Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[bis(2-methyl-1*H*-imidazole-κN^3)cadmium(II)]-μ-cyclohexane-1,4-dicarboxylato] dihydrate]

Yuan-Jing Li

Faculty of Chemistry and Biology, Beihua University, Jilin City 132013, People's Republic of China
Correspondence e-mail: jls_yjl@126.com

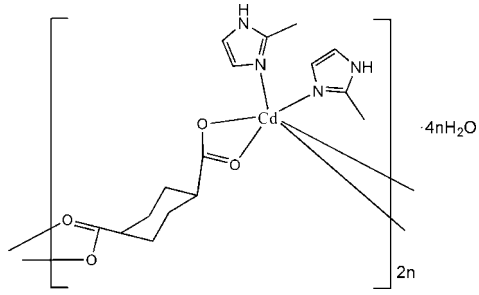
Received 3 May 2007; accepted 7 May 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.007 Å; R factor = 0.054; wR factor = 0.127; data-to-parameter ratio = 18.9.

In the title compound, $\{[Cd(C_8H_{10}O_2)(C_4H_6N_2)_2]\cdot 2H_2O\}_n$, each Cd^{II} atom is six-coordinated by two N atoms from two 2-methyl-1*H*-imidazole (mi) molecules and four O atoms from two cyclohexane-1,4-dicarboxylate (1,4-chdc) ligands in a distorted octahedral environment. The asymmetric unit consists of two independent mononuclear complex units and two solvent water molecules. Each 1,4-chdc acts as a bis-chelating ligand that binds two Cd^{II} atoms, thus forming two unique helical chains. These chains are decorated with mi ligands alternately on the two sides. Furthermore, O—H···O and N—H···O hydrogen bonds link the chains together, forming a three-dimensional supramolecular structure. There are weak π–π interactions between mi ligands in neighbouring chains at (x, y, z) and ($-x$, $-y$, 2 $-$ z), with an interplanar distance of 3.62 (2) Å.

Related literature

Two related helical coordination polymers with mixed ligands, $[Co_2(phen)_2(1,4\text{-chdc})_2(H_2O)_2]_n$ and $[Ni_2(phen)_2(1,4\text{-chdc})_2(H_2O)_2]_n$, have been prepared under hydrothermal conditions. The most attractive structural feature of the two isomorphous compounds is that they both exhibit an infinite helical chain-like structure with 2_1 helices. Moreover, adjacent chains are linked *via* hydrogen bonds and π–π interactions into three-dimensional supramolecular structures (Qi *et al.*, 2003). For related literature, see: Chen & Liu (2002); Lehn (1990); Li *et al.* (2002).



Experimental

Crystal data

$[Cd(C_8H_{10}O_2)(C_4H_6N_2)_2]\cdot 2H_2O$
M_r = 482.81
Orthorhombic, *Pbca*
a = 17.593 (4) Å
b = 16.005 (3) Å
c = 30.446 (6) Å
V = 8573 (3) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 292 (2) K
0.33 × 0.31 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.698, T_{max} = 0.742
71497 measured reflections
9751 independent reflections
6833 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.127
S = 1.01
9751 reflections
515 parameters
24 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.41 e Å^{-3}
$\Delta\rho_{min}$ = −1.01 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—HW11···O2	0.87 (5)	1.88 (5)	2.737 (6)	169 (7)
O2W—HW21···O4	0.85 (5)	1.92 (3)	2.708 (6)	153 (6)
O2W—HW22···O8^{i}	0.844 (19)	1.97 (2)	2.814 (5)	173 (5)
O3W—HW32···O3	0.86 (6)	1.90 (4)	2.727 (7)	160 (8)
O3W—HW31···O4W^{ii}	0.87 (6)	1.89 (6)	2.758 (8)	176 (9)
O4W—HW41···O1	0.87 (7)	1.97 (8)	2.797 (7)	160 (7)
O4W—HW42···O2W^{iii}	0.87 (6)	1.90 (3)	2.756 (7)	170 (9)
N2—H2···O3W	0.86	1.86	2.712 (7)	171
N4—H4A···O5^{iv}	0.86	1.99	2.845 (6)	171
N6—H6A···O7	0.86	1.93	2.776 (6)	167
N8—H8···O1W^{v}	0.86	1.98	2.839 (7)	173

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The author thanks Beihua University for supporting this work.

  doi:10.1107/S1600536807022416

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2287).

References

Chen, X. M. & Liu, G. F. (2002). *Chem. Eur. J.* **8**, 4811–4817.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Lehn, J. M. (1990). *Angew. Chem. Int. Ed. Engl.* **29**, 1304–1305.
Li, Y. G., Zhang, H., Wang, E., Hao, N., Hu, C., Yu, Y. & Hall, D. (2002). *New J. Chem.* **26**, 1619–1623.
Qi, Y., Wang, Y., Hu, C., Cao, M., Mao, L. & Wang, E. (2003). *Inorg. Chem.* **42**, 8519–8523.
Rigaku (1998). *PROCESS-AUTO*. Version 1.06. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, m1654-m1655 [**doi:10.1107/S1600536807022416**]

catena-Poly[[[bis(2-methyl-1*H*-imidazole-κN^3)cadmium(II)]-μ-cyclohexane-1,4-dicarboxylato] dihydrate]

