Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{[*N*,*N*′-Bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetato}bis(1*H*-imidazole-κN^3)cadmium(II) dihydrate

Min Zhang, She-Min Lan, Hui-Li Weng and Xing-Man Xu*

Department of Chemistry, Central China Normal University, Wuhan, Hubei 430079, People's Republic of China
Correspondence e-mail: zhangmin126_2005@126.com

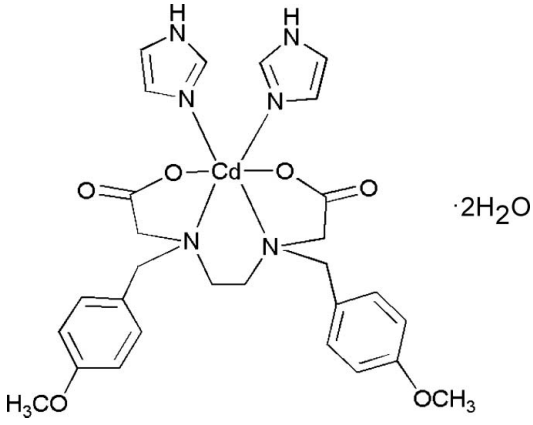
Received 4 June 2007; accepted 26 June 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.009 Å; disorder in main residue; R factor = 0.059; wR factor = 0.179; data-to-parameter ratio = 14.5.

In the title complex, $[Cd(C_{22}H_{26}N_2O_6)(C_3H_4N_2)_2]\cdot 2H_2O$, the Cd atom is in a distorted octahedral coordination environment. In the crystal structure, intermolecular hydrogen bonding links molecules into infinite one-dimensional chains. The atoms of one 4-methoxybenzyl group are disordered over two sites in approximately a 0.54:0.46 ratio.

Related literature

Recently, we have reported similar nickel and zinc complexes with [*N*,*N*′-bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetate (Zhang, Weng & Xu, 2007; Zhang, Weng, Hu & Xu, 2007).



Experimental

Crystal data

$[Cd(C_{22}H_{26}N_2O_6)(C_3H_4N_2)_2]\cdot 2H_2O$
M_r = 699.04
Orthorhombic, *Pcab*
a = 15.7646 (8) Å
b = 16.3172 (8) Å
c = 24.7351 (12) Å
V = 6362.7 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 292 (2) K
0.30 × 0.25 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.796, T_{max} = 0.949
63596 measured reflections
6253 independent reflections
3809 reflections with $I > 2\sigma(I)$
R_{int} = 0.088

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.179
S = 1.03
6253 reflections
430 parameters
102 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N3	2.261 (4)	Cd1—O2	2.325 (4)
Cd1—N5	2.276 (4)	Cd1—N1	2.415 (4)
Cd1—O4	2.311 (4)	Cd1—N2	2.426 (4)
N5—Cd1—O4	90.49 (13)	O4—Cd1—N2	72.21 (13)
N5—Cd1—O2	97.39 (14)	O2—Cd1—N2	96.99 (14)
N3—Cd1—N1	158.18 (13)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O3	0.85	1.91	2.756 (14)	173
N6—H6A···O3^{i}	0.86	1.85	2.703 (6)	172
C28—H28···O8^{ii}	0.93	2.67	3.58 (4)	167
N4—H4A···O5^{ii}	0.86	1.87	2.724 (6)	170

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2024).

References

Bruker (2000). *SMART*, *SAINT-Plus* and *SADABS* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2001). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Zhang, M., Weng, H.-L., Hu, B. & Xu, X.-M. (2007). *Acta Cryst.* E**63**, m1797.
Zhang, M., Weng, H.-L. & Xu, X.-M. (2007). *Acta Cryst.* E**63**, m1465–m1466.

 doi:10.1107/S1600536807031200

supplementary materials

Acta Cryst. (2007). E**63**, m2045 [**doi:10.1107/S1600536807031200**]

{[*N*,*N*'-Bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetato}bis(1*H*-imidazole-κN^3)cadmium(II) dihydrate

M. Zhang, S.-M. Lan, H.-L. Weng and X.-M. Xu

Comment

Recently, we have reported the nickel and zinc complexes with the [*N*,*N*'-bis(4-methoxylbenzyl)ethane-1,2-diyldiimino] diacetate (Zhang, Weng & Xu, 2007; Zhang, Weng, Hu & Xu, 2007). In this paper, we continue reporting the structure of the Cd(II) complex, Cd(L_a)(L_b)$_2$·2H$_2$O(L_a=[*N*,*N*'-bis(4-methoxyl- benzyl)ethane-1,2-diyldiimino]diacetate, L_b=imidazole)(1). In (1), the cadmium atom is also in a slightly distorted octahedral coordination environment (Fig. 1), which is similar to the zinc complex without the longer bond lengths (Table 1), and there is a disorder in one of the 4-methoxylbenzyl groups. In the crystal structure, the hydrogen bonds (Table 2) consolidate the crystal packing into infinite one-dimensional chains (Fig 2).

Experimental

The title complex was prepared according to the literature method (Zhang *et al.*, 2007*a*). Crystals were obtained by slow evaporation (one month) of a methanol solution(15 ml), with including the complex (1) (0.066 g, 0.1 mmol).

Refinement

H atoms bound to C atoms were included in calculated positions and allowed to ride during subsequent refinement, with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2, and C—H = 0.96Å and U_{iso} (H) = 1.5U_{eq}(C) for the methyl groups. H atoms bound to N atoms were located in difference Fourier map and refined with N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(N). In the crystal structure, the aromatic ring and methoxyl is disordered. The occupancy of the major component of disordered is 0.527, and the occupancy of the minor part is 0.473, the disorder was refined by using the AFIX, FLAT and ISOR restrains.

