
a = 13.167 (3) Å
b = 7.6750 (15) Å
c = 25.227 (5) Å
β = 92.568 (4)°
V = 2546.8 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 293 (2) K
0.22 × 0.21 × 0.19 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.82, T_{max} = 0.84
12190 measured reflections
4558 independent reflections
3767 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.105
S = 1.04
4558 reflections
349 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N2	2.348 (3)	Cd1—O3	2.430 (3)
Cd1—N1	2.369 (3)	Cd1—O8	2.433 (3)
Cd1—O6	2.399 (3)	Cd1—O4	2.523 (2)
Cd1—O5	2.415 (3)	Cd1—O10	2.673 (2)
N2—Cd1—N1	91.47 (10)	N1—Cd1—O8	133.87 (10)
N2—Cd1—O6	138.07 (10)	O6—Cd1—O8	76.09 (12)
N1—Cd1—O6	127.43 (11)	O5—Cd1—O8	85.66 (11)
N2—Cd1—O5	165.52 (12)	O3—Cd1—O8	154.93 (10)
N1—Cd1—O5	83.75 (11)	N2—Cd1—O4	71.36 (9)
O6—Cd1—O5	52.16 (11)	N1—Cd1—O4	126.54 (10)
N2—Cd1—O3	101.75 (10)	O6—Cd1—O4	72.42 (9)
N1—Cd1—O3	69.64 (10)	O5—Cd1—O4	122.27 (10)
O6—Cd1—O3	81.48 (10)	O3—Cd1—O4	65.46 (8)
O5—Cd1—O3	89.42 (12)	O8—Cd1—O4	96.74 (9)
N2—Cd1—O8	87.88 (11)		

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

We thank the National Natural Science Foundation of China (No. 20471014), the Program for New Century Excellent Talents in Chinese Universities (NCET-05-0320), the Fok Ying Tung Education Foundation, and the Analysis and Testing Foundation of Northeast Normal University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2056).

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  doi:10.1107/S1600536807056541

supplementary materials

Acta Cryst. (2008). E**64**, m322 [**doi:10.1107/S1600536807056541**]

(5,6:19,20-Dibenzo-1,4,11,14-tetraoxa-8,17-diazacycloeicosane-$\kappa^4 N^8,O^{11},O^{14},N^{17}$)dinitrato-$\kappa^4 O,O'$-cadmium(II)

T.-T. Han, J.-F. Ma, L.-P. Zhang and Q.-J. Li

Comment

In the last few decades, the modification of the macrocycles to control and tune the properties of coordinated metal atoms has been the subject of much interest (Meyerstein, 1990; Vicente *et al.*, 2003). We are involved in studies of oxaaza-macrocycles and their metal coordination compounds. In this paper, we report the preparation and crystal structure of the title macrocyclic complex of Cd^{II}.

In the structure of the title compound, Cd^{II} is eight-coordinated by two N atoms and two O atoms from ligand *L* and four O atoms from two nitrate groups. The title compound displays an antiprismatic geometry (Fig. 1). The bond distances and angles around the Cd atom are nomal (Popović *et al.*, 2006).

Experimental

Ligand *L* was synthesized according to the reported method (López-Deber *et al.*, 2005). A solution of $Cd(NO_3)_2.4H_2O$ (0.03 g, 0.10 mmol) in 5 ml e thanol was added dropwise to a solution of H_2L (0.039 g, 0.10 mmol) in 6 ml e thanol. After stirring for 30 min, the mixture was filtered. Colorless crystals were obtained by evaporating the filtrate at room temperature (yield 50%).

Refinement

The C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic and methylene H atoms. The disordered nitrate group was refined using O atom split over two sites, with a total occupancy of 1.

Figures

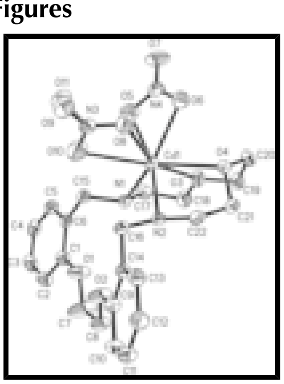


Fig. 1. A view of the molecule of I. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. Only one disorder site is shown for a nitrate.