Y.-J. Li

Comment

Helical structures have received much attention in coordination chemistry and materials chemistry (Lehn, 1990). So far, many helical complexes have been generated by self-assembly processes (Chen & Liu, 2002). An appropriate flexible bidentate organic acid bridge could be useful in the formation of helical chains in the presence of secondary ligands, such as 2,2'-bipyridine (bipy) and 1,10-phenanthroline (phen) (Li *et al.*, 2002). The N atoms from the secondary ligand may occupy two coordination positions of metal ions. The rest of the coordination positions are available for other carboxylate ligands to allow the formation of a helix. We selected cyclohexane-1,4-dicarboxylic acid (1,4-chdcH_2) as a bridging ligand and 2-methyl-1*H*-imidazole (mi) as a secondary ligand, generating a new helical chain coordination polymer, [Cd(1,4-chdc)(mi)$_2$]·2H_2O, (I), which is reported here.

In compound (I), the asymmetric unit contains two crystallographically nonequivalent Cd^{II} atoms (Cd1 and Cd2), two 1,4-chdc anions, four mi ligands, and four free water molecules (Fig. 1). Each Cd^{II} atom is six-coordinated by two N atoms from two mi molecules, and four O atoms from two 1,4-chdc ligands in a distorted octahedral environment (Fig. 1). The Cd—O distances range from 2.279 (5) to 2.457 (4) Å, and the Cd—N distances vary from 2.235 (5) to 2.269 (4) Å (Table 1). As shown in Fig. 2, each 1,4-chdc moiety acts as a bis-chelating ligand that binds two Cd^{II} atoms, forming two unique helical chains. These chains are decorated with mi ligands alternately at two sides. Furthermore, the O—H···O and N—H···O hydrogen bonds (Table 2) link the chains together, forming a three-dimensional supramolecular structure of (I). There are weak π—π interactions between 2-methyl- 1*H*-imidazole ligands in neighboring chains at (*x*, *y*, *z*) and (−*x*, −*y*, 2 − *z*), with the interplanar distance of 3.62 (2) Å.

Experimental

A mixture of $CdCl_2$·2H_2O (0.5 mmol), 1,4-chdc acid (0.5 mmol), mi (0.5 mmol), and H_2O (500 mmol) was adjusted to pH = 7 by addition of aqueous NaOH solution, and heated at 453 K for 6 days. After the mixture was slowly cooled to room temperature, colourless crystals of (I) were yielded (37% yield).

Refinement

All H atoms on C and N atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 Å) and refined as riding, with U_{iso}(H) =1.2U_{eq}(carrier). The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O—H = 0.85 Å; their temperature factors were tied to those of parent atoms by a factor of 1.2.

Figures

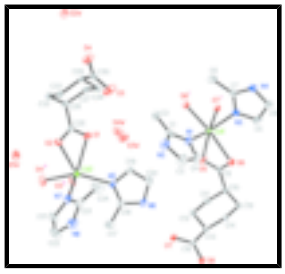


Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. (H atoms have been omitted). Symmetry code: (i) $x + 1/2, y, 1.5 - z$; (ii) $0.5 - x, 1/2 + y, z$.

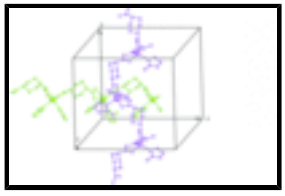


Fig. 2. View of the chain structure in (I). H atoms have been omitted.

catena-Poly[[[bis(2-methyl-1*H*-imidazole-κN^3)cadmium(II)]-μ- cyclohexane-1,4-dicarboxylato] dihydrate]

Crystal data

$[Cd(C_8H_{10}O_2)(C_4H_6N_2)_2]\cdot 2H_2O$	$F_{000} = 3936$
$M_r = 482.81$	$D_x = 1.496$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 51297 reflections
$a = 17.593$ (4) Å	θ = 3.2–27.5º
$b = 16.005$ (3) Å	μ = 1.06 mm^{-1}
$c = 30.446$ (6) Å	$T = 292$ (2) K
$V = 8573$ (3) Å^3	Block, colourless
$Z = 16$	0.33 × 0.31 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	9751 independent reflections
Radiation source: rotating anode	6833 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.074$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 292(2)$ K	$\theta_{min} = 3.2$º
ω scans	$h = -22\rightarrow22$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -20\rightarrow20$
$T_{min} = 0.698$, $T_{max} = 0.742$	$l = -39\rightarrow38$
71497 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
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 26.2686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.002$
9751 reflections	$\Delta\rho_{max} = 1.41$ e Å^{-3}
515 parameters	$\Delta\rho_{min} = -1.01$ e Å^{-3}
24 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}
C1	0.3487 (4)	0.0299 (4)	0.8365 (2)	0.0655 (16)
C2	0.3969 (4)	0.0552 (5)	0.8728 (2)	0.084 (2)
H2A	0.4082	0.0075	0.8908	0.125*
H2B	0.3710	0.0966	0.8900	0.125*
H2C	0.4433	0.0783	0.8615	0.125*
C3	0.2583 (6)	−0.0328 (6)	0.8009 (3)	0.117 (4)
H3	0.2163	−0.0658	0.7943	0.140*
C4	0.2962 (5)	0.0120 (5)	0.7727 (2)	0.093 (3)
H4	0.2862	0.0165	0.7428	0.111*
C5	0.4929 (5)	−0.0180 (4)	0.6884 (2)	0.086 (2)
H5	0.4682	0.0088	0.6654	0.104*
C6	0.5290 (5)	−0.0929 (5)	0.6857 (2)	0.091 (3)
H6	0.5335	−0.1268	0.6610	0.109*
C7	0.5378 (3)	−0.0443 (4)	0.75212 (19)	0.0567 (14)
C8	0.5594 (5)	−0.0398 (6)	0.7991 (2)	0.114 (3)
H8A	0.5626	−0.0953	0.8110	0.171*