Figures

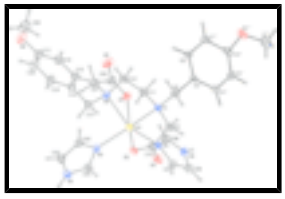


Fig. 1. Molecular structure of (I) showing 30% probability displacement ellipsoids. Omit the water molecule for clear.

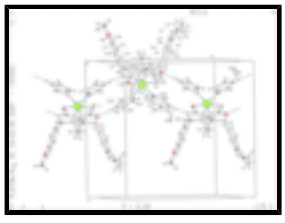


Fig. 2. Part of the crystal structure of (1), showing the formation of a chain of rings along [100]. Dashed lines denote hydrogen bonds.

{[*N*,*N*'-Bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetato}bis(1*H*- imidazole-kN^3)cadmium(II) dihydrate

Crystal data

$[Cd(C_{22}H_{26}N_2O_6)(C_3H_4N_2)_2]\cdot 2H_2O$	F_{000} = 2880
M_r = 699.04	D_x = 1.459 Mg m^{-3}
Orthorhombic, *Pcab*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2bc 2ac	Cell parameters from 5642 reflections
a = 15.7646 (8) Å	θ = 2.4–22.5º
b = 16.3172 (8) Å	μ = 0.74 mm^{-1}
c = 24.7351 (12) Å	*T* = 292 (2) K
V = 6362.7 (5) $Å^3$	Plate, colorless
Z = 8	0.30 × 0.25 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer	6253 independent reflections
Radiation source: fine-focus sealed tube	3809 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.088
T = 292(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	*h* = −19→19
T_{min} = 0.796, T_{max} = 0.949	*k* = −20→20
63596 measured reflections	*l* = −30→30

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H-atom parameters constrained
$wR(F^2)$ = 0.179	$w = 1/[\sigma^2(F_o^2) + (0.0819P)^2 + 6.7434P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
6253 reflections	$\Delta\rho_{max}$ = 0.69 e $Å^{-3}$
430 parameters	$\Delta\rho_{min}$ = −0.78 e $Å^{-3}$
102 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)
Cd1	0.36406 (3)	0.17511 (2)	0.249249 (14)	0.06385 (18)	
C1	0.606 (2)	−0.2625 (18)	0.4734 (13)	0.139 (10)	0.456 (14)
H1A	0.5778	−0.2972	0.4476	0.209*	0.456 (14)
H1B	0.6125	−0.2916	0.5068	0.209*	0.456 (14)
H1C	0.6601	−0.2466	0.4598	0.209*	0.456 (14)
O1	0.5578 (12)	−0.1948 (15)	0.4820 (10)	0.139 (7)	0.456 (14)
C2	0.5431 (13)	−0.1292 (13)	0.4356 (15)	0.118 (11)	0.456 (14)
C3	0.5056 (7)	−0.0690 (8)	0.4603 (4)	0.171 (13)	0.456 (14)
H3	0.5014	−0.0598	0.4973	0.205*	0.456 (14)
C4	0.4733 (7)	−0.0219 (8)	0.4186 (4)	0.113 (8)	0.456 (14)
H4	0.4312	0.0147	0.4290	0.136*	0.456 (14)
C5	0.4929 (7)	−0.0197 (8)	0.3641 (4)	0.087 (10)	0.456 (14)
C6	0.5234 (7)	−0.0970 (8)	0.3513 (4)	0.080 (5)	0.456 (14)
H6	0.5290	−0.1093	0.3148	0.096*	0.456 (14)
C7	0.5466 (7)	−0.1580 (8)	0.3877 (4)	0.081 (8)	0.456 (14)
H7	0.5714	−0.2071	0.3771	0.097*	0.456 (14)
C1'	0.595 (3)	−0.217 (2)	0.4931 (16)	0.194 (17)	0.544 (14)
H1'1	0.6369	−0.1757	0.4999	0.291*	0.544 (14)
H1'2	0.6137	−0.2685	0.5070	0.291*	0.544 (14)
H1'3	0.5426	−0.2016	0.5106	0.291*	0.544 (14)
O1'	0.5810 (9)	−0.2234 (7)	0.4373 (6)	0.145 (5)	0.544 (14)
C2'	0.5414 (8)	−0.1585 (11)	0.4180 (13)	0.107 (9)	0.544 (14)
C3'	0.5194 (5)	−0.0834 (5)	0.4385 (3)	0.114 (7)	0.544 (14)
H3'	0.5149	−0.0801	0.4760	0.137*	0.544 (14)
C4'	0.5029 (5)	−0.0118 (5)	0.4101 (3)	0.082 (5)	0.544 (14)
H4'	0.4965	0.0394	0.4262	0.099*	0.544 (14)
C5'	0.4973 (5)	−0.0255 (5)	0.3552 (3)	0.062 (5)	0.544 (14)
C6'	0.5277 (5)	−0.0922 (5)	0.3271 (3)	0.062 (3)	0.544 (14)
H6'	0.5296	−0.0921	0.2895	0.075*	0.544 (14)
C7'	0.5553 (5)	−0.1593 (5)	0.3564 (3)	0.078 (4)	0.544 (14)
H7'	0.5743	−0.2066	0.3393	0.094*	0.544 (14)
C8	0.4723 (3)	0.0483 (3)	0.3220 (2)	0.0719 (14)	
H8A	0.4929	0.1002	0.3360	0.086*	