[5,6:19,20-Dibenzo-1,4,11,14-tetraoxa-8,17-diazacycloeicosane- κ$^4N^8$,O^{11},O^{14},N^{17}]dinitrato-κ^4O,O'-cadmium(II)

Crystal data

$[Cd(NO_3)_2(C_{22}H_{30}N_2O_4)]$	F_{000} = 1272
M_r = 622.90	D_x = 1.625 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: -P 2ybc	Cell parameters from 3767 reflections
a = 13.167 (3) Å	θ = 1.6–25.2º
b = 7.6750 (15) Å	μ = 0.92 mm^{-1}
c = 25.227 (5) Å	T = 293 (2) K
β = 92.568 (4)º	Block, colourless
V = 2546.8 (9) Å^3	0.22 × 0.21 × 0.19 mm
Z = 4	

Data collection

Bruker APEX CCD area-detector diffractometer	4558 independent reflections
Radiation source: fine-focus sealed tube	3767 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.056
T = 293(2) K	θ_{max} = 25.2º
ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 14$
T_{min} = 0.82, T_{max} = 0.84	$k = -9 \rightarrow 8$
12190 measured reflections	$l = -30 \rightarrow 23$

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 atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.8726P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ < 0.001
4558 reflections	$\Delta\rho_{max}$ = 1.00 e Å^{-3}
349 parameters	$\Delta\rho_{min}$ = −1.00 e Å^{-3}
1 restraint	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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.237559 (19)	0.06536 (3)	0.068001 (9)	0.03453 (12)	
C1	0.3037 (3)	0.2975 (5)	0.26599 (15)	0.0463 (9)	
C2	0.3327 (4)	0.3662 (6)	0.31505 (16)	0.0567 (11)	
H2	0.2898	0.4418	0.3323	0.068*	
C3	0.4250 (3)	0.3218 (6)	0.33784 (16)	0.0556 (11)	
H3	0.4448	0.3669	0.3709	0.067*	
C4	0.4888 (3)	0.2114 (6)	0.31257 (17)	0.0566 (11)	
H4	0.5522	0.1839	0.3281	0.068*	
C5	0.4585 (3)	0.1415 (5)	0.26411 (16)	0.0501 (10)	
H5	0.5020	0.0665	0.2471	0.060*	
C6	0.3642 (3)	0.1809 (5)	0.24025 (14)	0.0422 (9)	
C7	0.1505 (5)	0.4558 (8)	0.2560 (3)	0.110 (3)	
H7A	0.1873	0.5651	0.2544	0.132*	
H7B	0.1373	0.4350	0.2930	0.132*	
C8	0.0537 (3)	0.4785 (6)	0.22754 (19)	0.0597 (12)	
H8A	0.0022	0.5032	0.2528	0.072*	
H8B	0.0579	0.5785	0.2042	0.072*	
C9	−0.0699 (3)	0.3258 (5)	0.17268 (16)	0.0460 (9)	
C10	−0.1521 (3)	0.4239 (5)	0.18653 (18)	0.0552 (11)	
H10	−0.1454	0.5067	0.2134	0.066*	
C11	−0.2452 (3)	0.3972 (6)	0.15981 (19)	0.0587 (11)	
H11	−0.3015	0.4611	0.1695	0.070*	
C12	−0.2557 (3)	0.2788 (6)	0.11950 (17)	0.0550 (10)	
H12	−0.3181	0.2642	0.1014	0.066*	
C13	−0.1727 (3)	0.1810 (5)	0.10590 (16)	0.0479 (9)	
H13	−0.1798	0.0994	0.0787	0.057*	
C14	−0.0788 (3)	0.2032 (5)	0.13236 (14)	0.0414 (8)	
C15	0.3261 (3)	0.0939 (5)	0.18976 (15)	0.0454 (9)	
H15A	0.3732	0.0017	0.1814	0.054*	
H15B	0.2612	0.0397	0.1960	0.054*	
C16	0.0130 (3)	0.1004 (4)	0.11704 (16)	0.0412 (8)	
H16A	0.0521	0.0678	0.1490	0.049*	
H16B	−0.0097	−0.0059	0.0994	0.049*	
C17	0.4099 (3)	0.2851 (5)	0.12706 (16)	0.0478 (9)	
H17A	0.4557	0.1927	0.1173	0.057*	
H17B	0.4415	0.3482	0.1567	0.057*	
C18	0.3922 (4)	0.4067 (5)	0.08089 (18)	0.0577 (11)	
H18A	0.3528	0.5068	0.0914	0.069*	