H8B	0.5218	−0.0085	0.8150	0.171*
H8C	0.6079	−0.0128	0.8018	0.171*
C9	0.3491 (3)	0.2185 (3)	0.70464 (16)	0.0418 (11)
C10	0.3014 (3)	0.2702 (3)	0.67294 (15)	0.0425 (11)
H10	0.3373	0.3010	0.6544	0.051*
C11	0.2531 (3)	0.3359 (3)	0.69652 (18)	0.0471 (12)
H11A	0.2352	0.3767	0.6753	0.057*
H11B	0.2842	0.3649	0.7179	0.057*
C12	0.1844 (3)	0.2963 (3)	0.71987 (16)	0.0464 (12)
H12A	0.2022	0.2592	0.7429	0.056*
H12B	0.1541	0.3399	0.7334	0.056*
C13	0.1358 (3)	0.2479 (3)	0.68804 (15)	0.0407 (11)
H13	0.1187	0.2866	0.6652	0.049*
C14	0.1845 (3)	0.1795 (3)	0.66569 (16)	0.0451 (12)
H14A	0.2019	0.1400	0.6876	0.054*
H14B	0.1536	0.1493	0.6446	0.054*
C15	0.2530 (3)	0.2179 (4)	0.64228 (15)	0.0500 (13)
H15A	0.2839	0.1736	0.6299	0.060*
H15B	0.2353	0.2527	0.6183	0.060*
C16	0.0660 (3)	0.2092 (3)	0.70850 (15)	0.0421 (11)
C17	0.0291 (5)	0.2609 (8)	0.8744 (3)	0.140 (4)
H17A	0.0182	0.3013	0.8519	0.210*
H17B	0.0254	0.2868	0.9027	0.210*
H17C	−0.0067	0.2158	0.8725	0.210*
C18	0.1073 (4)	0.2279 (4)	0.86811 (18)	0.0582 (15)
C19	0.2189 (5)	0.1846 (8)	0.8780 (2)	0.132 (4)
H19	0.2637	0.1674	0.8915	0.158*
C20	0.2070 (6)	0.1864 (7)	0.8342 (3)	0.125 (3)
H20	0.2414	0.1722	0.8122	0.150*
C21	−0.0350 (4)	0.1632 (5)	0.9842 (3)	0.088 (2)
H21	−0.0451	0.2114	1.0002	0.106*
C22	−0.0868 (5)	0.1091 (6)	0.9702 (3)	0.117 (3)
H22	−0.1390	0.1120	0.9746	0.140*
C23	0.0253 (4)	0.0665 (4)	0.9494 (2)	0.0644 (16)
C24	0.0853 (5)	0.0148 (5)	0.9297 (3)	0.116 (3)
H24A	0.1299	0.0170	0.9478	0.174*
H24B	0.0972	0.0354	0.9009	0.174*
H24C	0.0680	−0.0420	0.9276	0.174*
C25	0.2703 (3)	0.1530 (3)	1.01604 (16)	0.0446 (12)
C26	0.3384 (3)	0.1297 (3)	1.04391 (17)	0.0487 (12)
H26	0.3531	0.1802	1.0601	0.058*
C27	0.4074 (3)	0.1047 (3)	1.01558 (18)	0.0489 (13)
H27A	0.4141	0.1454	0.9923	0.059*
H27B	0.4529	0.1052	1.0336	0.059*
C28	0.3971 (3)	0.0188 (3)	0.99572 (16)	0.0440 (11)
H28A	0.4415	0.0048	0.9784	0.053*
H28B	0.3534	0.0193	0.9763	0.053*
C29	0.3855 (3)	−0.0475 (3)	1.03110 (15)	0.0414 (11)
H29	0.4294	−0.0461	1.0508	0.050*

