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catena-Poly[[[bis(2-methyl-1*H*-imidazole-κN^3)copper(II)]-μ-biphenyl-2,2′-dicarboxylato-$\kappa^2 O$:O'] dihydrate]

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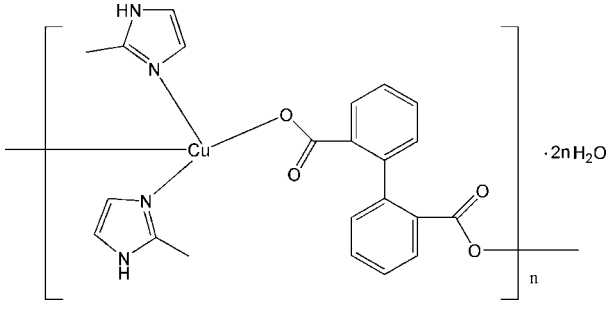
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.101; data-to-parameter ratio = 17.7.

In the title compound, $\{[Cu(C_{14}H_8O_4)(C_4H_6N_2)_2]\cdot 2H_2O\}_n$, each Cu^{II} atom is four-coordinated by two N atoms from two 2-methyl-1*H*-imidazole (mi) ligands and two O atoms from two biphenyl-2,2′-dicarboxylate (dpdc) anions in a distorted square-planar coordination environment. Each dpdc ligand bridges two neighboring Cu^{II} atoms in a bis-monodentate mode, forming a zigzag chain along the *b* axis. These chains are decorated with mi ligands alternately on the two sides. O—H···O and N—H···O hydrogen bonds involving the water molecules link the chains together, forming a supramolecular structure.

Related literature

For related literature, see: Chen & Liu (2002); De (2007); Lehn (1990).



Experimental

Crystal data

$[Cu(C_{14}H_8O_4)(C_4H_6N_2)_2]\cdot 2H_2O$
M_r = 503.99
Monoclinic, $P2_1/n$
a = 8.7554 (18) Å
b = 17.940 (4) Å
c = 16.116 (3) Å
β = 104.65 (3)°
V = 2449.0 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 293 (2) K
0.33 × 0.25 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.731, T_{max} = 0.836
23229 measured reflections
5578 independent reflections
4004 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.101
S = 1.03
5578 reflections
316 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.994 (2)	Cu1—O2	1.9488 (17)
Cu1—N3	1.960 (2)	Cu1—O4^{i}	2.0005 (18)
O2—Cu1—N3	165.28 (8)	O2—Cu1—O4^{i}	89.39 (8)
O2—Cu1—N1	91.99 (9)	N3—Cu1—O4^{i}	90.88 (9)
N3—Cu1—N1	90.72 (9)	N1—Cu1—O4^{i}	168.31 (8)

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—HW12···O2W^{ii}	0.840 (17)	1.94 (2)	2.757 (4)	163 (3)
O1W—HW11···O2W^{iii}	0.837 (17)	2.02 (2)	2.846 (4)	169 (3)
O2W—HW21···O1	0.842 (17)	1.922 (18)	2.761 (3)	174 (4)
O2W—HW22···O3	0.859 (18)	1.884 (18)	2.738 (3)	173 (4)
N2—H2···O4^{iv}	0.86	1.98	2.814 (3)	164
N4—H4A···O1W	0.86	1.90	2.738 (4)	163

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

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 authors thank Jilin Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2473).

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supplementary materials

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catena-Poly[[[bis(2-methyl-1*H*-imidazole-κN^3)copper(II)]-μ-biphenyl-2,2'-dicarboxylato-$\kappa^2 O$:O'] dihydrate]

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Comment

Helical or chain structures have received much attention in coordination chemistry (Chen & Liu, 2002). An appropriate bidentate carboxylate could be useful in the formation of helical chains in the presence of secondary ligands (Lehn, 1990). 2,2'-Diphenyldicarboxylic acid (H_2dpdc) is a benzoic acid-based ligand, where the two phenyl rings can freely twist to meet the requirements of the coordination geometries of metal ions in the assembly process. We selected H_2dpdc as a bridging ligand and 2-methyl-1*H*-imidazole (mi) as a secondary ligand, generating a new zigzag chain coordination polymer, $[Cu(dpdc)(mi)_2]\cdot 2H_2O$, (I), which is reported here.