H18B	0.4565	0.4476	0.0683	0.069*	
C19	0.3169 (4)	0.4064 (5)	−0.00699 (17)	0.0543 (11)	
H19A	0.3795	0.4405	−0.0230	0.065*	
H19B	0.2782	0.5105	0.0003	0.065*	
C20	0.2563 (3)	0.2872 (6)	−0.04333 (15)	0.0541 (10)	
H20A	0.2293	0.3534	−0.0735	0.065*	
H20B	0.3008	0.1979	−0.0565	0.065*	
C21	0.0930 (3)	0.3238 (5)	−0.00682 (16)	0.0474 (9)	
H21A	0.0550	0.3526	−0.0395	0.057*	
H21B	0.1202	0.4308	0.0086	0.057*	
C22	0.0255 (3)	0.2383 (5)	0.03056 (15)	0.0445 (9)	
H22A	−0.0314	0.3145	0.0370	0.053*	
H22B	−0.0012	0.1316	0.0148	0.053*	
N1	0.3131 (2)	0.2088 (4)	0.14301 (11)	0.0380 (7)	
N2	0.0799 (2)	0.1973 (4)	0.08151 (12)	0.0362 (7)	
N3	0.1614 (3)	−0.2792 (4)	0.09950 (14)	0.0510 (8)	
N4	0.3934 (3)	−0.1361 (4)	0.02528 (15)	0.0504 (8)	
O1	0.2109 (2)	0.3313 (4)	0.24031 (13)	0.0725 (10)	
O2	0.0240 (2)	0.3344 (4)	0.19770 (14)	0.0711 (10)	
O3	0.3384 (2)	0.3117 (3)	0.04042 (10)	0.0510 (7)	
O4	0.1745 (2)	0.2061 (3)	−0.01765 (9)	0.0444 (6)	
O5	0.3898 (3)	−0.1102 (5)	0.07408 (14)	0.0717 (9)	
O6	0.3226 (3)	−0.0730 (4)	−0.00288 (13)	0.0649 (9)	
O7	0.4605 (3)	−0.2216 (5)	0.00709 (18)	0.0926 (12)	
O8	0.1473 (3)	−0.2092 (4)	0.05524 (13)	0.0673 (8)	
O9	0.1617 (10)	−0.439 (3)	0.1075 (11)	0.067 (4)	0.50
O10	0.1959 (3)	−0.1895 (4)	0.13589 (14)	0.0847 (11)	
O11	0.1198 (10)	−0.424 (3)	0.1043 (11)	0.075 (4)	0.50
H1N	0.272 (4)	0.298 (7)	0.150 (2)	0.090*	
H2N	0.098 (4)	0.287 (8)	0.096 (2)	0.090*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04017 (18)	0.02992 (17)	0.03375 (17)	0.00307 (10)	0.00432 (12)	−0.00144 (9)
C1	0.049 (2)	0.047 (2)	0.043 (2)	−0.0025 (18)	0.0002 (18)	−0.0047 (17)
C2	0.070 (3)	0.055 (2)	0.045 (2)	−0.006 (2)	0.001 (2)	−0.0145 (19)
C3	0.067 (3)	0.062 (3)	0.037 (2)	−0.019 (2)	−0.004 (2)	−0.0040 (19)
C4	0.061 (3)	0.052 (2)	0.055 (2)	−0.013 (2)	−0.015 (2)	0.011 (2)
C5	0.056 (2)	0.043 (2)	0.051 (2)	0.0012 (19)	0.000 (2)	0.0005 (17)
C6	0.054 (2)	0.0334 (19)	0.0387 (19)	−0.0028 (17)	−0.0029 (18)	−0.0004 (15)
C7	0.088 (4)	0.077 (4)	0.160 (6)	0.035 (3)	−0.051 (4)	−0.068 (4)
C8	0.069 (3)	0.045 (2)	0.065 (3)	0.012 (2)	−0.002 (2)	−0.021 (2)
C9	0.049 (2)	0.040 (2)	0.049 (2)	0.0082 (18)	0.0055 (19)	−0.0021 (17)
C10	0.058 (3)	0.051 (2)	0.057 (3)	0.014 (2)	0.010 (2)	−0.0077 (19)
C11	0.052 (3)	0.058 (3)	0.068 (3)	0.020 (2)	0.015 (2)	0.003 (2)
C12	0.045 (2)	0.060 (3)	0.060 (3)	0.003 (2)	0.008 (2)	0.004 (2)
C13	0.047 (2)	0.046 (2)	0.051 (2)	−0.0023 (18)	0.0070 (19)	−0.0009 (17)