H8B	0.5037	0.0367	0.2891	0.086*
C9	0.3283 (3)	0.0752 (3)	0.3551 (2)	0.0689 (13)
H9A	0.3596	0.1101	0.3797	0.083*
H9B	0.3161	0.0242	0.3737	0.083*
C10	0.2442 (3)	0.1174 (4)	0.3402 (2)	0.0758 (15)
C11	0.3464 (3)	−0.0126 (3)	0.2774 (2)	0.0692 (13)
H11A	0.2849	−0.0113	0.2795	0.083*
H11B	0.3655	−0.0630	0.2943	0.083*
C12	0.3724 (3)	−0.0130 (3)	0.2191 (2)	0.0708 (14)
H12A	0.4337	−0.0159	0.2171	0.085*
H12B	0.3497	−0.0617	0.2020	0.085*
C13	0.2532 (3)	0.0536 (3)	0.1719 (2)	0.0711 (14)
H13A	0.2367	0.1062	0.1570	0.085*
H13B	0.2189	0.0446	0.2039	0.085*
C14	0.2313 (3)	−0.0116 (4)	0.1313 (2)	0.0719 (14)
C15	0.2008 (3)	−0.0873 (4)	0.1453 (3)	0.0824 (16)
H15	0.1925	−0.1001	0.1816	0.099*
C16	0.1814 (4)	−0.1468 (4)	0.1046 (3)	0.0864 (17)
H16	0.1607	−0.1983	0.1138	0.104*
C17	0.1943 (4)	−0.1258 (5)	0.0520 (3)	0.0930 (18)
C18	0.2213 (5)	−0.0515 (5)	0.0374 (3)	0.119 (3)
H18	0.2278	−0.0381	0.0011	0.143*
C19	0.2390 (4)	0.0038 (4)	0.0765 (2)	0.100 (2)
H19	0.2576	0.0554	0.0659	0.120*
C20	0.1472 (6)	−0.2579 (6)	0.0218 (4)	0.158 (4)
H20A	0.1911	−0.2975	0.0153	0.236*
H20B	0.0989	−0.2702	−0.0003	0.236*
H20C	0.1311	−0.2596	0.0593	0.236*
C21	0.4002 (4)	0.0757 (3)	0.1429 (2)	0.0767 (15)
H21A	0.3731	0.1142	0.1186	0.092*
H21B	0.4098	0.0251	0.1232	0.092*
C22	0.4853 (3)	0.1106 (4)	0.1615 (2)	0.0784 (15)
C23	0.2216 (3)	0.2934 (3)	0.1992 (2)	0.0703 (13)
H23	0.1878	0.2848	0.2295	0.084*
C24	0.3236 (3)	0.2919 (3)	0.1431 (2)	0.0717 (14)
H24	0.3761	0.2817	0.1274	0.086*
C25	0.2623 (4)	0.3350 (4)	0.1210 (2)	0.0786 (16)
H25	0.2633	0.3595	0.0871	0.094*
C26	0.5097 (3)	0.2857 (3)	0.3045 (2)	0.0728 (14)
H26	0.5452	0.2743	0.2754	0.087*
C27	0.4026 (3)	0.2913 (3)	0.3560 (2)	0.0693 (13)
H27	0.3483	0.2840	0.3700	0.083*
C28	0.4646 (4)	0.3341 (3)	0.3792 (2)	0.0770 (15)
H28	0.4615	0.3618	0.4120	0.092*
N1	0.3811 (2)	0.0579 (2)	0.30784 (17)	0.0612 (10)
N2	0.3434 (3)	0.0594 (3)	0.18910 (17)	0.0651 (11)
N3	0.2983 (3)	0.2641 (2)	0.19315 (15)	0.0650 (10)
N4	0.1983 (3)	0.3369 (3)	0.15648 (19)	0.0759 (12)
H4A	0.1507	0.3619	0.1523	0.091*

