Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[(μ_4-carbonyldibenzene-3,3′,4,4′-tetracarboxylato)tetrakis(1,10-phenanthroline)dicadmium(II)] dihydrate]

Yu-Xiang Gao,* Li-Bin Wang and Yan-Ling Niu

Department of Chemistry, Tonghua Teachers' College, Tonghua 134002, People's Republic of China
Correspondence e-mail: yxgao_tonghua@yahoo.com.cn

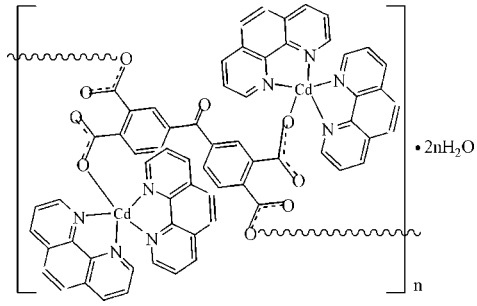
Received 4 June 2007; accepted 11 June 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.007 Å; R factor = 0.047; wR factor = 0.136; data-to-parameter ratio = 11.8.

In the title compound, $\{[Cd_2(C_{17}H_6O_9)(C_{12}H_8N_2)_4]\cdot 2H_2O\}_n$, each Cd^{II} atom is hexacoordinated by two carboxylate O atoms from two 3,3′,4,4′-benzophenone tetracarboxylate anions and four N atoms from two 1,10-phenanthroline ligands, showing a slightly distorted octahedral geometry. Neighboring Cd^{II} atoms are bridged by benzophenone tetracarboxylate anions, forming a dinuclear unit, which is further bridged by benzophenone tetracarboxylate anions to form an infinite chain. The benzophenone carbonyl group lies on a twofold rotation axis.

Related literature

For related compounds, see: Ngo *et al.* (2004); Evans *et al.* (2001); Vioux *et al.* (2004); Sanchez *et al.* (2003); Evans & Lin (2001); Jannasch (2003); Javaid *et al.* (2001); Honma *et al.* (2001); Sudik *et al.* (2005); Rowsell *et al.* (2004); Kitaura *et al.* (2002).



Experimental

Crystal data

$[Cd_2(C_{17}H_6O_9)(C_{12}H_8N_2)_4]\cdot 2H_2O$
M_r = 1335.87
Monoclinic, $C2/c$
a = 24.5326 (10) Å
b = 9.9826 (15) Å
c = 23.761 (3) Å
β = 110.797 (2)°
V = 5439.9 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.86 mm^{-1}
T = 273 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
20482 measured reflections
4681 independent reflections
3527 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.136
S = 1.00
4681 reflections
398 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.48 e Å^{-3}
$\Delta\rho_{min}$ = −1.39 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

The authors thank the NSFC (**expand abbreviation?**) (grant No. 20501017) and Tonghua Teachers' College.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2175).

References

Bruker (1999). *SAINT* and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Evans, O. R. & Lin, W. B. (2001). *Chem. Mater.* **13**, 3009–3017.
Evans, O. R., Ngo, H. L. & Lin, W. B. (2001). *J. Am. Chem. Soc.* **123**, 10395–10396.
Honma, I., Nomura, S. & Nakajima, H. (2001). *J. Membr. Sci.* **185**, 83–94.
Jannasch, P. (2003). *Curr. Opin. Colloid Interf. Sci.* **8**, 96–102.
Javaid, A., Hughey, M. P., Varutbangkul, V. & Ford, D. M. (2001). *J. Membr. Sci.* **187**, 141–150.
Kitaura, R., Kitagawa, S., Kubota, Y., Kobayashi, T. C., Kindo, K., Mita, Y., Matsuo, A., Kobayashi, M., Chang, H.-C., Ozawa, T. C., Suzuki, M., Sakata, M. & Takata, M. (2002). *Science*, **298**, 2358–2361.
Ngo, H. L., Hu, A. G. & Lin, W. B. (2004). *J. Mol. Catal. A*, **215**, 177–186.
Rowsell, J. L. C., Millward, A. R., Park, K. S. & Yaghi, O. M. (2004). *J. Am. Chem. Soc.* **126**, 5666–5667.
Sanchez, C., Lebeau, B., Chaput, F. & Boilet, J. P. (2003). *Adv. Mater.* **15**, 1969–1994.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sudik, A. C., Millward, A. R., Ockwig, N. W., Cote, A. P., Kim, J. & Yaghi, O. M. (2005). *J. Am. Chem. Soc.* **127**, 7110–7118.
Vioux, A., LeBideau, J., Mutin, P. H. & Leclercq, D. (2004). *New Aspects in Phosphorus Chemistry IV*, Vol. 232, pp. 145–174. New York: Springer.