C14	0.045 (2)	0.0354 (19)	0.044 (2)	0.0011 (16)	0.0102 (17)	0.0007 (16)
C15	0.058 (2)	0.036 (2)	0.041 (2)	0.0021 (17)	−0.0024 (19)	−0.0043 (15)
C16	0.047 (2)	0.0306 (18)	0.046 (2)	0.0049 (16)	0.0073 (18)	−0.0012 (15)
C17	0.043 (2)	0.050 (2)	0.050 (2)	−0.0066 (18)	0.0027 (18)	−0.0054 (18)
C18	0.067 (3)	0.048 (2)	0.057 (3)	−0.013 (2)	0.003 (2)	0.0000 (19)
C19	0.055 (2)	0.057 (3)	0.052 (2)	−0.002 (2)	0.020 (2)	0.0180 (19)
C20	0.063 (3)	0.063 (3)	0.038 (2)	0.006 (2)	0.0227 (19)	0.0073 (19)
C21	0.056 (2)	0.039 (2)	0.047 (2)	0.0117 (18)	−0.0001 (19)	0.0057 (17)
C22	0.047 (2)	0.037 (2)	0.050 (2)	0.0064 (17)	−0.0003 (18)	0.0011 (16)
N1	0.0424 (17)	0.0356 (16)	0.0361 (16)	0.0006 (13)	0.0027 (14)	−0.0016 (13)
N2	0.0402 (16)	0.0287 (15)	0.0401 (16)	0.0027 (13)	0.0037 (13)	−0.0051 (12)
N3	0.064 (2)	0.0343 (18)	0.055 (2)	−0.0062 (17)	0.0082 (18)	−0.0069 (16)
N4	0.051 (2)	0.0383 (18)	0.063 (2)	0.0029 (16)	0.0114 (18)	−0.0043 (16)
O1	0.0618 (19)	0.079 (2)	0.074 (2)	0.0264 (17)	−0.0188 (17)	−0.0395 (18)
O2	0.0611 (19)	0.0554 (19)	0.095 (2)	0.0182 (15)	−0.0221 (18)	−0.0349 (17)
O3	0.0648 (18)	0.0436 (15)	0.0444 (14)	−0.0110 (13)	0.0024 (13)	0.0079 (12)
O4	0.0554 (16)	0.0399 (14)	0.0385 (13)	0.0078 (12)	0.0076 (12)	−0.0001 (11)
O5	0.076 (2)	0.074 (2)	0.063 (2)	0.0211 (18)	−0.0111 (19)	−0.0101 (17)
O6	0.071 (2)	0.065 (2)	0.0579 (19)	0.0131 (16)	−0.0053 (17)	−0.0043 (14)
O7	0.075 (2)	0.071 (2)	0.135 (3)	0.0246 (19)	0.044 (2)	−0.018 (2)
O8	0.079 (2)	0.0600 (19)	0.0618 (19)	−0.0019 (16)	−0.0068 (17)	0.0067 (16)
O9	0.076 (9)	0.036 (5)	0.091 (7)	−0.017 (8)	0.008 (9)	−0.002 (4)
O10	0.122 (3)	0.054 (2)	0.075 (2)	−0.0126 (19)	−0.023 (2)	−0.0153 (17)
O11	0.090 (11)	0.048 (7)	0.087 (7)	−0.031 (9)	0.006 (11)	−0.004 (5)

Geometric parameters (Å, °)

Cd1—N2	2.348 (3)	C14—C16	1.508 (5)
Cd1—N1	2.369 (3)	C15—N1	1.476 (5)
Cd1—O6	2.399 (3)	C15—H15A	0.9700
Cd1—O5	2.415 (3)	C15—H15B	0.9700
Cd1—O3	2.430 (3)	C16—N2	1.484 (5)
Cd1—O8	2.433 (3)	C16—H16A	0.9700
Cd1—O4	2.523 (2)	C16—H16B	0.9700
Cd1—O10	2.673 (2)	C17—N1	1.475 (5)
C1—C6	1.380 (5)	C17—C18	1.503 (6)
C1—O1	1.382 (5)	C17—H17A	0.9700
C1—C2	1.383 (5)	C17—H17B	0.9700
C2—C3	1.364 (6)	C18—O3	1.418 (5)
C2—H2	0.9300	C18—H18A	0.9700
C3—C4	1.370 (6)	C18—H18B	0.9700
C3—H3	0.9300	C19—O3	1.417 (5)
C4—C5	1.378 (6)	C19—C20	1.499 (6)
C4—H4	0.9300	C19—H19A	0.9700
C5—C6	1.389 (5)	C19—H19B	0.9700
C5—H5	0.9300	C20—O4	1.425 (5)
C6—C15	1.504 (5)	C20—H20A	0.9700
C7—O1	1.315 (6)	C20—H20B	0.9700
C7—C8	1.445 (6)	C21—O4	1.439 (4)

