Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[diammonium [diaquabis(pyridine-2,4-dicarboxylato-κ^2N,O^2)cuprate(II)] [[diaquacopper(II)]-μ-pyridine-2,4-dicarboxylato-$\kappa^3N,O^2:O^{2'}$-[tetraaquacadmium(II)]-μ-pyridine-2,4-dicarboxylato-$\kappa^3O^2:N,O^{2'}$] hexahydrate]

Guan-Hua Wang,[a,b] Zhi-Gang Li,[a,b] Heng-Qing Jia,[a] Ning-Hai Hu[a]* and Jing-Wei Xu[a]

[a]The State Key Laboratory of Electroanalytical Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China, and [b]Graduate School, Chinese Academy of Sciences, Beijing 100039, People's Republic of China
Correspondence e-mail: hunh@ciac.jl.cn

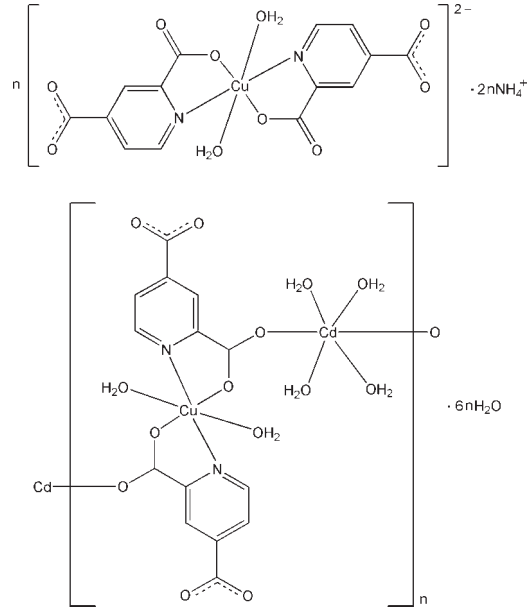
Received 21 October 2009; accepted 6 November 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.073; data-to-parameter ratio = 11.7.

The title mixed-metal complex, $\{(NH_4)_2[Cu(C_7H_3NO_4)_2(H_2O)_2][CdCu(C_7H_3NO_4)_2(H_2O)_6]\cdot 6H_2O\}_n$, contains one octahedrally coordinated Cd^{II} center and two octahedrally coordinated Cu^{II} centers, each lying on an inversion center. The two Cu^{II} atoms are each coordinated by two O atoms and two N atoms from two 2,4-pydc (2,4-H_2pydc = pyridine-2,4-dicarboxylic acid) ligands in the equatorial plane and two water molecules at the axial sites, thus producing two crystallographically independent $[Cu(2,4\text{-pydc})_2(H_2O)_2]^{2-}$ metalloligands. One metalloligand exists as a discrete anion and the other connects the $Cd(H_2O)_4$ units, forming a neutral chain. O—H···O and N—H···O hydrogen bonds connects the polymeric chains, complex anions, ammonium cations and uncoordinated water molecules into a three-dimensional supramolecular network.

Related literature

For general background to coordination polymers, see: Caneschi *et al.* (2001); Dong *et al.* (2000); Evans & Lin (2002); Kitagawa *et al.* (1999, 2004, 2006). For related structures, see: Li *et al.* (2008); Noro *et al.* (2002*a*,*b*); Wang *et al.* (2009).



Experimental

Crystal data

$(NH_4)_2[Cu(C_7H_3NO_4)_2(H_2O)_2]$-$[CdCu(C_7H_3NO_4)_2(H_2O)_6]\cdot 6H_2O$
M_r = 1188.20
Triclinic, $P\overline{1}$
a = 10.4520 (19) Å
b = 10.5252 (19) Å
c = 10.6733 (19) Å
α = 102.869 (2)°
β = 103.536 (2)°
γ = 94.834 (2)°
V = 1101.3 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.54 mm^{-1}
T = 293 K
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.720, T_{max} = 0.785
6205 measured reflections
4212 independent reflections
3869 reflections with $I > 2\sigma(I)$
R_{int} = 0.011

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.073
S = 1.05
4212 reflections
361 parameters
31 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O7^{i}	0.94 (2)	1.80 (1)	2.739 (2)	171 (2)
O1W—H1B···O4^{ii}	0.95 (2)	1.82 (1)	2.769 (2)	177 (3)
O2W—H2A···O3^{ii}	0.95 (1)	1.72 (1)	2.657 (3)	168 (2)
O2W—H2B···O8^{iii}	0.95 (1)	1.77 (1)	2.722 (2)	177 (2)
O3W—H3A···O6W^{iv}	0.94 (1)	1.84 (1)	2.781 (3)	172 (3)
O3W—H3B···O7^{iv}	0.94 (1)	1.84 (1)	2.776 (3)	172 (3)
O4W—H4A···O3W^{v}	0.95 (1)	1.89 (1)	2.827 (3)	169 (2)
O4W—H4B···O4^{i}	0.95 (1)	1.80 (1)	2.752 (3)	176 (2)
O5W—H5A···O4W^{vi}	0.95 (1)	2.10 (1)	3.048 (3)	170 (3)
O5W—H5B···O3	0.96 (1)	1.93 (1)	2.882 (3)	171 (3)
O6W—H6A···O6	0.95 (1)	1.79 (1)	2.742 (3)	173 (3)