N5	0.4319 (3)	0.2597 (2)	0.30825 (16)	0.0656 (10)
N6	0.5323 (3)	0.3302 (3)	0.34665 (19)	0.0773 (13)
H6A	0.5811	0.3524	0.3521	0.093*
O2	0.2394 (2)	0.1595 (2)	0.29840 (15)	0.0792 (10)
O3	0.1857 (3)	0.1072 (3)	0.37274 (18)	0.1179 (17)
O4	0.4891 (2)	0.1547 (2)	0.20236 (15)	0.0778 (10)
O5	0.5458 (3)	0.0944 (3)	0.1314 (2)	0.1219 (18)
O6	0.1771 (4)	−0.1803 (4)	0.0092 (2)	0.1312 (19)
O7	0.1167 (7)	0.0124 (8)	0.4537 (5)	0.337 (7)*
H7A	0.1411	0.0432	0.4308	0.404*
H7B	0.1498	−0.0274	0.4605	0.404*
O8	0.990 (3)	0.0651 (17)	0.5068 (17)	0.87 (3)*
H8C	0.9998	0.1160	0.5108	1.042*
H8D	0.9668	0.0586	0.4761	1.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0626 (3)	0.0620 (3)	0.0670 (3)	−0.00006 (17)	−0.00320 (17)	−0.00432 (18)
C1	0.133 (16)	0.17 (3)	0.119 (19)	0.078 (18)	0.017 (14)	0.032 (18)
O1	0.138 (13)	0.158 (16)	0.120 (16)	0.060 (11)	0.020 (10)	0.050 (12)
C2	0.147 (19)	0.050 (18)	0.16 (2)	−0.014 (12)	−0.055 (16)	−0.005 (15)
C3	0.24 (3)	0.20 (2)	0.076 (14)	0.11 (2)	−0.052 (15)	−0.047 (13)
C4	0.066 (10)	0.16 (2)	0.116 (15)	−0.002 (10)	−0.023 (9)	0.012 (14)
C5	0.057 (14)	0.050 (13)	0.16 (2)	0.003 (11)	0.001 (14)	−0.019 (16)
C6	0.080 (10)	0.105 (13)	0.055 (10)	−0.005 (9)	0.011 (8)	−0.008 (9)
C7	0.058 (9)	0.079 (13)	0.105 (17)	0.020 (7)	0.050 (12)	−0.017 (11)
C1'	0.26 (4)	0.19 (3)	0.13 (3)	0.10 (3)	0.01 (3)	0.07 (2)
O1'	0.171 (11)	0.121 (9)	0.142 (11)	0.054 (7)	0.004 (9)	0.060 (8)
C2'	0.089 (12)	0.035 (12)	0.20 (3)	0.003 (7)	−0.058 (12)	−0.001 (11)
C3'	0.190 (18)	0.089 (12)	0.062 (9)	0.047 (12)	−0.034 (9)	−0.005 (10)
C4'	0.100 (11)	0.083 (9)	0.063 (8)	0.026 (7)	−0.012 (7)	0.002 (7)
C5'	0.048 (10)	0.072 (14)	0.067 (7)	0.015 (9)	−0.014 (6)	−0.008 (8)
C6'	0.053 (6)	0.060 (6)	0.073 (8)	0.016 (5)	0.008 (5)	−0.008 (5)
C7'	0.060 (7)	0.077 (8)	0.097 (10)	0.025 (6)	0.016 (7)	−0.008 (8)
C8	0.057 (3)	0.072 (3)	0.087 (4)	0.002 (3)	−0.008 (3)	−0.009 (3)
C9	0.064 (3)	0.072 (3)	0.071 (3)	0.004 (3)	0.000 (3)	0.004 (3)
C10	0.061 (3)	0.084 (4)	0.082 (4)	0.012 (3)	0.004 (3)	0.004 (3)
C11	0.059 (3)	0.062 (3)	0.087 (4)	−0.007 (2)	−0.014 (3)	0.004 (3)
C12	0.060 (3)	0.064 (3)	0.088 (4)	0.002 (3)	−0.008 (3)	−0.017 (3)
C13	0.056 (3)	0.082 (3)	0.075 (3)	0.003 (3)	−0.007 (3)	−0.004 (3)
C14	0.051 (3)	0.084 (4)	0.080 (4)	−0.002 (3)	−0.009 (2)	−0.010 (3)
C15	0.051 (3)	0.109 (5)	0.087 (4)	−0.007 (3)	−0.006 (3)	−0.007 (4)
C16	0.065 (4)	0.081 (4)	0.113 (5)	−0.011 (3)	−0.011 (3)	−0.003 (4)
C17	0.084 (4)	0.123 (6)	0.072 (4)	0.000 (4)	0.000 (3)	−0.013 (4)
C18	0.144 (7)	0.137 (6)	0.077 (4)	−0.040 (6)	0.005 (4)	−0.013 (5)
C19	0.111 (5)	0.113 (5)	0.075 (4)	−0.026 (4)	−0.015 (4)	−0.008 (4)
C20	0.183 (9)	0.128 (7)	0.162 (9)	−0.060 (7)	−0.014 (7)	−0.027 (7)

C21	0.075 (4)	0.083 (4)	0.072 (3)	−0.003 (3)	0.001 (3)	−0.011 (3)
C22	0.063 (3)	0.085 (4)	0.087 (4)	−0.006 (3)	0.009 (3)	−0.017 (3)
C23	0.067 (3)	0.071 (3)	0.073 (3)	−0.005 (3)	0.012 (3)	0.006 (3)
C24	0.062 (3)	0.085 (4)	0.069 (3)	−0.010 (3)	0.009 (3)	−0.001 (3)
C25	0.071 (4)	0.098 (4)	0.066 (3)	−0.009 (3)	0.000 (3)	0.017 (3)
C26	0.069 (3)	0.076 (4)	0.073 (3)	−0.003 (3)	0.010 (3)	−0.005 (3)
C27	0.067 (3)	0.068 (3)	0.073 (3)	0.003 (3)	0.005 (3)	−0.003 (3)
C28	0.087 (4)	0.079 (4)	0.065 (3)	0.004 (3)	−0.003 (3)	−0.006 (3)
N1	0.049 (2)	0.064 (2)	0.070 (3)	−0.0001 (18)	−0.0074 (19)	−0.005 (2)
N2	0.054 (2)	0.070 (3)	0.071 (3)	−0.002 (2)	−0.003 (2)	−0.007 (2)
N3	0.061 (2)	0.067 (3)	0.067 (2)	−0.003 (2)	0.002 (2)	0.000 (2)
N4	0.059 (3)	0.079 (3)	0.090 (3)	0.000 (2)	−0.002 (2)	0.014 (2)
N5	0.062 (2)	0.064 (3)	0.071 (3)	0.000 (2)	−0.002 (2)	−0.001 (2)
N6	0.068 (3)	0.083 (3)	0.081 (3)	−0.014 (2)	−0.008 (3)	−0.011 (2)
O2	0.066 (2)	0.088 (3)	0.083 (2)	0.0163 (19)	0.0032 (19)	0.017 (2)
O3	0.082 (3)	0.161 (4)	0.111 (3)	0.040 (3)	0.032 (3)	0.050 (3)
O4	0.068 (2)	0.086 (3)	0.080 (2)	−0.0121 (19)	0.0034 (19)	−0.018 (2)
O5	0.074 (3)	0.159 (4)	0.133 (4)	−0.027 (3)	0.026 (3)	−0.067 (3)
O6	0.152 (5)	0.146 (5)	0.096 (3)	−0.027 (4)	0.004 (3)	−0.033 (3)