  doi:10.1107/S1600536807028425

supplementary materials

Acta Cryst. (2007). E**63**, m1844 [**doi:10.1107/S1600536807028425**]

Poly[[(μ_4-carbonyldibenzene-3,3',4,4'-tetracarboxylato)tetrakis(1,10-phenanthroline)dicadmium(II)] dihydrate]

Y.-X. Gao, L.-B. Wang and Y.-L. Niu

Comment

Hybrid organic-inorganic materials occupy a prominent position by virtue of their applications to catalysis, optical materials, membranes, and sorption (Ngo *et al.*, 2004; Evans *et al.*, 2001; Vioux *et al.*, 2004; Sanchez *et al.*, 2003; Evans & Lin, 2001; Jannasch, 2003; Javaid *et al.*, 2001; Honma *et al.*, 2001; Sudik *et al.*, 2005; Rowsell *et al.*, 2004; Kitaura *et al.*, 2002). The design of organic-inorganic hybrid materials is conceived of the metal, metal cluster, or metal oxide substructure as a node from which rigid or flexible multitopic organic ligands radiate to act as tethers to adjacent nodes in the bottom-up construction of complex extended architectures. While a variety of organic molecules have been investigated as potential tethers, materials incorporating multitopic carboxylates and pyridine ligands have witnessed the most significant development. However, ligands offering alternative tether lengths, different charge-balance requirements, and orientations of donor groups may afford advantages in the design of materials. Herein, We report the structure of the new title complex, (I). The cadmium cation is hexa-coordinated by two carboxylate oxygen atoms from two 3,3',4,4'-benzophenone tetracarboxylate and four nitrogen atoms from two 1,10-phenanthroline, showing a slightly distorted octahedral geometry (Fig. 1). Each two Cd atoms form one circle *via* two half of 3,3',4,4'-benzophenone tetracarboxylate, which are further linked to form chains (Fig. 2). The Cd—N and Cd—O bond lengths are in the range of 2.392 (4)–2.524 (4) and 2.255 (3)–2.275 (4) Å, respectively.

Experimental

A mixture of cadmium acetate (0.5 mmol), 3,3',4,4'-benzophenone tetracarboxylic acid (0.5 mmol) and 1,10-phenanthroline (0.5 mmol) in 20 ml solution of water and ethanol (1:1) was sealed in an 30 ml Teflon-lined stainless autoclave, and kept at 423 K for 2 days. Colorless block-shaped crystals were obtained in 16% yield after slowly cooling to room temperature. Anal. Calc. for $C_{65}H_{42}Cd_2N_8O_{11}$: C 58.38, H 3.14, N 8.38, Cd 16.83%; Found: C 58.31, H 3.11, N 8.29, Cd 16.76%.

Refinement

C-bound H atoms were generated geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H)= 1.2U_{eq}(C). H atoms of the water molecule were located in a difference map and were refined with distance restraints of H···H = 1.38 (2) and O–H = 0.82 (2) Å, and with a fixed U_{iso}(H) of 0.80 Å^2. The highest peak and deepest hole in the difference Fourier map are located 0.92 and 0.65 Å, respectively, from atoms Cd1 and O6.