D—H···A	D—H	H···A	D···A	D—H···A
O6W—H6B···O2W^{vii}	0.96 (3)	2.14 (2)	2.991 (3)	147 (2)
O7W—H7A···O2	0.95 (3)	2.09 (3)	3.009 (3)	163 (3)
O7W—H7B···O5W	0.95 (3)	1.93 (3)	2.861 (3)	165 (4)
N3—H31···O7W^{viii}	0.98 (2)	1.90 (2)	2.867 (3)	174 (2)
N3—H32···O8	0.99 (2)	1.92 (1)	2.886 (3)	164 (2)
N3—H33···O5W^{ix}	0.99 (1)	2.53 (2)	3.208 (4)	126 (2)
N3—H33···O5^{x}	0.99 (1)	2.30 (2)	3.131 (3)	140 (2)
N3—H33···O6^{x}	0.99 (1)	2.19 (2)	2.888 (3)	126 (2)
N3—H34···O8^{xi}	0.99 (2)	2.34 (1)	3.277 (3)	157 (2)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y, z+1$; (iii) $x-1, y-1, z$; (iv) $x, y-1, z$; (v) $x, y+1, z+1$; (vi) $x, y-1, z-1$; (vii) $x, y+1, z$; (viii) $-x+1, -y, -z+1$; (ix) $x+1, y+1, z+1$; (x) $x+1, y, z$; (xi) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the Changchun Institute of Applied Chemistry for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2303).

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supplementary materials

Acta Cryst. (2009). E**65**, m1568-m1569 [**doi:10.1107/S1600536809046911**]

catena-Poly[diammonium [diaquabis(pyridine-2,4-dicarboxylato-κ^2N,O^2)cuprate(II)] [[diaquacopper(II)]-μ-pyridine-2,4-dicarboxylato-$\kappa^3N,O^2:O^{2'}$-[tetraaquacadmium(II)]-μ-pyridine-2,4-dicarboxylato-$\kappa^3O^2:N,O^{2'}$] hexahydrate]

G.-H. Wang, Z.-G. Li, H.-Q. Jia, N.-H. Hu and J.-W. Xu

Comment

Coordination polymers constructed from metal ions and bridging ligands have been of great interest owing to their structural diversities and fascinating properties (Caneschi *et al.*, 2001; Evans & Lin, 2002; Kitagawa *et al.*, 1999, 2004). In recent years, the design and synthesis of mixed-metal coordination polymers have received much attention because such heterometallic materials might exhibit interesting physical properties, resulting from interactions between two neighboring metal centers connected by a suitable linker (Dong *et al.*, 2000; Kitagawa *et al.*, 2006). Noro *et al.* (2002*a*, b) have prepared mixed-metal coordination polymers by using the Et_3NH salt of a metalloligand, $[Cu(2,4\text{-pydc})_2]^{2-}$ (2,4-H_2pydc = pyridine-2,4-dicarboxylic acid). We prepared recently a mixed-metal complex with a metalloligand $[Cu(2,5\text{-pydc})_2]^{2-}$ by a simplified synthetic method (Wang *et al.*, 2009). As a continuation of our work, we report here the synthesis and structure of the title compound.

The asymmetric unit of the title compound contains one six-coordinated Cd^{II} atom and two six-coordinated Cu^{II} atoms, each lying on an inversion center, two 2,4-pydc ligands, one ammonium ion, four coordinated water molecules and three uncoordinated water molecules (Fig. 1). Both Cu1 and Cu2 atoms have an axially elongated octahedral coordination geometry, defined by two O atoms and two N atoms from two 2,4-pydc ligands in the equatorial plane and two water molecules at the axial sites, thus producing two crystallographically independent $[Cu(2,4\text{-pydc})_2(H_2O)_2]^{2-}$ metalloligands. In each metalloligand, the equatorial plane consists of *trans* N donors and *trans* O donors. The Cd^{II} ions coordinated by four water molecules are linked by the Cu1-metalloligands, *via* the bidentate-bridging 2-carboxylate groups, into a one-dimensional polymeric chain along the [100] direction (Fig. 2). The shortest Cu···Cd distance is 5.226 (1) Å. The 2,4-pydc ligand binds Cu1 and Cd1 atoms in a μ_2-($\kappa^3N,O^2:O^{2'}$) mode with the 4-carboxylate group uncoordinated (Li *et al.*, 2008). The Cu2-metalloligand acts as a discrete divalent anion and does not interact with a second metal ion. The 2,4-pydc ligand in the Cu2-metalloligand adopts a (κ^2N,O^2) chelating mode with the 4-carboxylate group remaining idle. Extensive O—H···O and N—H···O hydrogen bonds (Table 1) assemble the various components into a supramolecular network (Fig. 3).

