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catena-Poly[[[bis(2-methyl-1*H*-imidazole)copper(II)]-μ-1,4-cyclohexanedicarboxylato-κ^2O,O'] monohydrate]

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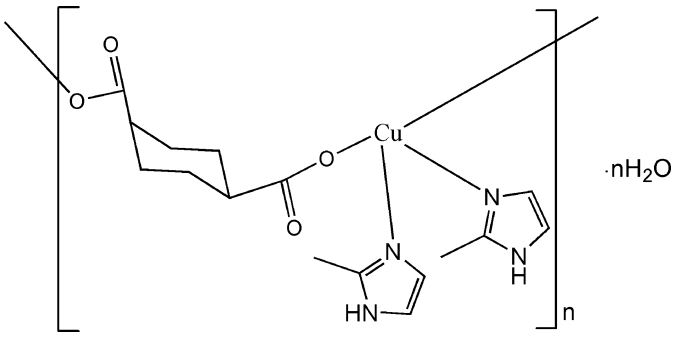
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.059; data-to-parameter ratio = 15.7.

In the title compound, $\{[Cu(1,4\text{-chdc})(L)_2]\cdot H_2O\}_n$, where 1,4-chdc is the 1,4-cyclohexanedicarboxylate dianion, $C_8H_{10}O_4^{2-}$, and L is 2-methyl-1*H*-imidazole, $C_4H_6N_2$, each Cu^{II} atom is four-coordinated by two N atoms from two L ligands and two O atoms from two 1,4-chdc anions in a distorted tetrahedral geometry. Each 1,4-chdc ligand bridges two neighbouring Cu^{II} atoms in a bidentate mode, forming a unique helical chain. These chains are decorated with L ligands alternately on the two sides. O—H···O and N—H···O hydrogen bonds complete the structure.

Related literature

The related compound, $[Zn(1,4\text{-chdc})(phen)(H_2O)]_n$ (phen is 1,10-phenanthroline), also has a chain structure. The central Zn^{II} cation is coordinated by four water and carboxylate O atoms and two N atoms from the phen ligand. Each 1,4-chdc ligand links two Zn^{II} cations in chelating and monodentate modes, forming an infinite helical chain-like structure with 2_1 helices (Bi *et al.*, 2004).

For related literature, see: Li *et al.* (2002).



Experimental

Crystal data

$[Cu(C_8H_{10}O_4)(C_4H_6N_2)_2]\cdot H_2O$
M_r = 415.93
Monoclinic, *Cc*
a = 13.179 (3) Å
b = 11.897 (2) Å
c = 12.314 (3) Å
β = 96.03 (3)°
V = 1920.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 293 (2) K
0.28 × 0.27 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.713, T_{max} = 0.758
9070 measured reflections
3853 independent reflections
3592 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.059
S = 1.09
3853 reflections
245 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1655 Friedel pairs
Flack parameter: 0.011 (10)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.9692 (17)	Cu1—O2	1.9951 (16)
Cu1—N3	1.9976 (18)	Cu1—O3^{i}	1.9627 (14)
O3^{i}—Cu1—N1	155.96 (6)	O3^{i}—Cu1—N3	93.83 (7)
O3^{i}—Cu1—O2	87.82 (7)	N1—Cu1—N3	94.84 (7)
N1—Cu1—O2	90.97 (8)	O2—Cu1—N3	161.53 (7)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—HW11···O4	0.807 (16)	1.989 (16)	2.794 (2)	174 (2)
O1W—HW12···O3^{ii}	0.822 (16)	2.115 (17)	2.921 (2)	167 (2)
N2—H2···O1W^{ii}	0.86	1.88	2.734 (2)	170
N4—H4···O1W^{iii}	0.86	2.01	2.861 (2)	172

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2052).