C30	0.3793 (3)	−0.1346 (3)	1.01204 (17)	0.0466 (12)
C32	0.3221 (4)	0.0625 (4)	1.07818 (16)	0.0561 (15)
H32A	0.3627	0.0619	1.0997	0.067*
H32B	0.2752	0.0760	1.0934	0.067*
C33	0.3150 (3)	−0.0239 (3)	1.05761 (16)	0.0500 (13)
H33A	0.2708	−0.0250	1.0385	0.060*
H33B	0.3072	−0.0649	1.0806	0.060*
N1	0.3556 (3)	0.0527 (3)	0.79580 (16)	0.0665 (14)
N2	0.2897 (3)	−0.0240 (4)	0.84165 (18)	0.0800 (17)
H2	0.2751	−0.0477	0.8656	0.096*
N3	0.4986 (3)	0.0114 (3)	0.73007 (15)	0.0572 (12)
N4	0.5567 (3)	−0.1078 (3)	0.72553 (18)	0.0638 (13)
H4A	0.5826	−0.1511	0.7331	0.077*
N5	0.1569 (3)	0.2111 (3)	0.89909 (14)	0.0599 (13)
N6	0.1345 (3)	0.2130 (4)	0.82889 (16)	0.0862 (19)
H6A	0.1109	0.2191	0.8044	0.103*
N7	0.0366 (3)	0.1368 (3)	0.97121 (16)	0.0603 (12)
N8	−0.0480 (4)	0.0483 (4)	0.9479 (2)	0.0862 (19)
H8	−0.0679	0.0056	0.9352	0.103*
O1	0.2783 (2)	0.1910 (3)	0.98117 (14)	0.0797 (14)
O2	0.2054 (2)	0.1357 (3)	1.02861 (14)	0.0738 (13)
O1W	0.1019 (3)	0.0996 (3)	1.09298 (15)	0.0737 (13)
HW11	0.139 (2)	0.113 (4)	1.0753 (18)	0.088*
HW12	0.067 (3)	0.138 (3)	1.090 (2)	0.088*
O3	0.3518 (4)	−0.1455 (3)	0.97550 (18)	0.112 (2)
O2W	0.4907 (3)	−0.2497 (3)	1.09893 (13)	0.0690 (12)
HW21	0.464 (3)	−0.218 (3)	1.0825 (15)	0.083*
HW22	0.491 (4)	−0.232 (4)	1.1251 (8)	0.083*
O4	0.4037 (3)	−0.1952 (3)	1.03138 (15)	0.0824 (15)
O3W	0.2434 (3)	−0.0813 (4)	0.92112 (18)	0.0933 (16)
HW31	0.209 (3)	−0.120 (4)	0.924 (2)	0.112*
HW32	0.277 (3)	−0.090 (5)	0.941 (2)	0.112*
O5	0.3690 (2)	0.2477 (2)	0.74102 (13)	0.0610 (11)
O4W	0.3630 (3)	0.2924 (4)	0.9246 (2)	0.1069 (19)
HW41	0.344 (4)	0.252 (4)	0.940 (3)	0.128*
HW42	0.407 (3)	0.275 (5)	0.915 (3)	0.128*
O6	0.3704 (3)	0.1473 (3)	0.69354 (13)	0.0691 (12)
O7	0.0579 (2)	0.2059 (3)	0.74928 (11)	0.0602 (11)
O8	0.0155 (2)	0.1791 (3)	0.68348 (11)	0.0533 (9)
Cd1	0.44158 (2)	0.12656 (2)	0.758212 (12)	0.04416 (11)
Cd2	0.14412 (2)	0.21222 (2)	0.973230 (11)	0.04324 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.060 (4)	0.071 (4)	0.065 (4)	−0.002 (3)	0.006 (3)	0.001 (3)
C2	0.068 (5)	0.123 (6)	0.060 (4)	−0.019 (4)	0.000 (3)	0.019 (4)
C3	0.127 (8)	0.136 (8)	0.087 (5)	−0.081 (7)	0.001 (5)	−0.013 (5)