Experimental

An aqueous solution (20 ml) of $Cu(NO_3)_2.3H_2O$ (0.125 g, 0.3 mmol) and a suspension of 2,4-H_2pydc (0.083 g, 0.3 mmol) in ethanol (10 ml) were mixed and refluxed for 24 h until a clear solution was obtained. To this solution, an aqueous solution (5 ml) of $CdCl_2$ (0.055 g, 0.5 mmol) was added. Aqueous NH_3 (25%, 0.06 ml) was then slowly added to the reaction mixture. The resulting solution was filtered off. Blue block crystals were obtained by allowing the filtrate to stand at room temperature for several days.

Refinement

H atoms on C atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). H atoms of water molecules and ammonium ion were located in a difference Fourier map and refined with distance restraints of O—H = 0.96 (1), H···H = 1.56 (1) Å, and N—H = 0.99 (1), H···H = 1.62 (1) Å, and with U_{iso}(H) = 1.2U_{eq}(O,*N*).

Figures

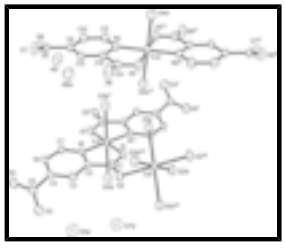

Fig. 1. The asymmetric unit of the title compound, together with symmetry-related atoms to complete the Cd1, Cu1 and Cu2 coordination. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) 1 - *x*, -*y*, 1 - *z*; (ii) 1 - *x*, 1 - *y*, 2 - *z*; (iii) -*x*, -*y*, 1 - *z*.]

Fig. 2. The one-dimensional chain in the title compound. H atoms have been omitted for clarity.

Fig. 3. The crystal packing of the title compound. Dashed lines denote hydrogen bonds.

catena-Poly[diammonium [diaquabis(pyridine-2,4-dicarboxylato-κ^2*N*,*O*^{2})cuprate(II)] [[diaquacopper(II)]-μ-pyridine-2,4-dicarboxylato- κ^3*N*,*O*^{2}:*O*$^{2'}$-[tetraaquacadmium(II)]- μ-pyridine-2,4-dicarboxylato-κ^3*O*^{2}:*N*,*O*$^{2'}$] hexahydrate]

Crystal data

$(NH_4)_2[Cu(C_7H_3NO_4)_2(H_2O)_2][CdCu(C_7H_3NO_4)_2(H_2O)_4]\cdot 6H_2O$	
M_r = 1188.20	F_{000} = 604
Triclinic, $P\overline{1}$	D_x = 1.792 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 10.4520 (19) Å	Cell parameters from 4140 reflections
b = 10.5252 (19) Å	θ = 2.5–26.1º
c = 10.6733 (19) Å	μ = 1.54 mm^{-1}
α = 102.869 (2)º	*T* = 293 K
β = 103.536 (2)º	Block, blue
γ = 94.834 (2)º	0.22 × 0.20 × 0.16 mm
V = 1101.3 (3) Å^3	

Data collection

Bruker SMART APEX CCD diffractometer	4212 independent reflections
Radiation source: fine-focus sealed tube	3869 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.011$
$T = 293$ K	$\theta_{max} = 26.1^{o}$
φ and ω scans	$\theta_{min} = 2.0^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 8$
$T_{min} = 0.720$, $T_{max} = 0.785$	$k = -12 \rightarrow 12$
6205 measured reflections	$l = -11 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.073$	$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.7186P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.004$
4212 reflections	$\Delta\rho_{max} = 0.67$ e Å^{-3}
361 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
31 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.0000	0.0000	0.5000	0.02604 (8)
Cu1	0.5000	0.0000	0.5000	0.02460 (10)
Cu2	0.5000	0.5000	1.0000	0.03268 (11)
N1	0.44406 (17)	0.04440 (17)	0.32615 (17)	0.0221 (4)
N2	0.60608 (19)	0.56353 (19)	0.88835 (18)	0.0282 (4)
O1	0.30942 (15)	−0.02363 (16)	0.48585 (15)	0.0281 (3)
O2	0.11497 (15)	−0.03483 (18)	0.34073 (16)	0.0342 (4)
O3	0.1713 (2)	−0.0467 (2)	−0.13119 (19)	0.0591 (6)
O4	0.30140 (19)	0.1332 (2)	−0.12763 (17)	0.0439 (5)
O5	0.35050 (16)	0.49779 (19)	0.84955 (17)	0.0369 (4)
O6	0.30210 (18)	0.5639 (2)	0.6633 (2)	0.0490 (5)
O7	0.71230 (17)	0.72200 (19)	0.51106 (18)	0.0391 (4)
O8	0.89977 (16)	0.65182 (18)	0.59992 (18)	0.0366 (4)
C1	0.2382 (2)	−0.0169 (2)	0.3746 (2)	0.0239 (4)
C2	0.3115 (2)	0.0180 (2)	0.2780 (2)	0.0227 (4)