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supplementary materials

Acta Cryst. (2007). E**63**, m1748-m1749 [**doi:10.1107/S1600536807023628**]

catena-Poly[[[bis(2-methyl-1*H*-imidazole)copper(II)]-μ-1,4-cyclohexanedicarboxylato-κ^2O,O'] monohydrate]

G. De

Comment

Rigid spacer ligands such as benzenedi- and tri-carboxylates have successfully produced various extended structures with metal cations (Li *et al.*, 2002). However, the studies on the structures composed of flexible carboxylate ligands still remains undeveloped probably because the low symmetry and the flexibility of the ligand make it difficult to control the final structure. We selected 1,4-cyclohexanedicarboxylic acid (1,4-chdcH_2) as a bridging ligand and 2-methyl-1*H*-imidazole (*L*) as a secondary ligand, generating a new helical chain coordination polymer, [Cu(1,4-chdc)(*L*)$_2$]·H_2O, (I), which is reported here.

Selected bond lengths and angles for (I) are given in Table 1. In compound (I), each Cu(II) atom is four-coordinated by two N atoms from two *L* ligands, and two O atoms from two 1,4-chdc molecules in a distorted tetrahedral geometry (Fig. 1). The Cu1—O2 and Cu1—O3^i distances are 1.9951 (16) and 1.9627 (14) Å, respectively (Table 1). The Cu1—N1 and Cu1—N3 distances are 1.9692 (17) and 1.9976 (18) Å, respectively (Table 1). Each 1,4-chdc ligand bridges two neighboring Cu(II) atoms in a bidentate mode, forming a unique helical chain (Fig. 2). These chains are decorated with *L* ligands alternately at two sides. In addition, the O—H···O and N—H···O hydrogen bonds complete structure of (I) (Table 2).

Experimental

A mixture of $CuCl_2$·$2H_2O$ (0.5 mmol), 1,4-chdc acid (0.5 mmol), and *L* (0.5 mmol) was adjusted to pH=6 by addition of aqueous NaOH solution. The resulting solution was filtered, the filtrate was allowed to stand in air at room temperature for two weeks, and the blue crystals of (I) were obtained (yield 31% based on Cu).

Refinement

All H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93–0.98 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

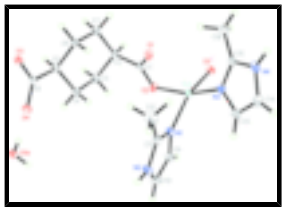

Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) $x - 1/2, y + 1/2, z$.

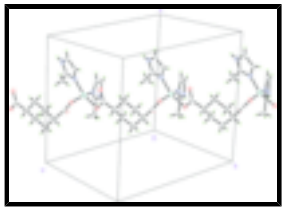

Fig. 2. View of the chain structure in (I).

catena-Poly[[[bis(2-methyl-1_H_-imidazole)copper(II)] -μ-1,4-cyclohexanedicarboxylato-κ^2_O_,_O_'] monohydrate]

Crystal data

$[Cu(C_8H_{10}O_4)(C_4H_6N_2)_2]\cdot H_2O$	F_{000} = 868
M_r = 415.93	D_x = 1.439 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 8581 reflections
a = 13.179 (3) Å	θ = 3.2–27.5º
b = 11.897 (2) Å	μ = 1.17 mm^{-1}
c = 12.314 (3) Å	*T* = 293 (2) K
β = 96.03 (3)º	Block, blue
V = 1920.1 (7) Å^3	0.28 × 0.27 × 0.24 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	3853 independent reflections
Radiation source: rotating anode	3592 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.1º
ω scan	*h* = −17→17
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*k* = −15→15
T_{min} = 0.713, T_{max} = 0.758	*l* = −15→15
9070 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.024	$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 0.0676P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.059	$(\Delta/\sigma)_{max} < 0.001$
S = 1.09	$\Delta\rho_{max}$ = 0.22 e Å^{-3}

3853 reflections	$\Delta\rho_{min} = -0.21$ e Å^{-3}
245 parameters	Extinction correction: none
5 restraints	Absolute structure: Flack (1983), 1655 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.011 (10)
Secondary atom site location: difference Fourier map	