Figures

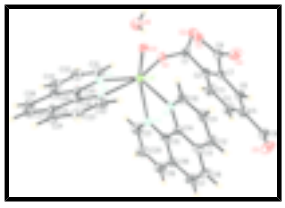


Fig. 1. The coordination of the Cd atom in the title compound, with displacement ellipsoids at the 30% probability level. The suffix I corresponds to symmetry code (−*x* + 3/2, −*y* + 1/2, −*z*).

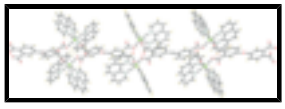


Fig. 2. A view of the chain structure of the title compound.

Poly[[(μ4-carbonyldibenzene-3,3',4,4'-tetracarboxylato)tetrakis(1,10- phenanthroline)dicadmium(II)] dihydrate]

Crystal data

$[Cd_2(C_{17}H_6O_9)(C_{12}H_8N_2)_4]\cdot 2H_2O$	F_{000} = 2688
M_r = 1335.87	D_x = 1.631 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3610 reflections
a = 24.5326 (10) Å	θ = 4.0–27.4º
b = 9.9826 (15) Å	μ = 0.86 mm^{-1}
c = 23.761 (3) Å	*T* = 273 (2) K
β = 110.797 (2)º	Block, colorless
V = 5439.9 (11) Å^3	0.10 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	3527 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.022
Monochromator: graphite	θ_{max} = 25.0º
T = 273(2) K	θ_{min} = 1.8º
φ and ω scans	*h* = −29→28
Absorption correction: none	*k* = −11→11
20482 measured reflections	*l* = −28→28
4681 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement

$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0734P)^2 + 4.4546P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
4681 reflections	$\Delta\rho_{max} = 1.48$ e Å^{-3}
398 parameters	$\Delta\rho_{min} = -1.39$ e Å^{-3}
3 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}
Cd1	0.672613 (12)	0.28062 (3)	0.051215 (14)	0.03039 (16)
C1	0.66588 (18)	0.4960 (5)	−0.0547 (2)	0.0350 (11)
C2	0.62528 (17)	0.4085 (5)	−0.10503 (19)	0.0317 (10)
C3	0.56796 (19)	0.4497 (6)	−0.1303 (2)	0.0522 (15)
H28	0.5560	0.5258	−0.1153	0.063*
C4	0.52773 (19)	0.3802 (6)	−0.1777 (2)	0.0536 (15)
H29	0.4896	0.4114	−0.1942	0.064*
C5	0.54344 (18)	0.2669 (5)	−0.2001 (2)	0.0392 (12)
C6	0.60108 (18)	0.2224 (5)	−0.1749 (2)	0.0341 (11)
H31	0.6121	0.1441	−0.1892	0.041*
C7	0.64206 (16)	0.2930 (4)	−0.1289 (2)	0.0283 (10)
C8	0.70458 (18)	0.2475 (5)	−0.1058 (2)	0.0335 (11)
C9	0.5000	0.1883 (8)	−0.2500	0.0427 (18)
C10	0.67162 (18)	0.0193 (5)	−0.0332 (2)	0.0346 (11)
H13	0.7116	0.0334	−0.0153	0.042*
C11	0.6526 (2)	−0.0881 (6)	−0.0740 (2)	0.0429 (12)
H14	0.6792	−0.1455	−0.0814	0.052*
C12	0.5939 (2)	−0.1053 (6)	−0.1023 (2)	0.0499 (14)
H15	0.5798	−0.1725	−0.1309	0.060*
C13	0.55538 (19)	−0.0220 (5)	−0.0881 (2)	0.0407 (12)
C14	0.57798 (16)	0.0817 (5)	−0.04594 (19)	0.0305 (10)
C15	0.53995 (16)	0.1662 (5)	−0.0282 (2)	0.0345 (11)
C16	0.47858 (17)	0.1462 (5)	−0.0548 (2)	0.0423 (12)
C17	0.4574 (2)	0.0417 (6)	−0.0988 (3)	0.0582 (16)