Selected bond lengths and angles are listed in Table 1. In the title compound, each Cu^{II} atom is four-coordinated by two N atoms from two mi ligands, and two O atoms from two dpdc ligands in a square-planar coordination environment (Fig. 1). The Cu—O distances vary from 1.9488 (17) to 2.0005 (18) Å (Table 1), and the Cu1—N3 and Cu1—N1 distances are 1.960 (2) and 1.994 (2) Å, respectively. Each dpdc ligand bridges two neighboring Cu^{II} atoms in a bis-monodentate mode, forming a zigzag chain along the *b* axis (Fig. 2). The chain is 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, resulting in a supramolecular structure.

Experimental

A mixture of $CuCl_2\cdot 2H_2O$ (0.5 mmol), H_2dpdc (0.5 mmol), mi (0.5 mmol), and H_2O (500 mmol) was adjusted to pH=5.8 by addition of aqueous NaOH solution, and heated at 458 K for 2 d. After the mixture was slowly cooled to room temperature, blue crystals of (I) were obtained (yield 27%).

Refinement

C– and N-bound H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93–0.96 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 The U^{ij} components of atom O1 were approximated to isotropic behaviour.

Figures

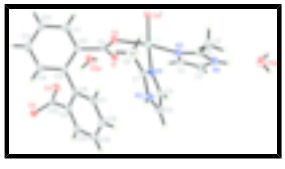

Fig. 1. The structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) 1/2 − *x*, *y* − 1/2, 3/1 − *z*.

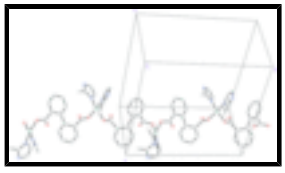

Fig. 2. View of the chain structure in the title compound.

catena-Poly[[[bis(2-methyl-1_H_-imidazole-κN^3)copper(II)]- μ-biphenyl-2,2'-dicarboxylato-κ^2O:O'] dihydrate]

Crystal data

$[Cu(C_{14}H_8O_4)(C_4H_6N_2)_2]\cdot 2H_2O$	F_{000} = 1044
M_r = 503.99	D_x = 1.367 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 17307 reflections
a = 8.7554 (18) Å	θ = 3.0–27.5º
b = 17.940 (4) Å	μ = 0.94 mm^{-1}
c = 16.116 (3) Å	T = 293 (2) K
β = 104.65 (3)º	Block, blue
V = 2449.0 (9) Å^3	0.33 × 0.25 × 0.19 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	5578 independent reflections
Radiation source: rotating anode	4004 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.056
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.0º
ω scans	h = −11→11
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −23→23
T_{min} = 0.731, T_{max} = 0.836	l = −20→20
23229 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
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.101	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 1.0153P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
5578 reflections	$\Delta\rho_{max}$ = 0.47 e Å^{-3}

316 parameters
12 restraints
Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -0.32$ e Å^{-3}
Extinction correction: none