C3	0.2475 (2)	0.0220 (2)	0.1505 (2)	0.0269 (5)
H3	0.1557	0.0001	0.1186	0.032*
C4	0.3247 (2)	0.0598 (2)	0.0707 (2)	0.0267 (5)
C5	0.2599 (2)	0.0495 (3)	−0.0752 (2)	0.0327 (5)
C6	0.4603 (2)	0.0970 (2)	0.1247 (2)	0.0262 (5)
H6	0.5124	0.1301	0.0763	0.031*
C7	0.5176 (2)	0.0845 (2)	0.2518 (2)	0.0255 (4)
H7	0.6094	0.1046	0.2858	0.031*
C8	0.7820 (2)	0.6710 (2)	0.5938 (2)	0.0280 (5)
C9	0.7192 (2)	0.6332 (2)	0.6975 (2)	0.0270 (5)
C10	0.7977 (2)	0.6251 (3)	0.8193 (2)	0.0337 (5)
H10	0.8898	0.6421	0.8379	0.040*
C11	0.7380 (2)	0.5914 (3)	0.9128 (2)	0.0340 (5)
H11	0.7913	0.5882	0.9948	0.041*
C12	0.5292 (2)	0.5726 (2)	0.7720 (2)	0.0261 (5)
C13	0.5820 (2)	0.6079 (2)	0.6751 (2)	0.0258 (4)
H13	0.5262	0.6147	0.5958	0.031*
C14	0.3820 (2)	0.5433 (2)	0.7580 (2)	0.0305 (5)
O1W	0.14804 (16)	0.17674 (17)	0.64065 (16)	0.0324 (4)
H1A	0.202 (2)	0.205 (3)	0.590 (2)	0.039*
H1B	0.201 (2)	0.159 (3)	0.7184 (16)	0.039*
O2W	0.08911 (16)	−0.15033 (17)	0.60774 (17)	0.0323 (4)
H2A	0.121 (2)	−0.102 (2)	0.6985 (13)	0.039*
H2B	0.023 (2)	−0.2214 (18)	0.603 (2)	0.039*
O3W	0.46396 (19)	−0.24026 (19)	0.37308 (18)	0.0397 (4)
H3A	0.3913 (16)	−0.275 (3)	0.399 (3)	0.048*
H3B	0.5449 (13)	−0.261 (3)	0.419 (3)	0.048*
O4W	0.4544 (2)	0.7280 (2)	1.10086 (19)	0.0445 (4)
H4A	0.447 (3)	0.731 (3)	1.1887 (15)	0.053*
H4B	0.5379 (17)	0.775 (3)	1.106 (3)	0.053*
O5W	0.1659 (2)	−0.2927 (2)	−0.0551 (2)	0.0585 (6)
H5A	0.2575 (14)	−0.294 (3)	−0.016 (3)	0.070*
H5B	0.158 (3)	−0.213 (2)	−0.084 (3)	0.070*
O6W	0.2430 (2)	0.6784 (2)	0.4538 (2)	0.0459 (5)
H6A	0.260 (3)	0.632 (2)	0.522 (2)	0.055*
H6B	0.210 (3)	0.7573 (18)	0.488 (3)	0.055*
O7W	0.0227 (3)	−0.2976 (3)	0.1422 (3)	0.0668 (7)
H7A	0.033 (3)	−0.2138 (19)	0.202 (3)	0.080*
H7B	0.083 (3)	−0.297 (3)	0.088 (3)	0.080*
N3	1.0503 (2)	0.4588 (2)	0.6944 (3)	0.0482 (6)
H31	1.020 (2)	0.406 (2)	0.749 (2)	0.058*
H32	0.9847 (18)	0.5165 (19)	0.666 (2)	0.058*
H33	1.1357 (14)	0.5156 (19)	0.745 (2)	0.058*
H34	1.065 (2)	0.4011 (19)	0.6132 (15)	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Cd1	0.02452 (13)	0.03503 (14)	0.02213 (13)	0.00417 (9)	0.00922 (9)	0.01115 (9)
Cu1	0.02026 (19)	0.0393 (2)	0.01908 (19)	0.00659 (15)	0.00640 (15)	0.01509 (16)
Cu2	0.0253 (2)	0.0519 (3)	0.0262 (2)	−0.00001 (18)	0.00792 (17)	0.02147 (19)
N1	0.0217 (9)	0.0281 (9)	0.0180 (8)	0.0046 (7)	0.0060 (7)	0.0077 (7)