C4	0.113 (7)	0.100 (6)	0.065 (4)	−0.048 (5)	0.006 (4)	−0.005 (4)
C5	0.123 (7)	0.066 (4)	0.070 (4)	0.030 (4)	−0.038 (4)	−0.010 (3)
C6	0.116 (7)	0.074 (5)	0.081 (5)	0.032 (5)	−0.031 (5)	−0.030 (4)
C7	0.048 (3)	0.057 (3)	0.064 (3)	0.014 (3)	0.005 (3)	0.008 (3)
C8	0.133 (8)	0.131 (8)	0.077 (5)	0.072 (6)	−0.019 (5)	0.013 (5)
C9	0.031 (2)	0.051 (3)	0.044 (3)	−0.007 (2)	−0.001 (2)	0.006 (2)
C10	0.029 (2)	0.058 (3)	0.040 (2)	−0.002 (2)	0.0027 (19)	0.010 (2)
C11	0.036 (3)	0.045 (3)	0.061 (3)	0.000 (2)	0.002 (2)	0.009 (2)
C12	0.038 (3)	0.055 (3)	0.046 (3)	−0.006 (2)	0.006 (2)	−0.008 (2)
C13	0.031 (3)	0.053 (3)	0.038 (2)	0.001 (2)	−0.0010 (19)	0.007 (2)
C14	0.032 (3)	0.061 (3)	0.042 (3)	−0.005 (2)	−0.001 (2)	−0.008 (2)
C15	0.035 (3)	0.078 (4)	0.036 (2)	0.002 (3)	0.000 (2)	−0.002 (3)
C16	0.032 (3)	0.055 (3)	0.039 (2)	0.003 (2)	0.000 (2)	0.003 (2)
C17	0.096 (7)	0.233 (13)	0.091 (6)	0.073 (8)	−0.003 (5)	0.037 (7)
C18	0.059 (4)	0.068 (4)	0.047 (3)	0.002 (3)	−0.006 (3)	0.003 (3)
C19	0.084 (6)	0.256 (13)	0.054 (4)	0.081 (7)	−0.015 (4)	−0.039 (6)
C20	0.114 (6)	0.188 (8)	0.072 (5)	0.056 (6)	0.000 (4)	−0.028 (5)
C21	0.077 (5)	0.077 (5)	0.110 (6)	−0.019 (4)	0.022 (4)	−0.024 (4)
C22	0.066 (5)	0.133 (8)	0.152 (8)	−0.030 (5)	0.025 (5)	−0.053 (7)
C23	0.084 (5)	0.046 (3)	0.064 (4)	−0.004 (3)	−0.010 (3)	0.001 (3)
C24	0.121 (8)	0.065 (5)	0.163 (9)	0.012 (5)	0.004 (7)	−0.037 (5)
C25	0.052 (3)	0.037 (3)	0.044 (3)	0.005 (2)	−0.003 (2)	−0.006 (2)
C26	0.056 (3)	0.042 (3)	0.048 (3)	0.001 (3)	−0.011 (2)	−0.009 (2)
C27	0.038 (3)	0.041 (3)	0.068 (3)	−0.001 (2)	−0.008 (2)	0.001 (2)
C28	0.036 (3)	0.049 (3)	0.048 (3)	0.001 (2)	0.006 (2)	−0.003 (2)
C29	0.041 (3)	0.042 (3)	0.041 (2)	0.006 (2)	−0.009 (2)	−0.003 (2)
C30	0.048 (3)	0.048 (3)	0.044 (3)	0.000 (3)	−0.006 (2)	−0.003 (2)
C32	0.071 (4)	0.062 (4)	0.035 (3)	0.018 (3)	−0.005 (2)	−0.006 (2)
C33	0.060 (4)	0.051 (3)	0.039 (3)	0.004 (3)	0.004 (2)	0.011 (2)
N1	0.072 (4)	0.065 (3)	0.062 (3)	−0.016 (3)	−0.002 (3)	0.003 (3)
N2	0.087 (4)	0.088 (4)	0.065 (3)	−0.039 (3)	0.003 (3)	0.010 (3)
N3	0.060 (3)	0.052 (3)	0.059 (3)	0.007 (2)	−0.007 (2)	0.002 (2)
N4	0.064 (3)	0.046 (3)	0.081 (3)	0.012 (2)	−0.009 (3)	0.000 (2)
N5	0.053 (3)	0.083 (4)	0.043 (2)	0.003 (3)	−0.007 (2)	−0.014 (2)
N6	0.077 (4)	0.137 (6)	0.044 (3)	0.022 (4)	−0.017 (3)	−0.008 (3)
N7	0.067 (3)	0.052 (3)	0.061 (3)	−0.010 (2)	−0.006 (2)	−0.002 (2)
N8	0.088 (5)	0.077 (4)	0.093 (4)	−0.040 (4)	−0.017 (4)	−0.006 (3)
O1	0.056 (3)	0.111 (4)	0.072 (3)	0.000 (3)	−0.006 (2)	0.040 (3)
O2	0.049 (3)	0.101 (4)	0.071 (3)	0.014 (2)	0.007 (2)	0.028 (2)
O1W	0.081 (3)	0.073 (3)	0.066 (3)	−0.024 (3)	0.014 (2)	−0.004 (2)
O3	0.175 (5)	0.058 (3)	0.102 (4)	0.009 (3)	−0.076 (4)	−0.016 (3)
O2W	0.069 (3)	0.088 (3)	0.049 (2)	0.014 (3)	0.001 (2)	−0.004 (2)
O4	0.124 (4)	0.045 (2)	0.078 (3)	0.015 (3)	−0.038 (3)	−0.005 (2)
O3W	0.074 (4)	0.115 (4)	0.091 (4)	−0.005 (3)	−0.004 (3)	0.042 (3)
O5	0.071 (3)	0.055 (2)	0.058 (2)	−0.012 (2)	−0.031 (2)	0.0038 (18)
O4W	0.072 (4)	0.112 (5)	0.136 (5)	0.011 (3)	0.014 (3)	0.041 (4)
O6	0.078 (3)	0.067 (3)	0.062 (2)	0.030 (2)	−0.017 (2)	−0.012 (2)
O7	0.045 (2)	0.099 (3)	0.0366 (18)	−0.019 (2)	0.0004 (16)	0.0044 (19)
O8	0.040 (2)	0.080 (3)	0.0404 (18)	−0.0171 (19)	−0.0017 (15)	−0.0007 (18)

Cd1	0.03687 (19)	0.0486 (2)	0.0470 (2)	0.00164 (17)	−0.01030 (16)	0.00212 (17)
Cd2	0.0455 (2)	0.0431 (2)	0.04110 (19)	0.00382 (17)	−0.00389 (16)	−0.00270 (16)

Geometric parameters (Å, °)