H18	0.4174	0.0282	−0.1164	0.070*
C18	0.4931 (2)	−0.0363 (6)	−0.1152 (3)	0.0539 (15)
H17	0.4775	−0.1012	−0.1446	0.065*
C19	0.4427 (2)	0.2264 (6)	−0.0360 (3)	0.0530 (16)
H20	0.4025	0.2140	−0.0520	0.064*
C20	0.4658 (2)	0.3252 (6)	0.0065 (3)	0.0557 (15)
H21	0.4419	0.3803	0.0192	0.067*
C21	0.5267 (2)	0.3397 (6)	0.0299 (3)	0.0512 (14)
H22	0.5426	0.4061	0.0584	0.061*
C22	0.69912 (18)	−0.0002 (5)	0.1315 (2)	0.0393 (12)
H1	0.7059	−0.0314	0.0977	0.047*
C23	0.70645 (19)	−0.0893 (6)	0.1788 (2)	0.0447 (13)
H2	0.7177	−0.1774	0.1762	0.054*
C24	0.69687 (19)	−0.0450 (5)	0.2296 (2)	0.0446 (13)
H3	0.7013	−0.1032	0.2615	0.054*
C25	0.68045 (18)	0.0886 (5)	0.2326 (2)	0.0385 (11)
C26	0.67419 (16)	0.1711 (5)	0.1821 (2)	0.0325 (10)
C27	0.6712 (2)	0.1433 (6)	0.2843 (2)	0.0492 (13)
H5	0.6750	0.0881	0.3170	0.059*
C28	0.6571 (3)	0.2734 (6)	0.2864 (3)	0.0540 (15)
H6	0.6512	0.3069	0.3203	0.065*
C29	0.65118 (19)	0.3610 (5)	0.2359 (2)	0.0423 (12)
C30	0.65990 (17)	0.3122 (5)	0.1843 (2)	0.0329 (10)
C31	0.6484 (2)	0.5214 (5)	0.1396 (3)	0.0458 (13)
H10	0.6484	0.5775	0.1083	0.055*
C32	0.6388 (2)	0.5774 (6)	0.1898 (3)	0.0563 (15)
H9	0.6316	0.6688	0.1905	0.068*
C33	0.6400 (2)	0.4995 (6)	0.2370 (3)	0.0551 (15)
H8	0.6335	0.5371	0.2699	0.066*
H1W	0.706 (10)	0.649 (5)	0.046 (9)	0.30 (17)*
H2W	0.730 (3)	0.774 (6)	0.047 (3)	0.08 (3)*
N1	0.68314 (14)	0.1253 (4)	0.13188 (16)	0.0310 (8)
N2	0.65750 (15)	0.3910 (4)	0.13560 (18)	0.0356 (9)
N3	0.63683 (13)	0.1007 (4)	−0.01870 (16)	0.0319 (9)
N4	0.56285 (16)	0.2636 (4)	0.0134 (2)	0.0412 (11)
O1	0.66782 (13)	0.4723 (3)	−0.00050 (14)	0.0382 (8)
O2	0.68981 (15)	0.5896 (4)	−0.06927 (16)	0.0516 (10)
O3	0.73871 (12)	0.3046 (3)	−0.06003 (14)	0.0375 (8)
O4	0.71910 (13)	0.1553 (4)	−0.13297 (17)	0.0534 (10)
O5	0.5000	0.0672 (6)	−0.2500	0.0660 (17)
O6	0.7101 (2)	0.7270 (5)	0.0619 (2)	0.0664 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0267 (2)	0.0350 (3)	0.0285 (2)	0.00281 (13)	0.00860 (13)	0.00070 (14)
C1	0.031 (2)	0.038 (3)	0.032 (3)	0.004 (2)	0.0066 (18)	−0.003 (2)
C2	0.0277 (19)	0.040 (3)	0.024 (2)	0.0007 (19)	0.0047 (16)	0.004 (2)