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	0.19772 (16)	0.23174 (15)	0.28646 (19)	0.0282 (4)
C2	0.30024 (17)	0.25386 (14)	0.2433 (2)	0.0329 (5)
H2A	0.2942	0.3261	0.2050	0.039*
C3	0.38580 (18)	0.26687 (17)	0.3369 (2)	0.0396 (5)
H3A	0.3637	0.3182	0.3909	0.047*
H3B	0.4453	0.2993	0.3086	0.047*
C4	0.41519 (17)	0.15402 (17)	0.39159 (18)	0.0373 (5)
H4A	0.4715	0.1651	0.4479	0.045*
H4B	0.3578	0.1247	0.4260	0.045*
C5	0.44610 (15)	0.06954 (15)	0.30770 (16)	0.0278 (4)
H5	0.5051	0.1011	0.2762	0.033*
C6	0.36148 (17)	0.05469 (16)	0.21444 (17)	0.0326 (4)
H6A	0.3029	0.0197	0.2422	0.039*
H6B	0.3850	0.0052	0.1598	0.039*
C7	0.32944 (18)	0.16732 (18)	0.16160 (17)	0.0370 (5)
H7A	0.3853	0.1966	0.1246	0.044*
H7B	0.2718	0.1552	0.1071	0.044*
C8	0.47826 (14)	−0.04401 (15)	0.35574 (16)	0.0281 (4)
C9	0.10618 (19)	0.22595 (19)	0.6122 (2)	0.0377 (5)
H9	0.1056	0.3037	0.6201	0.045*
C10	0.1344 (2)	0.1525 (2)	0.69177 (18)	0.0445 (6)
H10	0.1569	0.1691	0.7641	0.053*
C11	0.09062 (17)	0.06032 (17)	0.54026 (17)	0.0346 (4)
C12	0.0745 (3)	−0.0340 (2)	0.4619 (2)	0.0602 (8)
H12A	0.0586	−0.1010	0.5002	0.090*
H12B	0.1354	−0.0458	0.4270	0.090*
H12C	0.0190	−0.0162	0.4078	0.090*