C7—H7A	0.9700	C21—C22	1.477 (6)
C7—H7B	0.9700	C21—H21A	0.9700
C8—O2	1.384 (5)	C21—H21B	0.9700
C8—H8A	0.9700	C22—N2	1.477 (5)
C8—H8B	0.9700	C22—H22A	0.9700
C9—O2	1.364 (5)	C22—H22B	0.9700
C9—C10	1.377 (6)	N1—H1N	0.90 (6)
C9—C14	1.387 (5)	N2—H2N	0.81 (6)
C10—C11	1.387 (6)	N3—O10	1.219 (4)
C10—H10	0.9300	N3—O9	1.24 (2)
C11—C12	1.366 (6)	N3—O8	1.245 (4)
C11—H11	0.9300	N3—O11	1.25 (2)
C12—C13	1.381 (6)	N4—O7	1.207 (4)
C12—H12	0.9300	N4—O6	1.245 (4)
C13—C14	1.389 (5)	N4—O5	1.250 (5)
C13—H13	0.9300	O9—O11	0.57 (2)

N2—Cd1—N1	91.47 (10)	N2—C16—C14	113.4 (3)
N2—Cd1—O6	138.07 (10)	N2—C16—H16A	108.9
N1—Cd1—O6	127.43 (11)	C14—C16—H16A	108.9
N2—Cd1—O5	165.52 (12)	N2—C16—H16B	108.9
N1—Cd1—O5	83.75 (11)	C14—C16—H16B	108.9
O6—Cd1—O5	52.16 (11)	H16A—C16—H16B	107.7
N2—Cd1—O3	101.75 (10)	N1—C17—C18	110.6 (3)
N1—Cd1—O3	69.64 (10)	N1—C17—H17A	109.5
O6—Cd1—O3	81.48 (10)	C18—C17—H17A	109.5
O5—Cd1—O3	89.42 (12)	N1—C17—H17B	109.5
N2—Cd1—O8	87.88 (11)	C18—C17—H17B	109.5
N1—Cd1—O8	133.87 (10)	H17A—C17—H17B	108.1
O6—Cd1—O8	76.09 (12)	O3—C18—C17	107.1 (3)
O5—Cd1—O8	85.66 (11)	O3—C18—H18A	110.3
O3—Cd1—O8	154.93 (10)	C17—C18—H18A	110.3
N2—Cd1—O4	71.36 (9)	O3—C18—H18B	110.3
N1—Cd1—O4	126.54 (10)	C17—C18—H18B	110.3
O6—Cd1—O4	72.42 (9)	H18A—C18—H18B	108.6
O5—Cd1—O4	122.27 (10)	O3—C19—C20	106.5 (3)
O3—Cd1—O4	65.46 (8)	O3—C19—H19A	110.4
O8—Cd1—O4	96.74 (9)	C20—C19—H19A	110.4
C6—C1—O1	114.7 (3)	O3—C19—H19B	110.4
C6—C1—C2	121.8 (4)	C20—C19—H19B	110.4
O1—C1—C2	123.4 (4)	H19A—C19—H19B	108.6
C3—C2—C1	119.1 (4)	O4—C20—C19	112.4 (3)
C3—C2—H2	120.4	O4—C20—H20A	109.1
C1—C2—H2	120.4	C19—C20—H20A	109.1
C2—C3—C4	120.8 (4)	O4—C20—H20B	109.1
C2—C3—H3	119.6	C19—C20—H20B	109.1
C4—C3—H3	119.6	H20A—C20—H20B	107.9
C3—C4—C5	119.6 (4)	O4—C21—C22	108.5 (3)
C3—C4—H4	120.2	O4—C21—H21A	110.0
C5—C4—H4	120.2	C22—C21—H21A	110.0