N2	0.0284 (10)	0.0354 (10)	0.0239 (9)	0.0021 (8)	0.0081 (8)	0.0132 (8)
O1	0.0248 (8)	0.0418 (9)	0.0230 (8)	0.0056 (7)	0.0091 (6)	0.0158 (7)
O2	0.0214 (8)	0.0579 (11)	0.0241 (8)	0.0019 (7)	0.0082 (7)	0.0113 (8)
O3	0.0686 (15)	0.0667 (14)	0.0275 (10)	−0.0263 (12)	−0.0090 (10)	0.0183 (9)
O4	0.0468 (11)	0.0582 (12)	0.0280 (9)	−0.0027 (9)	0.0038 (8)	0.0235 (9)
O5	0.0264 (9)	0.0565 (11)	0.0323 (9)	−0.0003 (8)	0.0089 (7)	0.0214 (8)
O6	0.0295 (9)	0.0816 (15)	0.0422 (11)	0.0023 (9)	0.0037 (8)	0.0367 (11)
O7	0.0360 (9)	0.0528 (11)	0.0423 (10)	0.0131 (8)	0.0178 (8)	0.0298 (9)
O8	0.0295 (9)	0.0450 (10)	0.0460 (10)	0.0076 (7)	0.0177 (8)	0.0241 (8)
C1	0.0238 (11)	0.0291 (11)	0.0201 (10)	0.0040 (8)	0.0076 (8)	0.0068 (8)
C2	0.0219 (10)	0.0292 (11)	0.0199 (10)	0.0055 (8)	0.0077 (8)	0.0087 (8)
C3	0.0220 (11)	0.0375 (12)	0.0216 (11)	0.0040 (9)	0.0047 (9)	0.0096 (9)
C4	0.0305 (12)	0.0319 (12)	0.0191 (10)	0.0054 (9)	0.0063 (9)	0.0089 (9)
C5	0.0345 (13)	0.0440 (14)	0.0214 (11)	0.0053 (11)	0.0069 (10)	0.0124 (10)
C6	0.0290 (11)	0.0314 (11)	0.0213 (10)	0.0021 (9)	0.0110 (9)	0.0092 (9)
C7	0.0231 (11)	0.0322 (12)	0.0236 (11)	0.0030 (9)	0.0088 (9)	0.0095 (9)
C8	0.0308 (12)	0.0278 (11)	0.0310 (12)	0.0035 (9)	0.0139 (10)	0.0129 (9)
C9	0.0305 (12)	0.0263 (11)	0.0285 (11)	0.0041 (9)	0.0127 (9)	0.0104 (9)
C10	0.0257 (12)	0.0453 (14)	0.0328 (12)	0.0026 (10)	0.0090 (10)	0.0149 (11)
C11	0.0263 (12)	0.0498 (15)	0.0291 (12)	0.0031 (10)	0.0058 (10)	0.0190 (11)
C12	0.0277 (11)	0.0267 (11)	0.0263 (11)	0.0037 (9)	0.0092 (9)	0.0091 (9)
C13	0.0280 (11)	0.0299 (11)	0.0223 (10)	0.0035 (9)	0.0085 (9)	0.0104 (9)
C14	0.0280 (12)	0.0377 (13)	0.0274 (12)	0.0017 (10)	0.0076 (10)	0.0123 (10)
O1W	0.0271 (8)	0.0448 (10)	0.0260 (8)	−0.0001 (7)	0.0065 (7)	0.0126 (7)
O2W	0.0289 (9)	0.0393 (9)	0.0310 (9)	0.0019 (7)	0.0074 (7)	0.0150 (7)
O3W	0.0398 (10)	0.0460 (11)	0.0390 (10)	0.0101 (8)	0.0139 (8)	0.0168 (8)
O4W	0.0488 (12)	0.0475 (11)	0.0367 (10)	−0.0018 (9)	0.0118 (9)	0.0120 (9)
O5W	0.0555 (13)	0.0568 (13)	0.0681 (15)	0.0083 (11)	0.0205 (12)	0.0208 (11)
O6W	0.0532 (12)	0.0450 (11)	0.0466 (11)	0.0098 (9)	0.0174 (9)	0.0205 (9)
O7W	0.0744 (17)	0.0650 (15)	0.0564 (15)	−0.0103 (13)	0.0218 (13)	0.0085 (12)
N3	0.0302 (12)	0.0545 (15)	0.0682 (17)	0.0102 (10)	0.0157 (11)	0.0277 (13)