C13	−0.15859 (19)	0.1245 (2)	0.43684 (19)	0.0414 (5)
H13	−0.1426	0.1338	0.5117	0.050*
C14	−0.23970 (19)	0.0679 (2)	0.3894 (2)	0.0466 (6)
H14	−0.2896	0.0317	0.4246	0.056*
C15	−0.15176 (16)	0.13368 (17)	0.26216 (17)	0.0337 (4)
C16	−0.1217 (2)	0.1605 (3)	0.15148 (18)	0.0561 (7)
H16A	−0.1682	0.1248	0.0969	0.084*
H16B	−0.0538	0.1336	0.1459	0.084*
H16C	−0.1238	0.2404	0.1405	0.084*
N1	0.07791 (14)	0.16816 (14)	0.51644 (14)	0.0318 (4)
N2	0.12344 (16)	0.04764 (15)	0.64560 (15)	0.0392 (4)
H2	0.1356	−0.0153	0.6788	0.047*
N3	−0.10236 (13)	0.16677 (14)	0.35673 (14)	0.0316 (4)
N4	−0.23445 (14)	0.07396 (16)	0.28022 (16)	0.0395 (4)
H4	−0.2772	0.0444	0.2308	0.047*
O1	0.13847 (12)	0.15720 (12)	0.24666 (14)	0.0410 (4)
O2	0.17380 (11)	0.29511 (12)	0.36217 (13)	0.0352 (3)
O1W	0.61751 (13)	0.03906 (15)	0.63232 (14)	0.0424 (4)
O3	0.48379 (11)	−0.12457 (11)	0.28814 (11)	0.0329 (3)
O4	0.49861 (13)	−0.05853 (13)	0.45594 (12)	0.0434 (4)
Cu1	0.03143 (3)	0.246810 (16)	0.37949 (3)	0.02601 (6)
HW11	0.5812 (18)	0.015 (2)	0.5807 (15)	0.034 (6)*
HW12	0.5816 (18)	0.0736 (19)	0.6717 (17)	0.038 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0256 (10)	0.0215 (8)	0.0373 (11)	0.0054 (7)	0.0011 (8)	0.0044 (8)
C2	0.0296 (11)	0.0242 (9)	0.0456 (12)	0.0057 (7)	0.0081 (9)	0.0061 (8)
C3	0.0290 (11)	0.0260 (9)	0.0640 (16)	−0.0004 (8)	0.0063 (10)	−0.0086 (10)
C4	0.0340 (12)	0.0330 (10)	0.0428 (12)	0.0073 (8)	−0.0061 (9)	−0.0122 (9)
C5	0.0235 (10)	0.0260 (8)	0.0335 (10)	0.0018 (7)	0.0009 (8)	−0.0001 (8)
C6	0.0350 (11)	0.0295 (9)	0.0321 (10)	0.0095 (8)	−0.0021 (8)	−0.0033 (8)
C7	0.0375 (12)	0.0393 (11)	0.0344 (10)	0.0117 (9)	0.0052 (9)	0.0064 (9)
C8	0.0213 (10)	0.0298 (9)	0.0323 (10)	0.0017 (7)	−0.0013 (8)	0.0020 (8)
C9	0.0404 (13)	0.0341 (9)	0.0370 (12)	−0.0006 (9)	−0.0032 (9)	−0.0015 (9)
C10	0.0533 (15)	0.0444 (12)	0.0335 (11)	0.0018 (10)	−0.0062 (10)	0.0007 (10)
C11	0.0345 (12)	0.0303 (10)	0.0377 (11)	−0.0027 (8)	−0.0016 (9)	0.0052 (9)
C12	0.087 (2)	0.0346 (12)	0.0555 (16)	−0.0004 (13)	−0.0105 (15)	−0.0039 (12)
C13	0.0446 (14)	0.0477 (12)	0.0329 (10)	−0.0109 (10)	0.0085 (9)	0.0005 (10)
C14	0.0381 (13)	0.0501 (13)	0.0522 (14)	−0.0147 (10)	0.0077 (11)	0.0042 (12)
C15	0.0295 (11)	0.0382 (10)	0.0323 (10)	0.0006 (8)	−0.0028 (8)	−0.0032 (9)
C16	0.0512 (16)	0.086 (2)	0.0310 (11)	−0.0052 (14)	0.0015 (11)	−0.0031 (13)
N1	0.0335 (9)	0.0281 (8)	0.0325 (8)	−0.0024 (7)	−0.0029 (7)	0.0039 (7)
N2	0.0431 (11)	0.0339 (9)	0.0389 (10)	0.0014 (8)	−0.0041 (8)	0.0122 (8)
N3	0.0285 (9)	0.0347 (8)	0.0311 (9)	−0.0054 (7)	0.0004 (7)	0.0009 (7)
N4	0.0316 (10)	0.0413 (9)	0.0435 (10)	−0.0056 (7)	−0.0062 (8)	−0.0044 (9)
O1	0.0329 (8)	0.0346 (7)	0.0563 (10)	−0.0038 (6)	0.0080 (7)	−0.0166 (7)

O2	0.0315 (8)	0.0306 (7)	0.0444 (9)	−0.0022 (6)	0.0088 (6)	−0.0087 (7)
O1W	0.0373 (9)	0.0517 (9)	0.0370 (9)	0.0068 (8)	−0.0016 (7)	−0.0061 (8)
O3	0.0413 (9)	0.0244 (6)	0.0320 (7)	0.0060 (6)	−0.0015 (6)	0.0018 (6)
O4	0.0574 (11)	0.0431 (8)	0.0283 (7)	0.0119 (7)	−0.0022 (7)	−0.0007 (7)
Cu1	0.02640 (10)	0.02329 (9)	0.02761 (10)	−0.00107 (9)	−0.00064 (7)	0.00362 (9)

Geometric parameters (Å, °)