C1—N1	1.298 (8)	C21—N7	1.386 (9)
C1—N2	1.360 (8)	C21—H21	0.9300
C1—C2	1.449 (9)	C22—N8	1.368 (10)
C2—H2A	0.9600	C22—H22	0.9300
C2—H2B	0.9600	C23—N8	1.323 (8)
C2—H2C	0.9600	C23—N7	1.322 (7)
C3—C4	1.303 (10)	C23—C24	1.468 (10)
C3—N2	1.364 (9)	C24—H24A	0.9600
C3—H3	0.9300	C24—H24B	0.9600
C4—N1	1.416 (9)	C24—H24C	0.9600
C4—H4	0.9300	C25—O1	1.232 (6)
C5—C6	1.359 (9)	C25—O2	1.234 (7)
C5—N3	1.356 (7)	C25—C26	1.516 (7)
C5—H5	0.9300	C26—C32	1.527 (8)
C6—N4	1.329 (8)	C26—C27	1.542 (8)
C6—H6	0.9300	C26—H26	0.9800
C7—N3	1.313 (7)	C27—C28	1.513 (7)
C7—N4	1.342 (7)	C27—H27A	0.9700
C7—C8	1.482 (9)	C27—H27B	0.9700
C8—H8A	0.9600	C28—C29	1.525 (7)
C8—H8B	0.9600	C28—H28A	0.9700
C8—H8C	0.9600	C28—H28B	0.9700
C9—O6	1.246 (6)	C29—C30	1.515 (7)
C9—O5	1.252 (6)	C29—C33	1.527 (7)
C9—C10	1.523 (7)	C29—H29	0.9800
C10—C15	1.516 (7)	C30—O4	1.214 (6)
C10—C11	1.531 (7)	C30—O3	1.226 (6)
C10—H10	0.9800	C32—C33	1.523 (8)
C11—C12	1.538 (7)	C32—H32A	0.9700
C11—H11A	0.9700	C32—H32B	0.9700
C11—H11B	0.9700	C33—H33A	0.9700
C12—C13	1.508 (7)	C33—H33B	0.9700
C12—H12A	0.9700	Cd1—N1	2.235 (5)
C12—H12B	0.9700	N2—H2	0.8600
C13—C16	1.509 (7)	Cd1—N3	2.266 (5)
C13—C14	1.547 (7)	N4—H4A	0.8600
C13—H13	0.9800	Cd2—N5	2.269 (4)
C14—C15	1.530 (7)	N6—H6A	0.8600
C14—H14A	0.9700	Cd2—N7	2.244 (5)
C14—H14B	0.9700	N8—H8	0.8600
C15—H15A	0.9700	Cd2—O1	2.397 (4)
C15—H15B	0.9700	Cd2—O2	2.347 (4)
C16—O7	1.251 (6)	O1W—HW11	0.87 (5)
C16—O8	1.266 (6)	O1W—HW12	0.87 (5)

C17—C18	1.485 (10)	O2W—HW21	0.85 (5)
C17—H17A	0.9600	O2W—HW22	0.844 (19)
C17—H17B	0.9600	O3W—HW31	0.87 (6)
C17—H17C	0.9600	O3W—HW32	0.86 (6)
C18—N6	1.308 (7)	O4W—HW41	0.87 (7)
C18—N5	1.313 (7)	O4W—HW42	0.87 (6)
C19—N5	1.335 (8)	Cd1—O5	2.380 (4)
C19—C20	1.352 (10)	Cd1—O6	2.357 (4)
C19—H19	0.9300	Cd1—O8^{i}	2.355 (3)
C20—N6	1.354 (10)	Cd1—O7^{i}	2.419 (4)
C20—H20	0.9300	Cd2—O3^{ii}	2.279 (5)
C21—C22	1.327 (10)	Cd2—O4^{ii}	2.457 (4)
N1—C1—N2	111.0 (6)	C25—C26—C32	114.0 (5)
N1—C1—C2	126.5 (6)	C25—C26—C27	111.9 (4)
N2—C1—C2	122.5 (6)	C32—C26—C27	110.3 (4)
C1—C2—H2A	109.5	C25—C26—H26	106.7
C1—C2—H2B	109.5	C32—C26—H26	106.7
H2A—C2—H2B	109.5	C27—C26—H26	106.7
C1—C2—H2C	109.5	C28—C27—C26	111.4 (4)
H2A—C2—H2C	109.5	C28—C27—H27A	109.3
H2B—C2—H2C	109.5	C26—C27—H27A	109.3
C4—C3—N2	109.6 (7)	C28—C27—H27B	109.3
C4—C3—H3	125.2	C26—C27—H27B	109.3
N2—C3—H3	125.2	H27A—C27—H27B	108.0
C3—C4—N1	107.7 (7)	C27—C28—C29	111.5 (4)
C3—C4—H4	126.1	C27—C28—H28A	109.3
N1—C4—H4	126.1	C29—C28—H28A	109.3
C6—C5—N3	109.3 (6)	C27—C28—H28B	109.3
C6—C5—H5	125.4	C29—C28—H28B	109.3
N3—C5—H5	125.4	H28A—C28—H28B	108.0
N4—C6—C5	105.9 (6)	C30—C29—C28	112.3 (4)
N4—C6—H6	127.1	C30—C29—C33	111.9 (4)
C5—C6—H6	127.1	C28—C29—C33	108.1 (4)
N3—C7—N4	109.7 (5)	C30—C29—H29	108.2
N3—C7—C8	126.6 (6)	C28—C29—H29	108.2
N4—C7—C8	123.7 (6)	C33—C29—H29	108.2
C7—C8—H8A	109.5	O4—C30—O3	117.8 (5)
C7—C8—H8B	109.5	O4—C30—C29	121.7 (5)
H8A—C8—H8B	109.5	O3—C30—C29	120.5 (5)
C7—C8—H8C	109.5	O4—C30—Cd2^{iii}	63.2 (3)
H8A—C8—H8C	109.5	O3—C30—Cd2^{iii}	54.8 (3)
H8B—C8—H8C	109.5	C29—C30—Cd2^{iii}	174.5 (4)
O6—C9—O5	119.8 (5)	C33—C32—C26	112.0 (4)
O6—C9—C10	119.4 (4)	C33—C32—H32A	109.2
O5—C9—C10	120.8 (5)	C26—C32—H32A	109.2
C15—C10—C9	113.5 (4)	C33—C32—H32B	109.2
C15—C10—C11	110.8 (4)	C26—C32—H32B	109.2