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	−0.0628 (3)	0.14907 (16)	0.89714 (17)	0.0417 (6)
C2	0.0462 (4)	0.09492 (19)	0.9508 (2)	0.0650 (9)
H2A	−0.0049	0.0716	0.9902	0.097*
H2B	0.1394	0.1203	0.9822	0.097*
H2C	0.0748	0.0576	0.9147	0.097*
C3	−0.2843 (4)	0.2071 (2)	0.8369 (2)	0.0628 (9)
H3	−0.3902	0.2207	0.8210	0.075*
C4	−0.1646 (3)	0.23935 (19)	0.81210 (19)	0.0527 (8)
H4	−0.1740	0.2799	0.7752	0.063*
C5	0.1416 (4)	0.29497 (18)	1.00860 (19)	0.0521 (7)
H5	0.0352	0.3051	0.9852	0.063*
C6	0.2215 (4)	0.3096 (2)	1.0897 (2)	0.0588 (8)
H6	0.1819	0.3315	1.1322	0.071*
C7	0.3821 (3)	0.25763 (16)	1.02174 (17)	0.0444 (6)
C8	0.5277 (4)	0.2251 (2)	1.0070 (2)	0.0699 (10)
H8A	0.5976	0.2116	1.0610	0.105*
H8B	0.5784	0.2609	0.9788	0.105*
H8C	0.5017	0.1815	0.9717	0.105*
C9	0.3097 (3)	0.34777 (15)	0.78098 (17)	0.0381 (6)
C10	0.4314 (3)	0.40035 (15)	0.76376 (17)	0.0397 (6)
C11	0.5341 (4)	0.37354 (18)	0.7172 (2)	0.0581 (8)
H11	0.5226	0.3250	0.6964	0.070*
C12	0.6531 (4)	0.4179 (2)	0.7015 (2)	0.0695 (11)
H12	0.7201	0.3994	0.6699	0.083*
C13	0.6715 (4)	0.4893 (2)	0.7328 (2)	0.0679 (10)
H13	0.7528	0.5189	0.7236	0.081*
C14	0.5691 (4)	0.51740 (18)	0.7781 (2)	0.0558 (8)
H14	0.5817	0.5662	0.7981	0.067*
C15	0.4473 (3)	0.47388 (15)	0.79433 (17)	0.0398 (6)

C16	0.3490 (3)	0.50494 (15)	0.84949 (17)	0.0409 (6)
C17	0.3339 (4)	0.46496 (17)	0.92179 (19)	0.0540 (8)
H17	0.3793	0.4179	0.9322	0.065*
C18	0.2531 (5)	0.4938 (2)	0.9781 (2)	0.0700 (10)
H18	0.2425	0.4659	1.0249	0.084*
C19	0.1889 (5)	0.5637 (2)	0.9645 (2)	0.0805 (12)
H19	0.1351	0.5834	1.0024	0.097*
C20	0.2040 (5)	0.60497 (19)	0.8946 (2)	0.0682 (10)
H20	0.1615	0.6527	0.8863	0.082*
C21	0.2815 (3)	0.57618 (15)	0.83676 (17)	0.0429 (6)
C22	0.2822 (3)	0.62358 (15)	0.75948 (18)	0.0414 (6)
N1	0.2424 (3)	0.26251 (13)	0.96545 (14)	0.0411 (5)
N2	0.3718 (3)	0.28605 (15)	1.09724 (15)	0.0528 (6)
H2	0.4479	0.2889	1.1429	0.063*
N3	−0.0259 (2)	0.20308 (13)	0.84973 (13)	0.0394 (5)
N4	−0.2186 (3)	0.15028 (15)	0.89015 (16)	0.0530 (6)
H4A	−0.2689	0.1201	0.9152	0.064*
O1	0.1663 (2)	0.36111 (11)	0.75780 (13)	0.0527 (5)
O2	0.3644 (2)	0.28816 (10)	0.82080 (11)	0.0399 (4)
O1W	−0.3240 (3)	0.03831 (16)	0.9770 (2)	0.0705 (7)
O3	0.2146 (3)	0.60283 (11)	0.68615 (13)	0.0564 (5)
O2W	0.0770 (3)	0.46838 (15)	0.63200 (15)	0.0693 (7)
O4	0.3503 (2)	0.68677 (10)	0.77385 (11)	0.0412 (4)
Cu1	0.18444 (3)	0.234302 (17)	0.841723 (19)	0.03370 (10)
HW11	−0.343 (4)	0.040 (2)	1.0252 (14)	0.092 (15)*
HW12	−0.387 (3)	0.0107 (17)	0.9426 (16)	0.067 (12)*
HW21	0.098 (4)	0.4360 (15)	0.6711 (19)	0.085 (13)*
HW22	0.117 (5)	0.5101 (13)	0.653 (2)	0.104 (16)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0451 (15)	0.0391 (15)	0.0404 (15)	−0.0007 (12)	0.0100 (12)	−0.0022 (12)
C2	0.064 (2)	0.056 (2)	0.074 (2)	0.0047 (17)	0.0160 (18)	0.0243 (18)
C3	0.0450 (17)	0.091 (3)	0.055 (2)	0.0161 (17)	0.0183 (15)	0.0137 (18)
C4	0.0500 (16)	0.065 (2)	0.0435 (16)	0.0158 (15)	0.0132 (13)	0.0115 (15)
C5	0.0534 (17)	0.0579 (19)	0.0472 (18)	0.0024 (15)	0.0166 (14)	−0.0099 (15)
C6	0.065 (2)	0.069 (2)	0.0455 (18)	−0.0003 (17)	0.0192 (16)	−0.0166 (16)
C7	0.0541 (16)	0.0437 (16)	0.0335 (14)	0.0004 (13)	0.0075 (12)	−0.0014 (12)
C8	0.0571 (19)	0.095 (3)	0.052 (2)	0.0228 (19)	0.0043 (16)	−0.0044 (19)
C9	0.0462 (15)	0.0306 (14)	0.0399 (15)	0.0026 (12)	0.0150 (12)	−0.0013 (11)
C10	0.0447 (14)	0.0344 (14)	0.0419 (15)	0.0066 (12)	0.0144 (12)	0.0114 (12)
C11	0.071 (2)	0.0449 (18)	0.067 (2)	0.0132 (16)	0.0320 (18)	0.0109 (15)
C12	0.071 (2)	0.071 (3)	0.083 (3)	0.0221 (19)	0.049 (2)	0.032 (2)
C13	0.0544 (19)	0.062 (2)	0.095 (3)	0.0034 (17)	0.0333 (19)	0.034 (2)
C14	0.0557 (18)	0.0437 (17)	0.068 (2)	−0.0022 (15)	0.0153 (16)	0.0164 (15)
C15	0.0432 (14)	0.0341 (14)	0.0411 (15)	0.0018 (12)	0.0086 (12)	0.0127 (12)
C16	0.0511 (15)	0.0342 (15)	0.0371 (14)	−0.0044 (12)	0.0106 (12)	0.0030 (11)