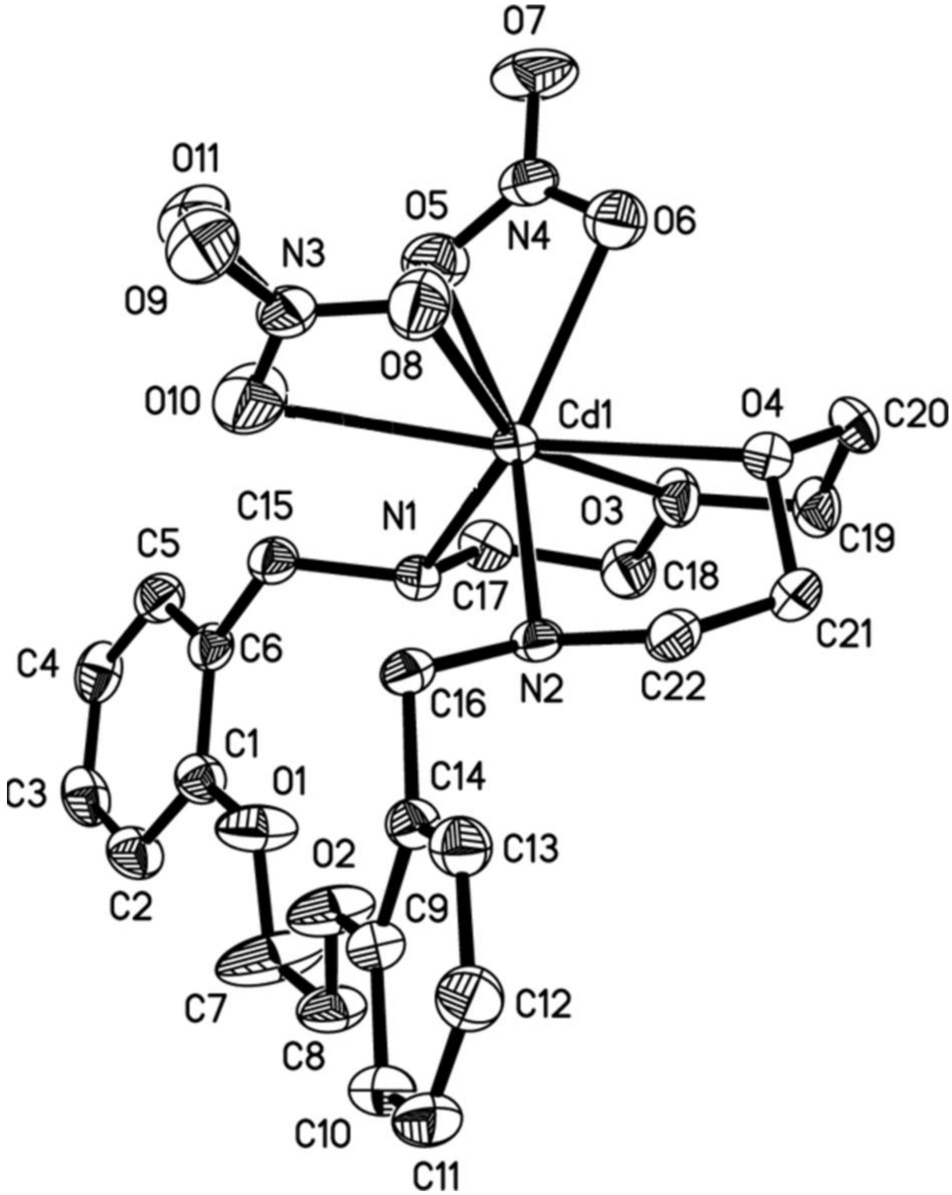
C4—C5—C6	121.1 (4)	O4—C21—H21B	110.0
C4—C5—H5	119.4	C22—C21—H21B	110.0
C6—C5—H5	119.4	H21A—C21—H21B	108.4
C1—C6—C5	117.5 (3)	N2—C22—C21	111.6 (3)
C1—C6—C15	120.6 (3)	N2—C22—H22A	109.3
C5—C6—C15	121.9 (4)	C21—C22—H22A	109.3
O1—C7—C8	118.0 (4)	N2—C22—H22B	109.3
O1—C7—H7A	107.8	C21—C22—H22B	109.3
C8—C7—H7A	107.8	H22A—C22—H22B	108.0
O1—C7—H7B	107.8	C17—N1—C15	112.6 (3)
C8—C7—H7B	107.8	C17—N1—Cd1	107.7 (2)
H7A—C7—H7B	107.1	C15—N1—Cd1	113.0 (2)
O2—C8—C7	113.3 (4)	C17—N1—H1N	107 (4)
O2—C8—H8A	108.9	C15—N1—H1N	110 (4)
C7—C8—H8A	108.9	Cd1—N1—H1N	106 (3)
O2—C8—H8B	108.9	C22—N2—C16	110.8 (3)
C7—C8—H8B	108.9	C22—N2—Cd1	111.3 (2)
H8A—C8—H8B	107.7	C16—N2—Cd1	115.1 (2)
O2—C9—C10	124.3 (4)	C22—N2—H2N	110 (4)
O2—C9—C14	114.7 (3)	C16—N2—H2N	109 (4)
C10—C9—C14	121.0 (4)	Cd1—N2—H2N	101 (4)
C9—C10—C11	118.9 (4)	O10—N3—O9	115.9 (12)
C9—C10—H10	120.5	O10—N3—O8	117.9 (3)
C11—C10—H10	120.5	O9—N3—O8	124.8 (13)
C12—C11—C10	121.1 (4)	O10—N3—O11	125.5 (13)
C12—C11—H11	119.4	O8—N3—O11	115.0 (12)
C10—C11—H11	119.4	O7—N4—O6	122.5 (4)
C11—C12—C13	119.5 (4)	O7—N4—O5	121.5 (4)
C11—C12—H12	120.3	O6—N4—O5	116.0 (4)
C13—C12—H12	120.3	C7—O1—C1	121.9 (3)
C12—C13—C14	120.7 (4)	C9—O2—C8	121.2 (3)
C12—C13—H13	119.6	C19—O3—C18	114.7 (3)
C14—C13—H13	119.6	C19—O3—Cd1	123.4 (2)
C9—C14—C13	118.7 (4)	C18—O3—Cd1	117.1 (2)
C9—C14—C16	120.0 (3)	C20—O4—C21	113.4 (3)
C13—C14—C16	121.3 (3)	C20—O4—Cd1	110.5 (2)
N1—C15—C6	115.7 (3)	C21—O4—Cd1	109.0 (2)
N1—C15—H15A	108.4	N4—O5—Cd1	95.4 (2)
C6—C15—H15A	108.4	N4—O6—Cd1	96.3 (2)
N1—C15—H15B	108.4	N3—O8—Cd1	101.7 (2)
C6—C15—H15B	108.4	O11—O9—N3	77 (5)
H15A—C15—H15B	107.4	O9—O11—N3	77 (4)