C3	0.035 (2)	0.063 (4)	0.050 (3)	0.015 (2)	0.004 (2)	−0.012 (3)
C4	0.030 (2)	0.071 (4)	0.048 (3)	0.015 (2)	−0.001 (2)	−0.007 (3)
C5	0.028 (2)	0.048 (3)	0.034 (3)	0.004 (2)	0.0012 (19)	0.005 (2)
C6	0.032 (2)	0.037 (3)	0.026 (2)	0.0014 (19)	0.0010 (18)	0.002 (2)
C7	0.0239 (19)	0.035 (3)	0.024 (2)	−0.0014 (17)	0.0058 (16)	0.0004 (19)
C8	0.028 (2)	0.040 (3)	0.030 (3)	0.0028 (19)	0.0090 (19)	0.006 (2)
C9	0.031 (3)	0.052 (5)	0.036 (4)	0.000	0.001 (3)	0.000
C10	0.032 (2)	0.038 (3)	0.033 (3)	0.0013 (19)	0.0110 (18)	−0.004 (2)
C11	0.043 (2)	0.049 (3)	0.040 (3)	0.005 (2)	0.018 (2)	−0.003 (3)
C12	0.048 (3)	0.057 (4)	0.042 (3)	−0.006 (2)	0.013 (2)	−0.019 (3)
C13	0.039 (2)	0.047 (3)	0.037 (3)	−0.009 (2)	0.0142 (19)	−0.005 (2)
C14	0.0276 (19)	0.035 (3)	0.027 (2)	−0.0025 (18)	0.0070 (16)	0.003 (2)
C15	0.026 (2)	0.040 (3)	0.036 (3)	−0.0054 (19)	0.0094 (17)	0.004 (2)
C16	0.025 (2)	0.052 (3)	0.048 (3)	0.002 (2)	0.0105 (19)	0.006 (3)
C17	0.029 (2)	0.070 (4)	0.068 (4)	−0.014 (2)	0.007 (2)	−0.009 (3)
C18	0.039 (3)	0.060 (4)	0.058 (4)	−0.017 (3)	0.011 (2)	−0.024 (3)
C19	0.027 (2)	0.063 (4)	0.067 (4)	0.004 (2)	0.013 (2)	0.006 (3)
C20	0.038 (2)	0.063 (4)	0.069 (4)	0.016 (3)	0.023 (2)	0.001 (3)
C21	0.041 (3)	0.053 (4)	0.056 (4)	0.006 (2)	0.014 (2)	−0.009 (3)
C22	0.035 (2)	0.037 (3)	0.048 (3)	0.003 (2)	0.018 (2)	0.004 (2)
C23	0.042 (2)	0.040 (3)	0.052 (3)	0.004 (2)	0.016 (2)	0.001 (3)
C24	0.043 (2)	0.045 (3)	0.044 (3)	0.002 (2)	0.013 (2)	0.013 (3)
C25	0.034 (2)	0.050 (3)	0.032 (3)	−0.004 (2)	0.0116 (18)	0.002 (2)
C26	0.0233 (18)	0.043 (3)	0.032 (2)	−0.0025 (18)	0.0097 (16)	−0.001 (2)
C27	0.069 (3)	0.047 (3)	0.035 (3)	−0.002 (3)	0.021 (2)	0.008 (3)
C28	0.068 (3)	0.070 (4)	0.033 (3)	−0.015 (3)	0.028 (3)	−0.011 (3)
C29	0.041 (2)	0.049 (3)	0.041 (3)	−0.007 (2)	0.019 (2)	−0.015 (3)
C30	0.0273 (19)	0.043 (3)	0.031 (2)	−0.0015 (19)	0.0126 (17)	−0.006 (2)
C31	0.047 (3)	0.035 (3)	0.058 (3)	0.006 (2)	0.021 (2)	0.003 (3)
C32	0.061 (3)	0.037 (3)	0.073 (4)	0.003 (3)	0.026 (3)	−0.011 (3)
C33	0.058 (3)	0.053 (4)	0.061 (4)	−0.003 (3)	0.029 (3)	−0.026 (3)
N1	0.0319 (17)	0.032 (2)	0.032 (2)	0.0018 (16)	0.0154 (15)	0.0049 (18)
N2	0.0333 (18)	0.034 (2)	0.040 (2)	0.0009 (16)	0.0137 (15)	0.000 (2)
N3	0.0233 (16)	0.038 (2)	0.032 (2)	−0.0034 (15)	0.0071 (14)	−0.0029 (18)
N4	0.0303 (19)	0.048 (3)	0.047 (3)	0.0035 (17)	0.0151 (18)	−0.003 (2)
O1	0.0489 (17)	0.0366 (19)	0.0269 (18)	0.0026 (15)	0.0106 (13)	−0.0013 (15)
O2	0.062 (2)	0.043 (2)	0.050 (2)	−0.0156 (19)	0.0203 (17)	0.0016 (19)
O3	0.0236 (14)	0.055 (2)	0.0314 (18)	−0.0001 (13)	0.0064 (12)	−0.0064 (16)
O4	0.0338 (16)	0.058 (2)	0.065 (3)	0.0066 (17)	0.0131 (16)	−0.019 (2)
O5	0.055 (3)	0.054 (4)	0.064 (4)	0.000	−0.009 (3)	0.000
O6	0.068 (3)	0.065 (3)	0.074 (3)	−0.006 (2)	0.034 (2)	−0.019 (2)