C17	0.076 (2)	0.0389 (17)	0.0474 (17)	−0.0025 (15)	0.0164 (16)	0.0080 (13)
C18	0.109 (3)	0.057 (2)	0.053 (2)	−0.001 (2)	0.039 (2)	0.0134 (16)
C19	0.132 (4)	0.057 (2)	0.074 (3)	0.013 (2)	0.065 (3)	0.0047 (19)
C20	0.106 (3)	0.0456 (19)	0.066 (2)	0.0128 (19)	0.045 (2)	0.0068 (16)
C21	0.0554 (16)	0.0351 (15)	0.0404 (15)	−0.0004 (13)	0.0163 (13)	0.0064 (12)
C22	0.0495 (15)	0.0342 (15)	0.0425 (16)	0.0069 (12)	0.0153 (13)	0.0036 (12)
N1	0.0453 (12)	0.0425 (13)	0.0351 (12)	−0.0010 (11)	0.0092 (10)	−0.0045 (10)
N2	0.0574 (15)	0.0622 (17)	0.0339 (13)	−0.0017 (13)	0.0027 (11)	−0.0090 (11)
N3	0.0407 (12)	0.0406 (13)	0.0352 (12)	0.0008 (10)	0.0066 (10)	0.0047 (10)
N4	0.0478 (14)	0.0635 (17)	0.0538 (15)	−0.0040 (13)	0.0239 (12)	0.0033 (13)
O1	0.0491 (8)	0.0475 (9)	0.0609 (9)	0.0017 (7)	0.0128 (7)	0.0060 (7)
O2	0.0460 (10)	0.0300 (9)	0.0425 (11)	−0.0002 (8)	0.0090 (8)	0.0062 (8)
O1W	0.0589 (15)	0.0783 (19)	0.0736 (18)	−0.0173 (13)	0.0155 (14)	0.0119 (15)
O3	0.0795 (15)	0.0430 (12)	0.0420 (12)	−0.0114 (11)	0.0065 (11)	0.0007 (9)
O2W	0.0917 (18)	0.0457 (15)	0.0552 (14)	−0.0042 (13)	−0.0099 (13)	0.0049 (12)
O4	0.0513 (11)	0.0327 (10)	0.0383 (10)	−0.0024 (8)	0.0089 (8)	0.0039 (8)
Cu1	0.03913 (17)	0.02943 (16)	0.03139 (16)	0.00027 (14)	0.00683 (12)	0.00007 (14)