C9—C10—C11	112.4 (4)	H32A—C32—H32B	107.9
C15—C10—H10	106.5	C32—C33—C29	112.0 (5)
C9—C10—H10	106.5	C32—C33—H33A	109.2
C11—C10—H10	106.5	C29—C33—H33A	109.2
C10—C11—C12	111.8 (4)	C32—C33—H33B	109.2
C10—C11—H11A	109.3	C29—C33—H33B	109.2
C12—C11—H11A	109.3	H33A—C33—H33B	107.9
C10—C11—H11B	109.3	C1—N1—C4	106.0 (6)
C12—C11—H11B	109.3	C1—N1—Cd1	134.5 (4)
H11A—C11—H11B	107.9	C4—N1—Cd1	119.2 (4)
C13—C12—C11	111.1 (4)	C1—N2—C3	105.7 (6)
C13—C12—H12A	109.4	C1—N2—H2	127.2
C11—C12—H12A	109.4	C3—N2—H2	127.2
C13—C12—H12B	109.4	C7—N3—C5	106.3 (5)
C11—C12—H12B	109.4	C7—N3—Cd1	126.3 (4)
H12A—C12—H12B	108.0	C5—N3—Cd1	127.1 (4)
C12—C13—C16	114.0 (4)	C6—N4—C7	108.9 (5)
C12—C13—C14	109.4 (4)	C6—N4—H4A	125.6
C16—C13—C14	110.0 (4)	C7—N4—H4A	125.6
C12—C13—H13	107.7	C18—N5—C19	105.3 (5)
C16—C13—H13	107.7	C18—N5—Cd2	130.3 (4)
C14—C13—H13	107.7	C19—N5—Cd2	124.2 (4)
C15—C14—C13	110.9 (4)	C18—N6—C20	107.1 (6)
C15—C14—H14A	109.5	C18—N6—H6A	126.4
C13—C14—H14A	109.5	C20—N6—H6A	126.4
C15—C14—H14B	109.5	C23—N7—C21	105.4 (6)
C13—C14—H14B	109.5	C23—N7—Cd2	126.7 (5)
H14A—C14—H14B	108.0	C21—N7—Cd2	126.5 (4)
C10—C15—C14	112.2 (4)	C23—N8—C22	108.3 (6)
C10—C15—H15A	109.2	C23—N8—H8	125.9
C14—C15—H15A	109.2	C22—N8—H8	125.9
C10—C15—H15B	109.2	C25—O1—Cd2	92.5 (4)
C14—C15—H15B	109.2	C25—O2—Cd2	94.9 (3)
H15A—C15—H15B	107.9	HW11—O1W—HW12	107 (3)
O7—C16—O8	120.0 (4)	C30—O3—Cd2^{iii}	99.1 (4)
O7—C16—C13	121.4 (4)	HW21—O2W—HW22	111 (3)
O8—C16—C13	118.6 (4)	C30—O4—Cd2^{iii}	90.6 (3)
C18—C17—H17A	109.5	HW31—O3W—HW32	108 (3)
C18—C17—H17B	109.5	C9—O5—Cd1	92.3 (3)
H17A—C17—H17B	109.5	HW41—O4W—HW42	107 (7)
C18—C17—H17C	109.5	C9—O6—Cd1	93.5 (3)
H17A—C17—H17C	109.5	C16—O7—Cd1^{iv}	91.5 (3)
H17B—C17—H17C	109.5	C16—O8—Cd1^{iv}	94.0 (3)
N6—C18—N5	112.0 (6)	N1—Cd1—N3	93.62 (19)
N6—C18—C17	121.4 (6)	N1—Cd1—O8^{i}	100.17 (15)
N5—C18—C17	126.6 (6)	N3—Cd1—O8^{i}	109.32 (16)
N5—C19—C20	110.0 (7)	N1—Cd1—O6	98.18 (18)
N5—C19—H19	125.0	N3—Cd1—O6	91.94 (15)