Geometric parameters (Å, °)

Cd1—N3	2.261 (4)	C11—H11A	0.9700
Cd1—N5	2.276 (4)	C11—H11B	0.9700
Cd1—O4	2.311 (4)	C12—N2	1.468 (7)
Cd1—O2	2.325 (4)	C12—H12A	0.9700
Cd1—N1	2.415 (4)	C12—H12B	0.9700
Cd1—N2	2.426 (4)	C13—N2	1.487 (6)
C1—O1	1.35 (4)	C13—C14	1.504 (7)
C1—H1A	0.9600	C13—H13A	0.9700
C1—H1B	0.9600	C13—H13B	0.9700
C1—H1C	0.9600	C14—C15	1.372 (8)
O1—C2	1.59 (4)	C14—C19	1.383 (7)
C2—C7	1.28 (3)	C15—C16	1.432 (8)
C2—C3	1.30 (3)	C15—H15	0.9300
C3—C4	1.3829	C16—C17	1.361 (8)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.3841	C17—C18	1.334 (9)
C4—H4	0.9300	C17—O6	1.409 (7)
C4—H4'	1.0807	C18—C19	1.351 (8)
C5—C6	1.3860	C18—H18	0.9300
C5—C8	1.556 (13)	C19—H19	0.9300
C6—C7	1.3910	C20—O6	1.386 (9)
C6—H6	0.9300	C20—H20A	0.9600
C7—H7	0.9300	C20—H20B	0.9600
C1'—O1'	1.40 (5)	C20—H20C	0.9600
C1'—H1'1	0.9600	C21—N2	1.475 (7)
C1'—H1'2	0.9600	C21—C22	1.528 (8)
C1'—H1'3	0.9600	C21—H21A	0.9700

O1'—C2'	1.32 (2)	C21—H21B	0.9700
C2'—C3'	1.37 (2)	C22—O5	1.239 (6)
C2'—C7'	1.54 (3)	C22—O4	1.241 (6)
C3'—C4'	1.3893	C23—N3	1.309 (6)
C3'—H3'	0.9300	C23—N4	1.324 (6)
C4'—C5'	1.3786	C23—H23	0.9300
C4'—H4	1.2981	C24—C25	1.314 (7)
C4'—H4'	0.9300	C24—N3	1.376 (6)
C5'—C6'	1.3787	C24—H24	0.9300
C5'—C8	1.509 (9)	C25—N4	1.337 (7)
C6'—C7'	1.3835	C25—H25	0.9300
C6'—H6	0.4131	C26—N5	1.301 (6)
C6'—H6'	0.9300	C26—N6	1.320 (6)
C7'—H7	0.9680	C26—H26	0.9300
C7'—H7'	0.9300	C27—C28	1.332 (7)
C8—N1	1.489 (6)	C27—N5	1.370 (6)
C8—H8A	0.9700	C27—H27	0.9300
C8—H8B	0.9700	C28—N6	1.339 (7)
C9—N1	1.462 (7)	C28—H28	0.9300
C9—C10	1.538 (7)	N4—H4A	0.8600
C9—H9A	0.9700	N6—H6A	0.8600
C9—H9B	0.9700	O7—H7A	0.8501
C10—O3	1.235 (6)	O7—H7B	0.8500
C10—O2	1.244 (6)	O8—H8C	0.8501
C11—N1	1.479 (6)	O8—H8D	0.8500
C11—C12	1.499 (8)		
N3—Cd1—N5	102.70 (14)	N1—C11—H11A	109.0
N3—Cd1—O4	100.12 (14)	C12—C11—H11A	109.0
N5—Cd1—O4	90.49 (13)	N1—C11—H11B	109.0
N3—Cd1—O2	90.21 (13)	C12—C11—H11B	109.0
N5—Cd1—O2	97.39 (14)	H11A—C11—H11B	107.8
O4—Cd1—O2	165.35 (14)	N2—C12—C11	113.5 (4)
N3—Cd1—N1	158.18 (13)	N2—C12—H12A	108.9
N5—Cd1—N1	92.47 (14)	C11—C12—H12A	108.9
O4—Cd1—N1	95.28 (13)	N2—C12—H12B	108.9
O2—Cd1—N1	72.15 (13)	C11—C12—H12B	108.9
N3—Cd1—N2	93.55 (14)	H12A—C12—H12B	107.7
N5—Cd1—N2	158.19 (14)	N2—C13—C14	117.0 (4)
O4—Cd1—N2	72.21 (13)	N2—C13—H13A	108.0
O2—Cd1—N2	96.99 (14)	C14—C13—H13A	108.0
N1—Cd1—N2	76.49 (16)	N2—C13—H13B	108.0
C1—O1—C2	121 (2)	C14—C13—H13B	108.0
C7—C2—C3	137 (3)	H13A—C13—H13B	107.3
C7—C2—O1	114.6 (19)	C15—C14—C19	116.2 (5)
C3—C2—O1	104 (2)	C15—C14—C13	123.3 (5)
C2—C3—C4	103.8 (17)	C19—C14—C13	120.5 (6)
C2—C3—H3	128.1	C14—C15—C16	120.5 (6)
C4—C3—H3	128.1	C14—C15—H15	119.8
C3—C4—C5	131.2	C16—C15—H15	119.8