Geometric parameters (Å, °)

C1—N3	1.324 (3)	C12—H12	0.93
C1—N4	1.340 (3)	C13—C14	1.386 (5)
C1—C2	1.478 (4)	C13—H13	0.93
C2—H2A	0.96	C14—C15	1.399 (4)
C2—H2B	0.96	C14—H14	0.93
C2—H2C	0.96	C15—C16	1.493 (4)
C3—C4	1.344 (4)	C16—C21	1.401 (4)
C3—N4	1.363 (4)	C16—C17	1.403 (4)
C3—H3	0.93	C17—C18	1.384 (4)
C4—N3	1.376 (3)	C17—H17	0.93
C4—H4	0.93	C18—C19	1.369 (5)
C5—C6	1.343 (4)	C18—H18	0.93
C5—N1	1.383 (4)	C19—C20	1.383 (4)
C5—H5	0.93	C19—H19	0.93
C6—N2	1.357 (4)	C20—C21	1.384 (4)
C6—H6	0.93	C20—H20	0.93
C7—N1	1.328 (4)	C21—C22	1.509 (4)
C7—N2	1.343 (3)	C22—O3	1.238 (3)
C7—C8	1.475 (4)	C22—O4	1.274 (3)
C8—H8A	0.96	Cu1—N1	1.994 (2)
C8—H8B	0.96	N2—H2	0.86
C8—H8C	0.96	Cu1—N3	1.960 (2)
C9—O1	1.240 (3)	N4—H4A	0.86
C9—O2	1.276 (3)	Cu1—O2	1.9488 (17)
C9—C10	1.500 (4)	O1W—HW11	0.837 (17)
C10—C11	1.395 (4)	O1W—HW12	0.840 (17)
C10—C15	1.403 (4)	O2W—HW21	0.842 (17)
C11—C12	1.384 (5)	O2W—HW22	0.859 (18)
C11—H11	0.93	O4—Cu1^{i}	2.0005 (18)