Geometric parameters (Å, °)

Cd1—O1	2.255 (3)	C16—C17	1.438 (8)
Cd1—O3^{i}	2.275 (3)	C17—C18	1.328 (8)
Cd1—N3	2.392 (4)	C17—H18	0.9300
Cd1—N1	2.407 (4)	C18—H17	0.9300
Cd1—N2	2.429 (4)	C19—C20	1.380 (8)

Cd1—N4	2.524 (4)	C19—H20	0.9300
C1—O2	1.217 (6)	C20—C21	1.405 (7)
C1—O1	1.293 (6)	C20—H21	0.9300
C1—C2	1.529 (6)	C21—N4	1.327 (7)
C2—C3	1.381 (6)	C21—H22	0.9300
C2—C7	1.410 (6)	C22—N1	1.314 (6)
C3—C4	1.390 (7)	C22—C23	1.394 (7)
C3—H28	0.9300	C22—H1	0.9300
C4—C5	1.363 (7)	C23—C24	1.382 (7)
C4—H29	0.9300	C23—H2	0.9300
C5—C6	1.398 (6)	C24—C25	1.402 (7)
C5—C9	1.503 (6)	C24—H3	0.9300
C6—C7	1.386 (6)	C25—C26	1.419 (7)
C6—H31	0.9300	C25—C27	1.434 (7)
C7—C8	1.504 (6)	C26—N1	1.366 (6)
C8—O4	1.246 (6)	C26—C30	1.458 (7)
C8—O3	1.250 (6)	C27—C28	1.349 (8)
C9—O5	1.209 (9)	C27—H5	0.9300
C9—C5^{ii}	1.503 (6)	C28—C29	1.449 (8)
C10—N3	1.310 (6)	C28—H6	0.9300
C10—C11	1.409 (7)	C29—C30	1.405 (7)
C10—H13	0.9300	C29—C33	1.411 (8)
C11—C12	1.368 (7)	C30—N2	1.383 (6)
C11—H14	0.9300	C31—N2	1.330 (6)
C12—C13	1.386 (7)	C31—C32	1.411 (8)
C12—H15	0.9300	C31—H10	0.9300
C13—C14	1.410 (7)	C32—C33	1.357 (8)
C13—C18	1.440 (6)	C32—H9	0.9300
C14—N3	1.370 (5)	C33—H8	0.9300
C14—C15	1.427 (6)	O3—Cd1^{i}	2.275 (3)
C15—N4	1.357 (7)	O6—H1W	0.85 (5)
C15—C16	1.425 (5)	O6—H2W	0.84 (7)
C16—C19	1.376 (8)		
O1—Cd1—O3^{i}	103.33 (12)	C16—C17—H18	118.9
O1—Cd1—N3	108.88 (12)	C17—C18—C13	121.1 (5)
O3^{i}—Cd1—N3	83.48 (11)	C17—C18—H17	119.5
O1—Cd1—N1	161.97 (12)	C13—C18—H17	119.4
O3^{i}—Cd1—N1	81.79 (12)	C16—C19—C20	120.6 (4)
N3—Cd1—N1	88.77 (13)	C16—C19—H20	119.7
O1—Cd1—N2	94.07 (12)	C20—C19—H20	119.7
O3^{i}—Cd1—N2	120.99 (11)	C19—C20—C21	117.8 (5)
N3—Cd1—N2	142.01 (13)	C19—C20—H21	121.1
N1—Cd1—N2	68.88 (13)	C21—C20—H21	121.1
O1—Cd1—N4	91.18 (13)	N4—C21—C20	123.5 (5)
O3^{i}—Cd1—N4	150.69 (13)	N4—C21—H22	118.2
N3—Cd1—N4	67.65 (13)	C20—C21—H22	118.2
N1—Cd1—N4	92.26 (13)	N1—C22—C23	123.7 (5)