C3—C4—H4	114.4	C17—C16—C15	118.0 (6)
C5—C4—H4	114.4	C17—C16—H16	121.0
C3—C4—H4'	105.2	C15—C16—H16	121.0
C5—C4—H4'	94.0	C18—C17—C16	122.4 (6)
H4—C4—H4'	66.3	C18—C17—O6	115.6 (6)
C4—C5—C6	106.0	C16—C17—O6	122.0 (7)
C4—C5—C8	128.6 (4)	C17—C18—C19	118.6 (7)
C6—C5—C8	124.7 (5)	C17—C18—H18	120.7
C5—C6—C7	126.5	C19—C18—H18	120.7
C5—C6—H6	116.8	C18—C19—C14	124.2 (7)
C7—C6—H6	116.8	C18—C19—H19	117.9
C5—C6—H6'	101.6	C14—C19—H19	117.9
C7—C6—H6'	131.8	O6—C20—H20A	109.5
C2—C7—C6	109.1 (14)	O6—C20—H20B	109.5
C2—C7—H7	126.7	H20A—C20—H20B	109.5
C6—C7—H7	123.0	O6—C20—H20C	109.5
C2—C7—H7'	161.4	H20A—C20—H20C	109.5
C6—C7—H7'	86.5	H20B—C20—H20C	109.5
O1'—C1'—H1'1	109.5	N2—C21—C22	111.5 (5)
O1'—C1'—H1'2	109.5	N2—C21—H21A	109.3
H1'1—C1'—H1'2	109.5	C22—C21—H21A	109.3
O1'—C1'—H1'3	109.5	N2—C21—H21B	109.3
H1'1—C1'—H1'3	109.5	C22—C21—H21B	109.3
H1'2—C1'—H1'3	109.5	H21A—C21—H21B	108.0
C2'—O1'—C1'	112 (2)	O5—C22—O4	125.1 (5)
O1'—C2'—C3'	135 (2)	O5—C22—C21	114.6 (5)
O1'—C2'—C7'	106.6 (17)	O4—C22—C21	120.2 (5)
C3'—C2'—C7'	114.2 (17)	N3—C23—N4	111.2 (5)
O1'—C2'—H7	68.9	N3—C23—H23	124.4
C3'—C2'—H7	151.5	N4—C23—H23	124.4
C2'—C3'—C4'	127.7 (13)	C25—C24—N3	109.7 (5)
C2'—C3'—H3'	116.2	C25—C24—H24	125.1
C4'—C3'—H3'	116.2	N3—C24—H24	125.1
C5'—C4'—C3'	112.0	C24—C25—N4	107.2 (5)
C5'—C4'—H4	110.7	C24—C25—H25	126.4
C3'—C4'—H4	105.1	N4—C25—H25	126.4
C5'—C4'—H4'	124.0	N5—C26—N6	112.2 (5)
C3'—C4'—H4'	124.0	N5—C26—H26	123.9
H4—C4'—H4'	56.8	N6—C26—H26	123.9
C4'—C5'—C6'	127.1	C28—C27—N5	108.7 (5)
C4'—C5'—C8	115.0 (4)	C28—C27—H27	125.6
C6'—C5'—C8	116.5 (4)	N5—C27—H27	125.6
C5'—C6'—C7'	118.0	C27—C28—N6	107.5 (5)
C5'—C6'—H6	157.3	C27—C28—H28	126.2
C7'—C6'—H6	80.5	N6—C28—H28	126.2
C5'—C6'—H6'	121.0	C9—N1—C11	110.2 (4)
C7'—C6'—H6'	121.0	C9—N1—C8	112.5 (4)
C6'—C7'—C2'	117.9 (7)	C11—N1—C8	113.3 (4)
C2'—C7'—H6	133.8	C9—N1—Cd1	105.3 (3)