C1—O1	1.247 (2)	C10—H10	0.9300
C1—O2	1.264 (3)	C11—N1	1.323 (3)
C1—C2	1.526 (3)	C11—N2	1.332 (3)
C2—C7	1.517 (3)	C11—C12	1.480 (3)
C2—C3	1.533 (4)	C12—H12A	0.9600
C2—H2A	0.9800	C12—H12B	0.9600
C3—C4	1.534 (3)	C12—H12C	0.9600
C3—H3A	0.9700	C13—C14	1.344 (3)
C3—H3B	0.9700	C13—N3	1.389 (3)
C4—C5	1.527 (3)	C13—H13	0.9300
C4—H4A	0.9700	C14—N4	1.356 (3)
C4—H4B	0.9700	C14—H14	0.9300
C5—C8	1.517 (3)	C15—N3	1.333 (3)
C5—C6	1.525 (3)	C15—N4	1.339 (3)
C5—H5	0.9800	C15—C16	1.493 (3)
C6—C7	1.530 (3)	C16—H16A	0.9600
C6—H6A	0.9700	C16—H16B	0.9600
C6—H6B	0.9700	C16—H16C	0.9600
C7—H7A	0.9700	Cu1—N1	1.9692 (17)
C7—H7B	0.9700	N2—H2	0.8600
C8—O4	1.247 (2)	Cu1—N3	1.9976 (18)
C8—O3	1.277 (2)	N4—H4	0.8600
C9—C10	1.336 (3)	Cu1—O2	1.9951 (16)
C9—N1	1.382 (3)	O1W—HW11	0.807 (16)
C9—H9	0.9300	O1W—HW12	0.822 (16)
C10—N2	1.372 (3)	Cu1—O3^{i}	1.9627 (14)
O1—C1—O2	121.3 (2)	N2—C10—H10	126.8
O1—C1—C2	121.78 (19)	N1—C11—N2	110.27 (19)
O2—C1—C2	116.89 (18)	N1—C11—C12	125.7 (2)
C7—C2—C1	114.17 (18)	N2—C11—C12	124.0 (2)
C7—C2—C3	110.44 (18)	C11—C12—H12A	109.5
C1—C2—C3	111.4 (2)	C11—C12—H12B	109.5
C7—C2—H2A	106.8	H12A—C12—H12B	109.5
C1—C2—H2A	106.8	C11—C12—H12C	109.5
C3—C2—H2A	106.8	H12A—C12—H12C	109.5
C2—C3—C4	111.95 (17)	H12B—C12—H12C	109.5
C2—C3—H3A	109.2	C14—C13—N3	109.4 (2)
C4—C3—H3A	109.2	C14—C13—H13	125.3
C2—C3—H3B	109.2	N3—C13—H13	125.3
C4—C3—H3B	109.2	C13—C14—N4	106.5 (2)
H3A—C3—H3B	107.9	C13—C14—H14	126.8