N2—Cd1—N4	82.44 (13)	N1—C22—H1	118.1
O2—C1—O1	124.9 (4)	C23—C22—H1	118.1
O2—C1—C2	117.5 (4)	C24—C23—C22	119.2 (5)
O1—C1—C2	117.3 (4)	C24—C23—H2	120.4
C3—C2—C7	117.7 (4)	C22—C23—H2	120.4
C3—C2—C1	116.8 (4)	C23—C24—C25	119.3 (5)
C7—C2—C1	125.4 (4)	C23—C24—H3	120.3
C2—C3—C4	121.6 (5)	C25—C24—H3	120.3
C2—C3—H28	119.2	C24—C25—C26	117.1 (5)
C4—C3—H28	119.2	C24—C25—C27	122.8 (5)
C5—C4—C3	120.8 (4)	C26—C25—C27	120.1 (5)
C5—C4—H29	119.6	N1—C26—C25	122.8 (4)
C3—C4—H29	119.6	N1—C26—C30	118.1 (4)
C4—C5—C6	118.6 (4)	C25—C26—C30	119.0 (4)
C4—C5—C9	121.5 (4)	C28—C27—C25	121.2 (5)
C6—C5—C9	119.9 (5)	C28—C27—H5	119.4
C7—C6—C5	121.1 (4)	C25—C27—H5	119.4
C7—C6—H31	119.4	C27—C28—C29	120.2 (5)
C5—C6—H31	119.5	C27—C28—H6	119.9
C6—C7—C2	120.0 (4)	C29—C28—H6	119.9
C6—C7—C8	119.6 (4)	C30—C29—C33	116.5 (5)
C2—C7—C8	120.4 (4)	C30—C29—C28	120.7 (5)
O4—C8—O3	124.1 (4)	C33—C29—C28	122.7 (5)
O4—C8—C7	118.4 (4)	N2—C30—C29	124.0 (4)
O3—C8—C7	117.5 (4)	N2—C30—C26	117.3 (4)
O5—C9—C5	121.5 (3)	C29—C30—C26	118.7 (4)
O5—C9—C5^{ii}	121.5 (3)	N2—C31—C32	122.0 (5)
C5—C9—C5^{ii}	117.1 (7)	N2—C31—H10	119.0
N3—C10—C11	124.4 (4)	C32—C31—H10	119.0
N3—C10—H13	117.8	C33—C32—C31	120.7 (5)
C11—C10—H13	117.8	C33—C32—H9	119.6
C12—C11—C10	117.8 (5)	C31—C32—H9	119.6
C12—C11—H14	121.1	C32—C33—C29	119.6 (5)
C10—C11—H14	121.1	C32—C33—H8	120.2
C11—C12—C13	119.7 (5)	C29—C33—H8	120.2
C11—C12—H15	120.1	C22—N1—C26	117.8 (4)
C13—C12—H15	120.2	C22—N1—Cd1	123.8 (3)
C12—C13—C14	118.9 (4)	C26—N1—Cd1	118.3 (3)
C12—C13—C18	122.6 (5)	C31—N2—C30	117.1 (5)
C14—C13—C18	118.5 (5)	C31—N2—Cd1	125.5 (4)
N3—C14—C13	121.3 (4)	C30—N2—Cd1	117.3 (3)
N3—C14—C15	117.9 (4)	C10—N3—C14	117.8 (4)
C13—C14—C15	120.7 (4)	C10—N3—Cd1	122.4 (3)
N4—C15—C16	121.4 (5)	C14—N3—Cd1	119.8 (3)
N4—C15—C14	119.5 (3)	C21—N4—C15	118.5 (4)
C16—C15—C14	119.0 (4)	C21—N4—Cd1	126.6 (3)
C19—C16—C15	118.2 (5)	C15—N4—Cd1	114.9 (3)
C19—C16—C17	123.4 (4)	C1—O1—Cd1	132.4 (3)