C6'—C7'—H7	176.9	C11—N1—Cd1	105.6 (3)
C2'—C7'—H7	61.2	C8—N1—Cd1	109.4 (3)
H6—C7'—H7	162.4	C12—N2—C21	110.3 (4)
C6'—C7'—H7'	121.4	C12—N2—C13	113.1 (4)
C2'—C7'—H7'	120.1	C21—N2—C13	111.7 (4)
H6—C7'—H7'	104.5	C12—N2—Cd1	105.9 (3)
N1—C8—C5'	117.6 (5)	C21—N2—Cd1	104.7 (3)
N1—C8—C5	115.7 (6)	C13—N2—Cd1	110.7 (3)
N1—C8—H8A	108.4	C23—N3—C24	104.5 (4)
C5'—C8—H8A	114.5	C23—N3—Cd1	126.1 (3)
C5—C8—H8A	108.4	C24—N3—Cd1	129.1 (4)
N1—C8—H8B	108.4	C23—N4—C25	107.5 (5)
C5'—C8—H8B	99.6	C23—N4—H4A	126.2
C5—C8—H8B	108.4	C25—N4—H4A	126.2
H8A—C8—H8B	107.4	C26—N5—C27	104.9 (4)
N1—C9—C10	112.8 (4)	C26—N5—Cd1	126.5 (4)
N1—C9—H9A	109.0	C27—N5—Cd1	128.5 (3)
C10—C9—H9A	109.0	C26—N6—C28	106.6 (5)
N1—C9—H9B	109.0	C26—N6—H6A	126.7
C10—C9—H9B	109.0	C28—N6—H6A	126.7
H9A—C9—H9B	107.8	C10—O2—Cd1	116.3 (3)
O3—C10—O2	124.8 (5)	C22—O4—Cd1	116.8 (3)
O3—C10—C9	115.3 (5)	C20—O6—C17	118.2 (6)
O2—C10—C9	119.9 (5)	H7A—O7—H7B	107.7
N1—C11—C12	113.0 (4)	H8C—O8—H8D	107.7
C1—O1—C2—C7	28 (3)	O4—Cd1—N1—C8	36.9 (3)
C1—O1—C2—C3	−171 (2)	O2—Cd1—N1—C8	−150.8 (3)
C7—C2—C3—C4	−11.3 (16)	N2—Cd1—N1—C8	107.1 (3)
O1—C2—C3—C4	−165.1 (11)	C11—C12—N2—C21	153.7 (4)
C2—C3—C4—C5	−17.6 (5)	C11—C12—N2—C13	−80.3 (5)
C3—C4—C5—C6	26.7	C11—C12—N2—Cd1	41.0 (4)
C3—C4—C5—C8	−162.5 (6)	C22—C21—N2—C12	−73.1 (5)
C4—C5—C6—C7	−12.3	C22—C21—N2—C13	160.2 (4)
C8—C5—C6—C7	176.5 (6)	C22—C21—N2—Cd1	40.4 (5)
C3—C2—C7—C6	21.6 (16)	C14—C13—N2—C12	−65.7 (6)
O1—C2—C7—C6	173.4 (11)	C14—C13—N2—C21	59.5 (6)
C5—C6—C7—C2	−6.1 (6)	C14—C13—N2—Cd1	175.7 (4)
C1'—O1'—C2'—C3'	9(3)	N3—Cd1—N2—C12	−173.3 (3)
C1'—O1'—C2'—C7'	162 (2)	N5—Cd1—N2—C12	48.3 (6)
O1'—C2'—C3'—C4'	157.1 (17)	O4—Cd1—N2—C12	87.2 (3)
C7'—C2'—C3'—C4'	4.8 (9)	O2—Cd1—N2—C12	−82.6 (3)
C2'—C3'—C4'—C5'	10.0 (5)	N1—Cd1—N2—C12	−12.9 (3)
C3'—C4'—C5'—C6'	−18.9	N3—Cd1—N2—C21	70.1 (3)
C3'—C4'—C5'—C8	175.2 (4)	N5—Cd1—N2—C21	−68.3 (5)
C4'—C5'—C6'—C7'	11.0	O4—Cd1—N2—C21	−29.4 (3)
C8—C5'—C6'—C7'	176.7 (4)	O2—Cd1—N2—C21	160.8 (3)
C5'—C6'—C7'—C2'	6.3 (4)	N1—Cd1—N2—C21	−129.5 (3)
O1'—C2'—C7'—C6'	−173.0 (8)	N3—Cd1—N2—C13	−50.4 (3)
C3'—C2'—C7'—C6'	−13.3 (8)	N5—Cd1—N2—C13	171.2 (4)