Geometric parameters (Å, °)

Cd1—O2	2.2850 (16)	C3—H3	0.9300
Cd1—O2^{i}	2.2850 (16)	C4—C6	1.384 (3)
Cd1—O1W	2.3004 (17)	C4—C5	1.521 (3)
Cd1—O2W^{i}	2.2915 (17)	C6—C7	1.389 (3)
Cd1—O2W	2.2915 (17)	C6—H6	0.9300
Cd1—O1W^{i}	2.3004 (17)	C7—H7	0.9300
Cu1—O1^{ii}	1.9523 (15)	C8—C9	1.519 (3)
Cu1—O1	1.9523 (15)	C9—C13	1.390 (3)
Cu1—N1	1.9819 (17)	C9—C10	1.389 (3)
Cu1—N1^{ii}	1.9819 (17)	C10—C11	1.386 (3)

Cu1—O3W^{ii}	2.539 (2)	C10—H10	0.9300
Cu1—O3W	2.539 (2)	C11—H11	0.9300
Cu2—O5	1.9553 (17)	C12—C13	1.385 (3)
Cu2—O5^{iii}	1.9553 (17)	C12—C14	1.509 (3)
Cu2—N2	1.9862 (18)	C13—H13	0.9300
Cu2—N2^{iii}	1.9862 (18)	O1W—H1A	0.94 (2)
Cu2—O4W^{iii}	2.535 (2)	O1W—H1B	0.95 (2)
Cu2—O4W	2.535 (2)	O2W—H2A	0.95 (1)
N1—C7	1.334 (3)	O2W—H2B	0.95 (1)
N1—C2	1.342 (3)	O3W—H3A	0.94 (1)
N2—C11	1.336 (3)	O3W—H3B	0.94 (1)
N2—C12	1.340 (3)	O4W—H4A	0.95 (1)
O1—C1	1.266 (3)	O4W—H4B	0.95 (1)
O2—C1	1.239 (3)	O5W—H5A	0.95 (1)
O3—C5	1.246 (3)	O5W—H5B	0.96 (1)
O4—C5	1.244 (3)	O6W—H6A	0.95 (1)
O5—C14	1.275 (3)	O6W—H6B	0.96 (3)
O6—C14	1.224 (3)	O7W—H7A	0.95 (3)
O7—C8	1.255 (3)	O7W—H7B	0.95 (3)
O8—C8	1.253 (3)	N3—H31	0.98 (2)
C1—C2	1.509 (3)	N3—H32	0.99 (2)
C2—C3	1.379 (3)	N3—H33	0.99 (1)
C3—C4	1.397 (3)	N3—H34	0.99 (2)
O2—Cd1—O2^{i}	180.00 (6)	N1—C2—C3	122.80 (19)
O2—Cd1—O2W^{i}	84.25 (6)	N1—C2—C1	114.40 (18)
O2^{i}—Cd1—O2W^{i}	95.75 (6)	C3—C2—C1	122.80 (19)
O2—Cd1—O2W	95.75 (6)	C2—C3—C4	118.1 (2)
O2^{i}—Cd1—O2W	84.25 (6)	C2—C3—H3	121.0
O2W^{i}—Cd1—O2W	180.0	C4—C3—H3	121.0
O2—Cd1—O1W	95.40 (6)	C6—C4—C3	118.78 (19)
O2^{i}—Cd1—O1W	84.60 (6)	C6—C4—C5	121.7 (2)
O2W^{i}—Cd1—O1W	85.58 (6)	C3—C4—C5	119.4 (2)
O2W—Cd1—O1W	94.42 (6)	O4—C5—O3	126.5 (2)
O2—Cd1—O1W^{i}	84.60 (6)	O4—C5—C4	118.3 (2)
O2^{i}—Cd1—O1W^{i}	95.40 (6)	O3—C5—C4	115.1 (2)
O2W^{i}—Cd1—O1W^{i}	94.43 (6)	C4—C6—C7	119.3 (2)
O2W—Cd1—O1W^{i}	85.57 (6)	C4—C6—H6	120.3
O1W—Cd1—O1W^{i}	179.999 (1)	C7—C6—H6	120.3
O1^{ii}—Cu1—O1	180.0	N1—C7—C6	121.5 (2)
O1^{ii}—Cu1—N1	96.26 (7)	N1—C7—H7	119.2
O1—Cu1—N1	83.74 (7)	C6—C7—H7	119.2
O1^{ii}—Cu1—N1^{ii}	83.74 (7)	O8—C8—O7	125.5 (2)
O1—Cu1—N1^{ii}	96.26 (7)	O8—C8—C9	117.5 (2)
N1—Cu1—N1^{ii}	180.0	O7—C8—C9	117.0 (2)