C15—C16—C17	118.4 (5)	C8—O3—Cd1^{i}	103.5 (3)
C18—C17—C16	122.2 (4)	H1W—O6—H2W	109 (16)
C18—C17—H18	118.9		

Symmetry codes: (i) −*x*+3/2, −*y*+1/2, −*z*; (ii) −*x*+1, *y*, −*z*−1/2.

Fig. 1

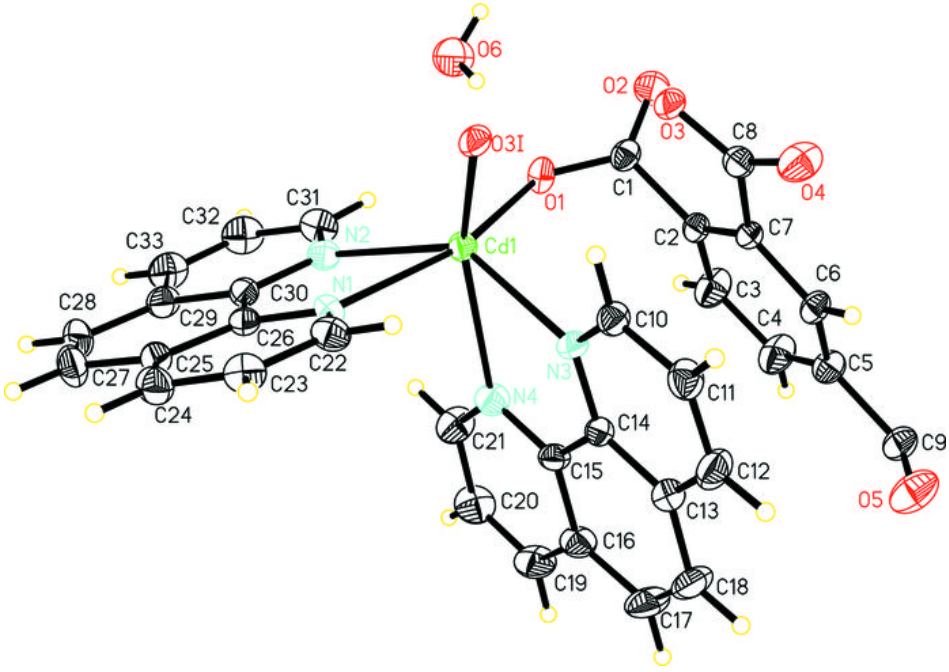

O6
O2
O3
O3I
C8
O1
C1
O4
C31
C32
N2
Cd1
C33
C2
C7
N1
C3
C6
C28
C30
C10
C29
C4
C26
C22
N3
C5
C25
C27
C23
C11
N4
C14
C21
C9
C15
C12
C20
C13
O5
C16
C19
C18
C17

Fig. 2