C6—C1—C2—C3	2.1 (7)	C10—C9—O2—C8	−20.9 (7)
O1—C1—C2—C3	178.4 (4)	C14—C9—O2—C8	161.5 (4)
C1—C2—C3—C4	0.4 (7)	C7—C8—O2—C9	173.2 (6)
C2—C3—C4—C5	−1.4 (7)	C20—C19—O3—C18	−177.5 (3)
C3—C4—C5—C6	0.0 (6)	C20—C19—O3—Cd1	−22.8 (4)
O1—C1—C6—C5	−180.0 (4)	C17—C18—O3—C19	−178.7 (4)
C2—C1—C6—C5	−3.4 (6)	C17—C18—O3—Cd1	24.9 (4)

O1—C1—C6—C15	−3.1 (6)	N2—Cd1—O3—C19	−64.3 (3)
C2—C1—C6—C15	173.5 (4)	N1—Cd1—O3—C19	−151.5 (3)
C4—C5—C6—C1	2.3 (6)	O6—Cd1—O3—C19	73.2 (3)
C4—C5—C6—C15	−174.6 (4)	O5—Cd1—O3—C19	125.0 (3)
O1—C7—C8—O2	18.3 (10)	O8—Cd1—O3—C19	46.5 (4)
O2—C9—C10—C11	−176.8 (4)	O4—Cd1—O3—C19	−1.3 (3)
C14—C9—C10—C11	0.7 (7)	N2—Cd1—O3—C18	89.8 (3)
C9—C10—C11—C12	−1.5 (7)	N1—Cd1—O3—C18	2.7 (3)
C10—C11—C12—C13	1.5 (7)	O6—Cd1—O3—C18	−132.7 (3)
C11—C12—C13—C14	−0.7 (6)	O5—Cd1—O3—C18	−80.9 (3)
O2—C9—C14—C13	177.8 (4)	O8—Cd1—O3—C18	−159.3 (3)
C10—C9—C14—C13	0.1 (6)	O4—Cd1—O3—C18	152.8 (3)
O2—C9—C14—C16	−3.8 (5)	C19—C20—O4—C21	71.5 (4)
C10—C9—C14—C16	178.5 (4)	C19—C20—O4—Cd1	−51.3 (4)
C12—C13—C14—C9	−0.1 (6)	C22—C21—O4—C20	−166.5 (3)
C12—C13—C14—C16	−178.5 (4)	C22—C21—O4—Cd1	−43.0 (3)
C1—C6—C15—N1	68.8 (5)	N2—Cd1—O4—C20	140.1 (2)
C5—C6—C15—N1	−114.5 (4)	N1—Cd1—O4—C20	62.6 (3)
C9—C14—C16—N2	−80.7 (4)	O6—Cd1—O4—C20	−61.4 (2)
C13—C14—C16—N2	97.7 (4)	O5—Cd1—O4—C20	−45.4 (3)
N1—C17—C18—O3	−54.4 (5)	O3—Cd1—O4—C20	27.1 (2)
O3—C19—C20—O4	48.3 (5)	O8—Cd1—O4—C20	−134.5 (2)
O4—C21—C22—N2	61.4 (4)	N2—Cd1—O4—C21	14.8 (2)
C18—C17—N1—C15	−177.6 (3)	N1—Cd1—O4—C21	−62.7 (2)
C18—C17—N1—Cd1	57.3 (3)	O6—Cd1—O4—C21	173.3 (2)
C6—C15—N1—C17	63.5 (4)	O5—Cd1—O4—C21	−170.7 (2)