C12—C13	1.371 (5)	Cu1—O4^{ii}	2.0005 (18)
N3—C1—N4	109.4 (2)	C15—C14—H14	119.3
N3—C1—C2	127.1 (3)	C14—C15—C10	118.2 (3)
N4—C1—C2	123.6 (3)	C14—C15—C16	119.0 (3)
C1—C2—H2A	109.5	C10—C15—C16	122.6 (2)
C1—C2—H2B	109.5	C21—C16—C17	117.6 (2)
H2A—C2—H2B	109.5	C21—C16—C15	122.6 (2)
C1—C2—H2C	109.5	C17—C16—C15	119.6 (3)
H2A—C2—H2C	109.5	C18—C17—C16	121.6 (3)
H2B—C2—H2C	109.5	C18—C17—H17	119.2
C4—C3—N4	105.8 (3)	C16—C17—H17	119.2
C4—C3—H3	127.1	C19—C18—C17	119.7 (3)
N4—C3—H3	127.1	C19—C18—H18	120.1
C3—C4—N3	109.5 (3)	C17—C18—H18	120.1
C3—C4—H4	125.3	C18—C19—C20	120.0 (3)
N3—C4—H4	125.3	C18—C19—H19	120.0
C6—C5—N1	109.3 (3)	C20—C19—H19	120.0
C6—C5—H5	125.4	C19—C20—C21	120.9 (3)
N1—C5—H5	125.4	C19—C20—H20	119.5
C5—C6—N2	106.3 (3)	C21—C20—H20	119.5
C5—C6—H6	126.8	C20—C21—C16	120.2 (3)
N2—C6—H6	126.8	C20—C21—C22	116.8 (3)
N1—C7—N2	109.4 (3)	C16—C21—C22	123.0 (2)
N1—C7—C8	126.9 (3)	O3—C22—O4	122.0 (2)
N2—C7—C8	123.7 (3)	O3—C22—C21	121.2 (3)
C7—C8—H8A	109.5	O4—C22—C21	116.8 (2)
C7—C8—H8B	109.5	C7—N1—C5	106.2 (2)
H8A—C8—H8B	109.5	C7—N1—Cu1	128.57 (19)
C7—C8—H8C	109.5	C5—N1—Cu1	125.17 (19)
H8A—C8—H8C	109.5	C7—N2—C6	108.8 (3)
H8B—C8—H8C	109.5	C7—N2—H2	125.6
O1—C9—O2	122.4 (2)	C6—N2—H2	125.6
O1—C9—C10	122.4 (2)	C1—N3—C4	106.5 (2)
O2—C9—C10	115.3 (2)	C1—N3—Cu1	128.17 (19)
C11—C10—C15	119.5 (3)	C4—N3—Cu1	125.1 (2)
C11—C10—C9	117.9 (3)	C1—N4—C3	108.9 (2)
C15—C10—C9	122.6 (2)	C1—N4—H4A	125.6
C12—C11—C10	121.2 (3)	C3—N4—H4A	125.6
C12—C11—H11	119.4	C9—O2—Cu1	106.61 (16)
C10—C11—H11	119.4	HW11—O1W—HW12	112 (3)
C13—C12—C11	119.6 (3)	HW21—O2W—HW22	109 (3)
C13—C12—H12	120.2	C22—O4—Cu1^{i}	104.84 (16)
C11—C12—H12	120.2	O2—Cu1—N3	165.28 (8)
C12—C13—C14	120.1 (3)	O2—Cu1—N1	91.99 (9)
C12—C13—H13	119.9	N3—Cu1—N1	90.72 (9)
C14—C13—H13	119.9	O2—Cu1—O4^{ii}	89.39 (8)
C13—C14—C15	121.4 (3)	N3—Cu1—O4^{ii}	90.88 (9)
C13—C14—H14	119.3	N1—Cu1—O4^{ii}	168.31 (8)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—HW12···O2W^{iii}	0.840 (17)	1.94 (2)	2.757 (4)	163 (3)
O1W—HW11···O2W^{iv}	0.837 (17)	2.02 (2)	2.846 (4)	169 (3)
O2W—HW21···O1	0.842 (17)	1.922 (18)	2.761 (3)	174 (4)
O2W—HW22···O3	0.859 (18)	1.884 (18)	2.738 (3)	173 (4)
N2—H2···O4^{v}	0.86	1.98	2.814 (3)	164
N4—H4A···O1W	0.86	1.90	2.738 (4)	163

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

Fig. 1

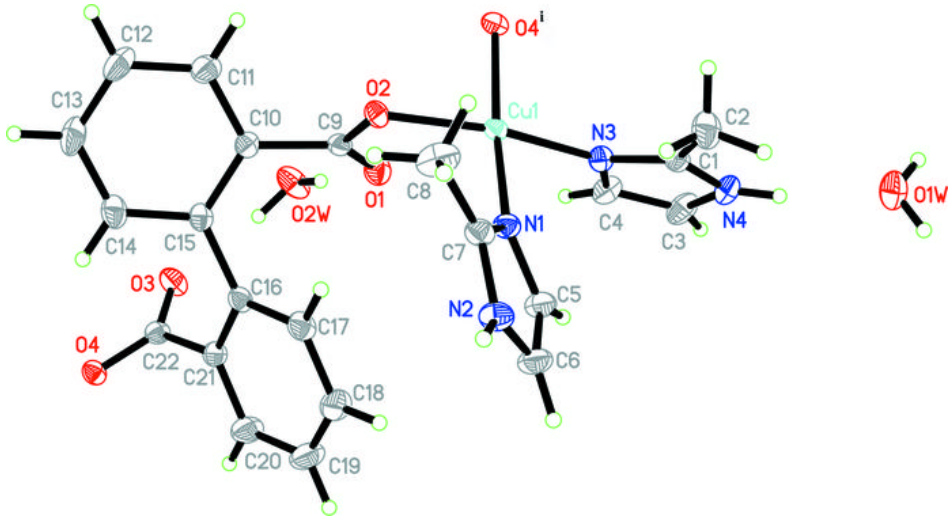
O4i
C12
C11
C13
C10
C9
O2
Cu1
N3
C2
C1
O1
C8
O2W
C14
C15
N1
C4
C3
N4
O1W
C7
O3
C16
C5
N2
C17
O4
C22
C21
C6
C18
C20
C19

Fig. 2