C20—C19—H19	125.0	O8^{i}—Cd1—O6	150.77 (15)
N6—C20—C19	105.6 (7)	N1—Cd1—O5	100.37 (18)
N6—C20—H20	127.2	N3—Cd1—O5	144.75 (15)
C19—C20—H20	127.2	O8^{i}—Cd1—O5	99.87 (13)
C22—C21—N7	109.5 (7)	O6—Cd1—O5	54.29 (13)
C22—C21—H21	125.2	N1—Cd1—O7^{i}	153.96 (16)
N7—C21—H21	125.2	N3—Cd1—O7^{i}	90.96 (17)
C21—C22—N8	106.3 (7)	O8^{i}—Cd1—O7^{i}	54.33 (11)
C21—C22—H22	126.9	O6—Cd1—O7^{i}	107.27 (15)
N8—C22—H22	126.9	O5—Cd1—O7^{i}	90.33 (15)
N8—C23—N7	110.5 (6)	N7—Cd2—N5	92.99 (18)
N8—C23—C24	124.3 (7)	N7—Cd2—O3^{ii}	124.4 (2)
N7—C23—C24	125.2 (7)	N5—Cd2—O3^{ii}	91.99 (19)
C23—C24—H24A	109.5	N7—Cd2—O2	97.27 (17)
C23—C24—H24B	109.5	N5—Cd2—O2	131.71 (17)
H24A—C24—H24B	109.5	O3^{ii}—Cd2—O2	119.0 (2)
C23—C24—H24C	109.5	N7—Cd2—O1	139.16 (18)
H24A—C24—H24C	109.5	N5—Cd2—O1	90.09 (16)
H24B—C24—H24C	109.5	O3^{ii}—Cd2—O1	96.1 (2)
O1—C25—O2	119.0 (5)	O2—Cd2—O1	53.20 (14)
O1—C25—C26	120.9 (5)	N7—Cd2—O4^{ii}	93.16 (18)
O2—C25—C26	120.1 (5)	N5—Cd2—O4^{ii}	139.08 (18)
O1—C25—Cd2	60.8 (3)	O3^{ii}—Cd2—O4^{ii}	52.18 (15)
O2—C25—Cd2	58.5 (3)	O2—Cd2—O4^{ii}	87.38 (17)
C26—C25—Cd2	172.4 (3)	O1—Cd2—O4^{ii}	110.49 (19)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—HW11···O2	0.87 (5)	1.88 (5)	2.737 (6)	169 (7)
O2W—HW21···O4	0.85 (5)	1.92 (3)	2.708 (6)	153 (6)
O2W—HW22···O8^{v}	0.844 (19)	1.97 (2)	2.814 (5)	173 (5)
O3W—HW32···O3	0.86 (6)	1.90 (4)	2.727 (7)	160 (8)
O3W—HW31···O4W^{iii}	0.87 (6)	1.89 (6)	2.758 (8)	176 (9)
O4W—HW41···O1	0.87 (7)	1.97 (8)	2.797 (7)	160 (7)
O4W—HW42···O2W^{vi}	0.87 (6)	1.90 (3)	2.756 (7)	170 (9)
N2—H2···O3W	0.86	1.86	2.712 (7)	171
N4—H4A···O5^{vii}	0.86	1.99	2.845 (6)	171
N6—H6A···O7	0.86	1.93	2.776 (6)	167
N8—H8···O1W^{viii}	0.86	1.98	2.839 (7)	173

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

Fig. 1

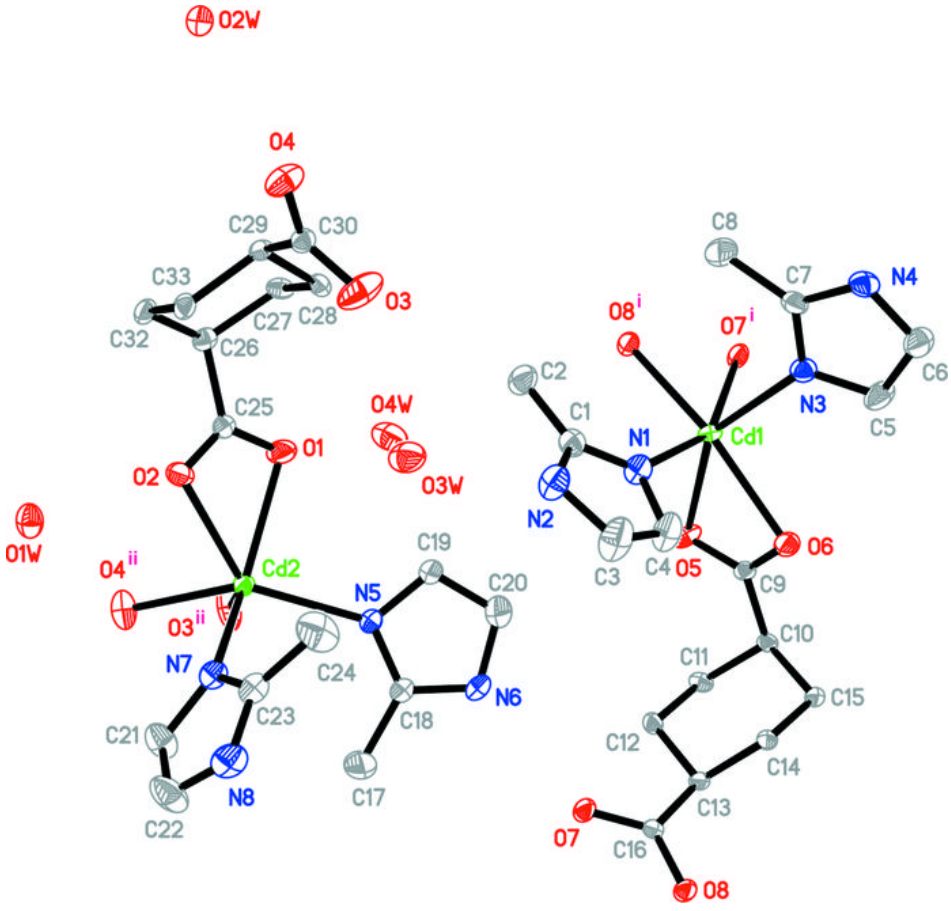

O2W
O4
C29
C30
C33
O3
C27
C28
C32
C26
C25
O1
O2
O4W
O3W
O1W
O4ii
Cd2
C19
C20
N5
O3ii
N7
C24
C23
N6
C18
C21
N8
C17
C22
C8
C7
N4
O8i
O7i
C2
C6
C1
N3
C5
N1
Cd1
N2
C3
C4
O5
O6
C9
C10
C11
C15
C12
C14
C13
O7
C16
O8

Fig. 2