O1^{ii}—Cu1—O3W^{ii}	85.99 (6)	C13—C9—C10	117.8 (2)
O1—Cu1—O3W^{ii}	94.01 (6)	C13—C9—C8	121.3 (2)
N1—Cu1—O3W^{ii}	92.15 (7)	C10—C9—C8	120.8 (2)
N1^{ii}—Cu1—O3W^{ii}	87.85 (7)	C11—C10—C9	119.8 (2)
O1^{ii}—Cu1—O3W	94.01 (6)	C11—C10—H10	120.1
O1—Cu1—O3W	85.99 (6)	C9—C10—H10	120.1
N1—Cu1—O3W	87.85 (7)	N2—C11—C10	121.8 (2)
N1^{ii}—Cu1—O3W	92.15 (7)	N2—C11—H11	119.1
O3W^{ii}—Cu1—O3W	180.00 (4)	C10—C11—H11	119.1
O5—Cu2—O5^{iii}	180.0	N2—C12—C13	122.2 (2)
O5—Cu2—N2	83.06 (7)	N2—C12—C14	114.18 (19)
O5^{iii}—Cu2—N2	96.94 (7)	C13—C12—C14	123.7 (2)
O5—Cu2—N2^{iii}	96.95 (7)	C12—C13—C9	119.4 (2)
O5^{iii}—Cu2—N2^{iii}	83.05 (7)	C12—C13—H13	120.3
N2—Cu2—N2^{iii}	179.998 (1)	C9—C13—H13	120.3
O5—Cu2—O4W^{iii}	94.09 (7)	O6—C14—O5	124.6 (2)
O5^{iii}—Cu2—O4W^{iii}	85.91 (7)	O6—C14—C12	119.9 (2)
N2—Cu2—O4W^{iii}	86.13 (7)	O5—C14—C12	115.49 (19)
N2^{iii}—Cu2—O4W^{iii}	93.87 (7)	Cd1—O1W—H1A	106.3 (16)
O5—Cu2—O4W	85.91 (7)	Cd1—O1W—H1B	114.8 (16)
O5^{iii}—Cu2—O4W	94.09 (7)	H1A—O1W—H1B	110 (1)
N2—Cu2—O4W	93.87 (7)	Cd1—O2W—H2A	104.0 (16)
N2^{iii}—Cu2—O4W	86.13 (7)	Cd1—O2W—H2B	112.0 (16)
O4W^{iii}—Cu2—O4W	180.0	H2A—O2W—H2B	108 (1)
C7—N1—C2	119.16 (18)	H3A—O3W—H3B	112 (1)
C7—N1—Cu1	129.85 (15)	H4A—O4W—H4B	109 (3)
C2—N1—Cu1	110.76 (13)	H5A—O5W—H5B	108 (3)
C11—N2—C12	119.09 (19)	H6A—O6W—H6B	108 (1)
C11—N2—Cu2	128.85 (15)	H7A—O7W—H7B	110 (3)
C12—N2—Cu2	112.00 (15)	H31—N3—H32	112 (1)
C1—O1—Cu1	113.79 (13)	H31—N3—H33	110 (1)
C1—O2—Cd1	119.57 (14)	H32—N3—H33	108 (1)
C14—O5—Cu2	114.67 (15)	H31—N3—H34	111 (1)
O2—C1—O1	125.21 (19)	H32—N3—H34	108 (1)
O2—C1—C2	118.48 (18)	H33—N3—H34	108 (1)
O1—C1—C2	116.30 (18)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1A···O7^{iv}	0.94 (2)	1.80 (1)	2.739 (2)	171 (2)
O1W—H1B···O4^{v}	0.95 (2)	1.82 (1)	2.769 (2)	177 (3)
O2W—H2A···O3^{v}	0.95 (1)	1.72 (1)	2.657 (3)	168 (2)

O2W—H2B···O8^{vi}	0.95 (1)	1.77 (1)	2.722 (2)	177 (2)
O3W—H3A···O6W^{vii}	0.94 (1)	1.84 (1)	2.781 (3)	172 (3)
O3W—H3B···O7^{vii}	0.94 (1)	1.84 (1)	2.776 (3)	172 (3)
O4W—H4A···O3W^{viii}	0.95 (1)	1.89 (1)	2.827 (3)	169 (2)
O4W—H4B···O4^{iv}	0.95 (1)	1.80 (1)	2.752 (3)	176 (2)
O5W—H5A···O4W^{ix}	0.95 (1)	2.10 (1)	3.048 (3)	170 (3)
O5W—H5B···O3	0.96 (1)	1.93 (1)	2.882 (3)	171 (3)
O6W—H6A···O6	0.95 (1)	1.79 (1)	2.742 (3)	173 (3)
O6W—H6B···O2W^{x}	0.96 (3)	2.14 (2)	2.991 (3)	147 (2)
O7W—H7A···O2	0.95 (3)	2.09 (3)	3.009 (3)	163 (3)
O7W—H7B···O5W	0.95 (3)	1.93 (3)	2.861 (3)	165 (4)
N3—H31···O7W^{ii}	0.98 (2)	1.90 (2)	2.867 (3)	174 (2)
N3—H32···O8	0.99 (2)	1.92 (1)	2.886 (3)	164 (2)
N3—H33···O5W^{xi}	0.99 (1)	2.53 (2)	3.208 (4)	126 (2)
N3—H33···O5^{xii}	0.99 (1)	2.30 (2)	3.131 (3)	140 (2)
N3—H33···O6^{xii}	0.99 (1)	2.19 (2)	2.888 (3)	126 (2)
N3—H34···O8^{xiii}	0.99 (2)	2.34 (1)	3.277 (3)	157 (2)

Symmetry codes: (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*, *y*, *z*+1; (vi) *x*−1, *y*−1, *z*; (vii) *x*, *y*−1, *z*; (viii) *x*, *y*+1, *z*+1; (ix) *x*, *y*−1, *z*−1; (x) *x*, *y*+1, *z*; (ii) −*x*+1, −*y*, −*z*+1; (xi) *x*+1, *y*+1, *z*+1; (xii) *x*+1, *y*, *z*; (xiii) −*x*+2, −*y*+1, −*z*+1.