C4'—C5'—C8—N1	−95.8 (4)	O4—Cd1—N2—C13	−149.9 (4)
C6'—C5'—C8—N1	96.8 (5)	O2—Cd1—N2—C13	40.3 (3)
C4'—C5'—C8—C5	−16 (4)	N1—Cd1—N2—C13	109.9 (4)
C6'—C5'—C8—C5	177 (5)	N4—C23—N3—C24	0.0 (6)
C4—C5—C8—N1	−68.9 (7)	N4—C23—N3—Cd1	−173.1 (3)
C6—C5—C8—N1	100.2 (5)	C25—C24—N3—C23	−0.8 (6)
C4—C5—C8—C5'	−173 (5)	C25—C24—N3—Cd1	172.1 (4)
C6—C5—C8—C5'	−4(4)	N5—Cd1—N3—C23	−90.8 (4)
N1—C9—C10—O3	154.8 (5)	O4—Cd1—N3—C23	176.4 (4)
N1—C9—C10—O2	−26.5 (7)	O2—Cd1—N3—C23	6.9 (4)
N1—C11—C12—N2	−61.1 (5)	N1—Cd1—N3—C23	42.2 (6)
N2—C13—C14—C15	95.5 (6)	N2—Cd1—N3—C23	103.9 (4)
N2—C13—C14—C19	−86.6 (7)	N5—Cd1—N3—C24	97.7 (4)
C19—C14—C15—C16	2.2 (8)	O4—Cd1—N3—C24	4.9 (4)
C13—C14—C15—C16	−179.8 (5)	O2—Cd1—N3—C24	−164.6 (4)
C14—C15—C16—C17	0.0 (8)	N1—Cd1—N3—C24	−129.3 (5)
C15—C16—C17—C18	−2.3 (10)	N2—Cd1—N3—C24	−67.6 (4)
C15—C16—C17—O6	−180.0 (6)	N3—C23—N4—C25	0.7 (6)
C16—C17—C18—C19	2.2 (12)	C24—C25—N4—C23	−1.2 (6)
O6—C17—C18—C19	180.0 (7)	N6—C26—N5—C27	1.1 (6)
C17—C18—C19—C14	0.3 (12)	N6—C26—N5—Cd1	−176.4 (3)
C15—C14—C19—C18	−2.4 (10)	C28—C27—N5—C26	−0.8 (6)
C13—C14—C19—C18	179.5 (7)	C28—C27—N5—Cd1	176.6 (3)
N2—C21—C22—O5	151.3 (6)	N3—Cd1—N5—C26	−93.5 (4)
N2—C21—C22—O4	−32.2 (8)	O4—Cd1—N5—C26	7.0 (4)
N3—C24—C25—N4	1.2 (6)	O2—Cd1—N5—C26	174.6 (4)
N5—C27—C28—N6	0.3 (6)	N1—Cd1—N5—C26	102.3 (4)
C10—C9—N1—C11	−74.8 (5)	N2—Cd1—N5—C26	43.8 (7)
C10—C9—N1—C8	157.6 (4)	N3—Cd1—N5—C27	89.7 (4)
C10—C9—N1—Cd1	38.6 (5)	O4—Cd1—N5—C27	−169.8 (4)
C12—C11—N1—C9	156.1 (4)	O2—Cd1—N5—C27	−2.2 (4)
C12—C11—N1—C8	−76.8 (5)	N1—Cd1—N5—C27	−74.5 (4)
C12—C11—N1—Cd1	42.9 (4)	N2—Cd1—N5—C27	−133.1 (5)
C5'—C8—N1—C9	67.8 (6)	N5—C26—N6—C28	−1.0 (6)
C5—C8—N1—C9	57.8 (7)	C27—C28—N6—C26	0.4 (6)
C5'—C8—N1—C11	−58.1 (7)	O3—C10—O2—Cd1	175.2 (5)
C5—C8—N1—C11	−68.1 (7)	C9—C10—O2—Cd1	−3.4 (7)
C5'—C8—N1—Cd1	−175.6 (5)	N3—Cd1—O2—C10	−174.2 (4)
C5—C8—N1—Cd1	174.4 (5)	N5—Cd1—O2—C10	−71.3 (4)
N3—Cd1—N1—C9	−67.2 (5)	O4—Cd1—O2—C10	50.7 (7)
N5—Cd1—N1—C9	67.2 (3)	N1—Cd1—O2—C10	18.9 (4)
O4—Cd1—N1—C9	158.0 (3)	N2—Cd1—O2—C10	92.2 (4)
O2—Cd1—N1—C9	−29.7 (3)	O5—C22—O4—Cd1	178.9 (6)
N2—Cd1—N1—C9	−131.8 (3)	C21—C22—O4—Cd1	2.7 (7)
N3—Cd1—N1—C11	49.5 (5)	N3—Cd1—O4—C22	−74.9 (4)
N5—Cd1—N1—C11	−176.1 (3)	N5—Cd1—O4—C22	−177.9 (4)
O4—Cd1—N1—C11	−85.4 (3)	O2—Cd1—O4—C22	59.3 (7)
O2—Cd1—N1—C11	86.9 (3)	N1—Cd1—O4—C22	89.5 (4)
N2—Cd1—N1—C11	−15.2 (3)	N2—Cd1—O4—C22	15.6 (4)

N3—Cd1—N1—C8	171.7 (4)	C18—C17—O6—C20	−178.8 (8)
N5—Cd1—N1—C8	−53.9 (3)	C16—C17—O6—C20	−0.9 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7A···O3	0.85	1.91	2.756 (14)	173
N6—H6A···O3^{i}	0.86	1.85	2.703 (6)	172
C28—H28···O8^{ii}	0.93	2.67	3.58 (4)	167
N4—H4A···O5^{ii}	0.86	1.87	2.724 (6)	170

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

Fig. 1

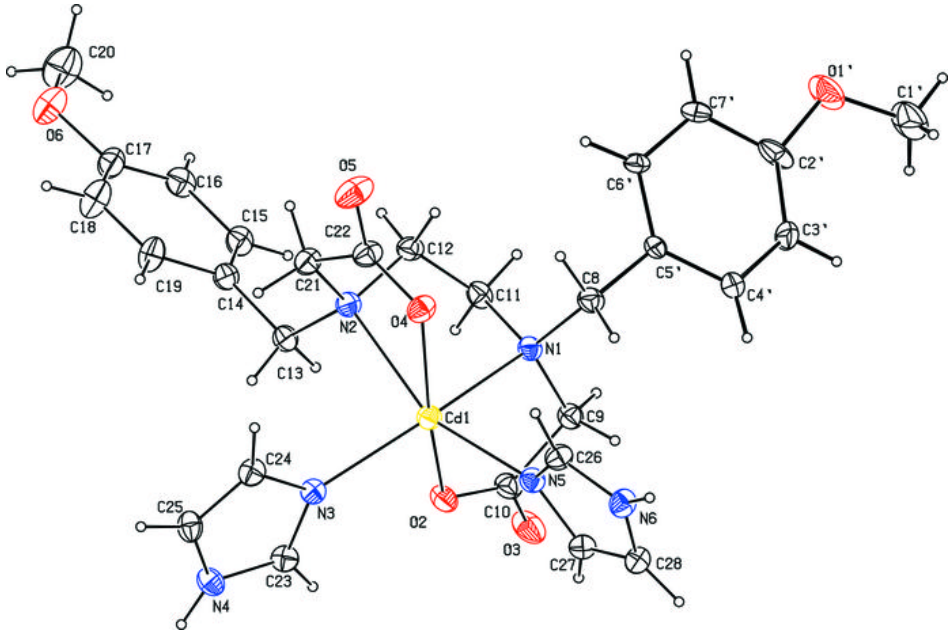

C20
O6
C17
C16
C18
C15
C19
C14
C22
O5
C21
C12
N2
O4
C13
C11
C8
C5'
C4'
C3'
C2'
C6'
C7'
O1'
C1'
N1
Cd1
C9
C24
C26
N5
C25
N3
O2
C10
N6
O3
C27
C28
C23
N4

Fig. 2