C6—C15—N1—Cd1	−174.3 (3)	O3—Cd1—O4—C21	−98.2 (2)
N2—Cd1—N1—C17	−132.3 (2)	O8—Cd1—O4—C21	100.2 (2)
O6—Cd1—N1—C17	30.8 (3)	O7—N4—O5—Cd1	179.6 (4)
O5—Cd1—N1—C17	61.4 (2)	O6—N4—O5—Cd1	−2.4 (4)
O3—Cd1—N1—C17	−30.3 (2)	N2—Cd1—O5—N4	140.9 (4)
O8—Cd1—N1—C17	139.2 (2)	N1—Cd1—O5—N4	−147.8 (3)
O4—Cd1—N1—C17	−64.6 (3)	O6—Cd1—O5—N4	1.4 (2)
N2—Cd1—N1—C15	102.8 (3)	O3—Cd1—O5—N4	−78.2 (3)
O6—Cd1—N1—C15	−94.1 (3)	O8—Cd1—O5—N4	77.1 (3)
O5—Cd1—N1—C15	−63.5 (3)	O4—Cd1—O5—N4	−18.1 (3)
O3—Cd1—N1—C15	−155.2 (3)	O7—N4—O6—Cd1	−179.6 (4)
O8—Cd1—N1—C15	14.3 (3)	O5—N4—O6—Cd1	2.4 (4)
O4—Cd1—N1—C15	170.5 (2)	N2—Cd1—O6—N4	−167.3 (2)
C21—C22—N2—C16	−176.0 (3)	N1—Cd1—O6—N4	38.4 (3)
C21—C22—N2—Cd1	−46.6 (3)	O5—Cd1—O6—N4	−1.4 (2)
C14—C16—N2—C22	−62.8 (4)	O3—Cd1—O6—N4	94.5 (2)
C14—C16—N2—Cd1	169.9 (2)	O8—Cd1—O6—N4	−96.8 (2)
N1—Cd1—N2—C22	144.3 (2)	O4—Cd1—O6—N4	161.4 (2)
O6—Cd1—N2—C22	−15.5 (3)	O10—N3—O8—Cd1	12.1 (4)
O5—Cd1—N2—C22	−145.3 (4)	O9—N3—O8—Cd1	−153.4 (9)
O3—Cd1—N2—C22	74.8 (2)	O11—N3—O8—Cd1	178.3 (10)
O8—Cd1—N2—C22	−81.9 (2)	N2—Cd1—O8—N3	−99.4 (3)
O4—Cd1—N2—C22	16.0 (2)	N1—Cd1—O8—N3	−9.4 (3)

N1—Cd1—N2—C16	−88.7 (2)	O6—Cd1—O8—N3	119.7 (3)
O6—Cd1—N2—C16	111.5 (2)	O5—Cd1—O8—N3	67.6 (3)
O5—Cd1—N2—C16	−18.3 (5)	O3—Cd1—O8—N3	146.9 (3)
O3—Cd1—N2—C16	−158.2 (2)	O4—Cd1—O8—N3	−170.4 (3)
O8—Cd1—N2—C16	45.2 (2)	O10—N3—O9—O11	118 (5)
O4—Cd1—N2—C16	143.0 (2)	O8—N3—O9—O11	−76 (6)
C8—C7—O1—C1	−178.4 (5)	O10—N3—O11—O9	−76 (6)
C6—C1—O1—C7	−170.9 (6)	O8—N3—O11—O9	118 (5)
C2—C1—O1—C7	12.6 (8)		

Fig. 1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