Fig. 1

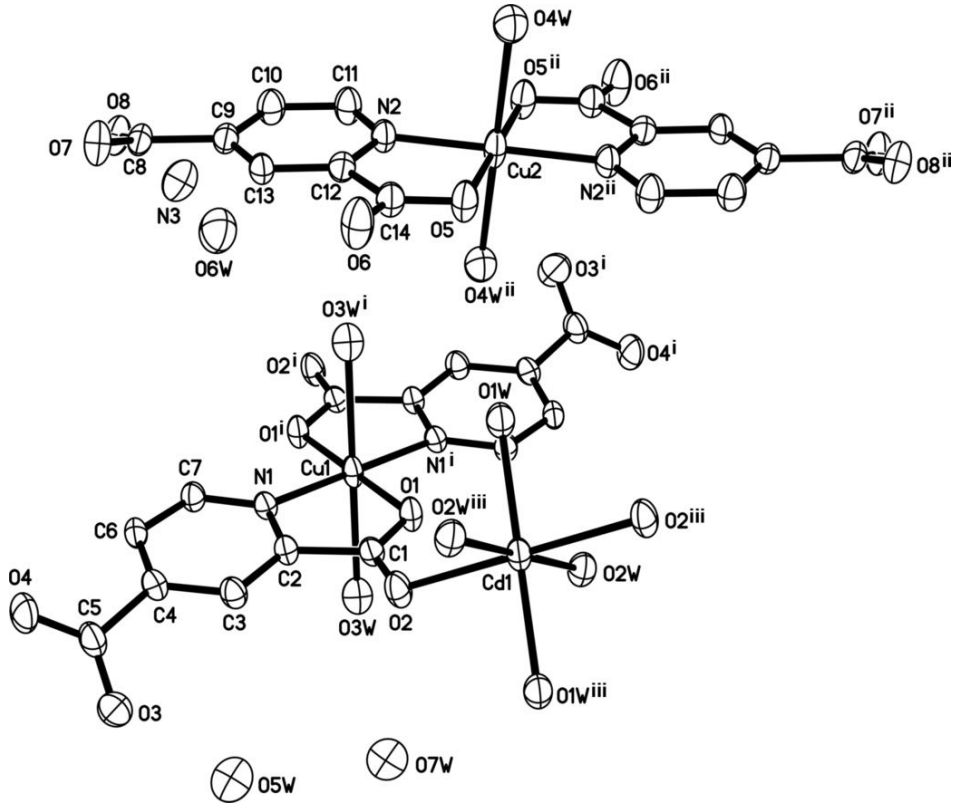
O4W
O5ii
O6ii
C10
C11
O8
C9
N2
O7ii
O7
C8
Cu2
O8ii
N2ii
N3
C13
C12
C14
O5
O6W
O6
O4Wii
O3i
O3Wi
O4i
O2i
O1W
O1i
N1i
C7
N1
Cu1
O1
O2Wiii
O2iii
C6
C1
O2W
C2
Cd1
O4
C5
C4
C3
O3W
O2
O1Wiii
O3
O5W
O7W

Fig. 2

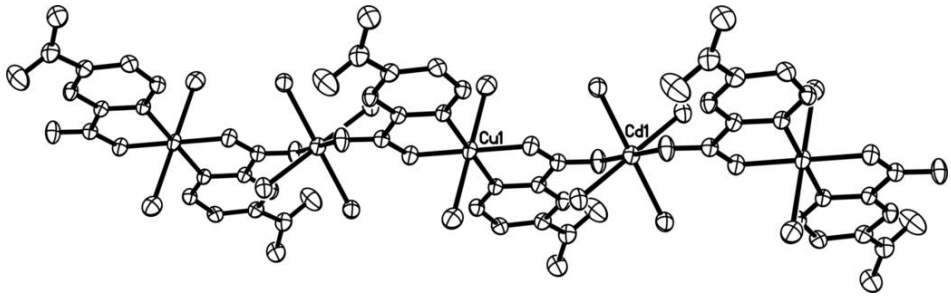
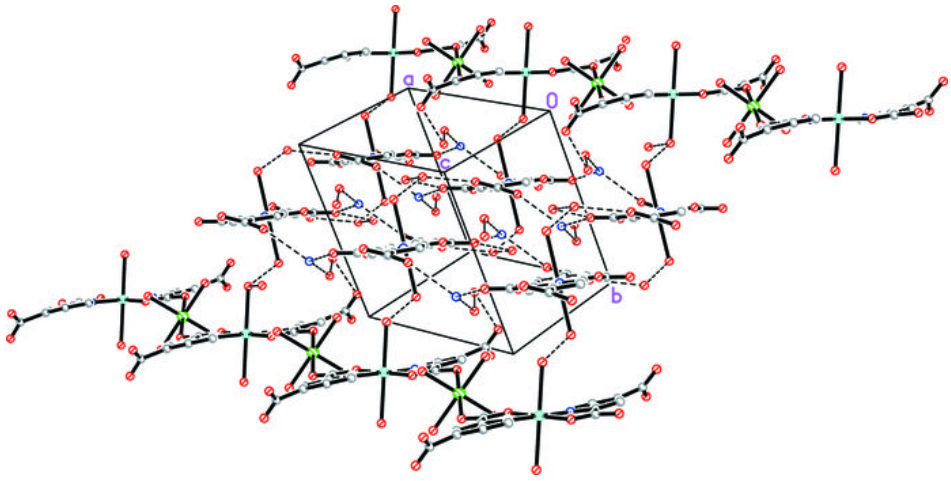
Fig. 3