C5—C4—C3	110.6 (2)	N4—C14—H14	126.8
C5—C4—H4A	109.5	N3—C15—N4	110.06 (19)
C3—C4—H4A	109.5	N3—C15—C16	125.6 (2)
C5—C4—H4B	109.5	N4—C15—C16	124.31 (19)
C3—C4—H4B	109.5	C15—C16—H16A	109.5
H4A—C4—H4B	108.1	C15—C16—H16B	109.5
C8—C5—C6	110.05 (15)	H16A—C16—H16B	109.5
C8—C5—C4	113.94 (17)	C15—C16—H16C	109.5
C6—C5—C4	111.09 (16)	H16A—C16—H16C	109.5
C8—C5—H5	107.1	H16B—C16—H16C	109.5
C6—C5—H5	107.1	C11—N1—C9	106.06 (17)
C4—C5—H5	107.1	C11—N1—Cu1	132.18 (14)
C5—C6—C7	111.49 (17)	C9—N1—Cu1	121.75 (14)
C5—C6—H6A	109.3	C11—N2—C10	108.04 (18)
C7—C6—H6A	109.3	C11—N2—H2	126.0
C5—C6—H6B	109.3	C10—N2—H2	126.0
C7—C6—H6B	109.3	C15—N3—C13	105.40 (18)
H6A—C6—H6B	108.0	C15—N3—Cu1	127.33 (15)
C2—C7—C6	112.96 (17)	C13—N3—Cu1	127.01 (14)
C2—C7—H7A	109.0	C15—N4—C14	108.68 (18)
C6—C7—H7A	109.0	C15—N4—H4	125.7
C2—C7—H7B	109.0	C14—N4—H4	125.7
C6—C7—H7B	109.0	C1—O2—Cu1	102.54 (13)
H7A—C7—H7B	107.8	HW11—O1W—HW12	108 (2)
O4—C8—O3	121.34 (17)	C8—O3—Cu1^{ii}	104.38 (12)
O4—C8—C5	122.11 (17)	O3^{i}—Cu1—N1	155.96 (6)
O3—C8—C5	116.55 (16)	O3^{i}—Cu1—O2	87.82 (7)
C10—C9—N1	109.24 (19)	N1—Cu1—O2	90.97 (8)
C10—C9—H9	125.4	O3^{i}—Cu1—N3	93.83 (7)
N1—C9—H9	125.4	N1—Cu1—N3	94.84 (7)
C9—C10—N2	106.37 (19)	O2—Cu1—N3	161.53 (7)
C9—C10—H10	126.8		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—HW11···O4	0.807 (16)	1.989 (16)	2.794 (2)	174 (2)
O1W—HW12···O3^{iii}	0.822 (16)	2.115 (17)	2.921 (2)	167 (2)
N2—H2···O1^{iii}	0.86	1.88	2.734 (2)	170
N4—H4···O1W^{iv}	0.86	2.01	2.861 (2)	172

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

Fig. 1

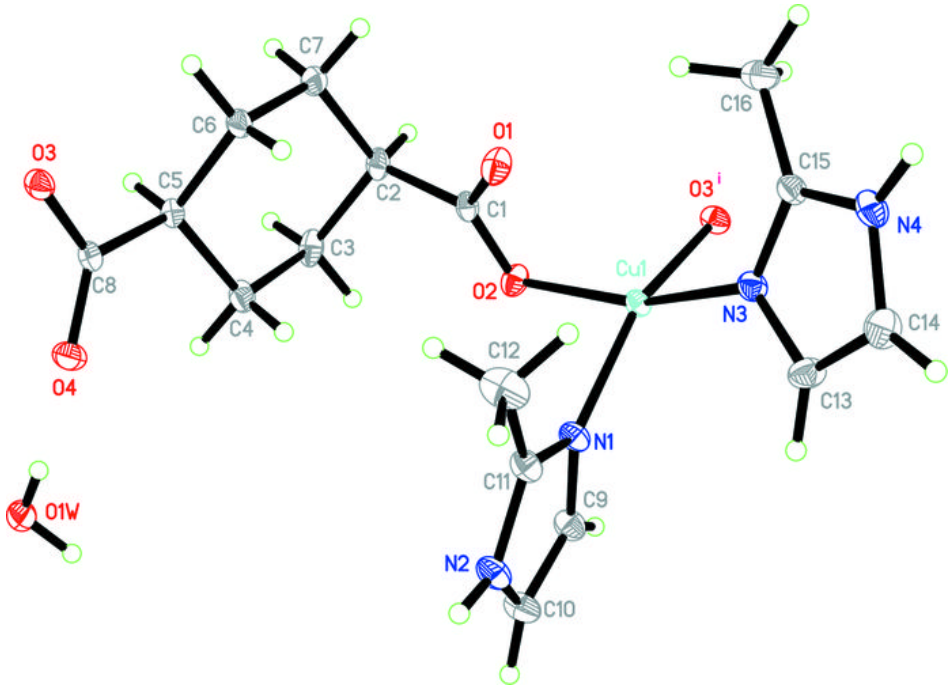
C7
C6
O3
C5
C2
O1
C1
C16
C15
O3 i
N4
C3
C8
O2
Cu1
N3
C14
C4
C12
O4
C13
N1
C11
C9
O1W
N2
C10

Fig. 2