Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaqua[(*Z*)-4,4′-ethylenedipyridine *N*,*N*′-dioxide-κ*O*](malonato-κ^2*O*:*O*)copper(II) trihydrate

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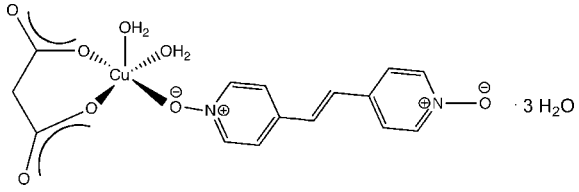
Received 9 July 2007; accepted 13 July 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.106; data-to-parameter ratio = 14.6.

In the title compound, $[Cu(C_3H_2O_4)(C_{12}H_{10}N_2O_2)(H_2O)_2]\cdot 3H_2O$, a Cu^{II} center with '4+1' Jahn–Teller-distorted square-pyramidal coordination is bound by a chelating malonate dianion, two aqua ligands and a monodentate *Z*-4,4′-ethylenedipyridine *N*,*N*′-dioxide ligand. Three uncoordinated water molecules cocrystallize with each complex molecule. Individual molecules are connected into one-dimensional ribbons and two-dimensional sheets through extensive hydrogen-bonding patterns mediated by both aqua ligands and water molecules of crystallization.

Related literature

For related literature, see: Li *et al.* (1997); Rodriguez-Martin *et al.* (2001); Simpson *et al.* (1963).



Experimental

Crystal data

$[Cu(C_3H_2O_4)(C_{12}H_{10}N_2O_2)(H_2O)_2]\cdot 3H_2O$
M_r = 469.89
Triclinic, $P\overline{1}$
a = 7.526 (3) Å
b = 11.781 (4) Å
c = 12.723 (5) Å
α = 111.701 (6)°
β = 99.270 (6)°
γ = 106.219 (6)°
V = 961.2 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.20 mm^{-1}
T = 293 (2) K
0.75 × 0.12 × 0.12 mm

Data collection

Bruker SMART 1K diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.635, T_{max} = 0.866
10713 measured reflections
4273 independent reflections
3606 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.106
S = 1.07
4273 reflections
292 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O3	1.9263 (17)	Cu1—O7	1.9766 (18)
Cu1—O5	1.9357 (17)	Cu1—O8	2.350 (2)
Cu1—O1	1.9450 (17)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O4^{i}	0.857 (18)	1.929 (19)	2.786 (3)	178 (4)
O1*W*—H1*WB*···O4^{ii}	0.842 (18)	2.11 (2)	2.883 (3)	152 (3)
O2*W*—H2*WB*···O5^{iii}	0.850 (18)	2.33 (3)	2.963 (3)	131 (3)
O2*W*—H2*WB*···O5^{iv}	0.850 (18)	2.62 (3)	3.271 (3)	134 (3)
O2*W*—H2*WA*···O1*W*	0.866 (18)	1.923 (19)	2.780 (4)	170 (4)
O3*W*—H3*WB*···O6^{i}	0.861 (18)	1.960 (19)	2.818 (3)	174 (3)
O3*W*—H3*WA*···O2*W*	0.871 (17)	1.845 (18)	2.707 (3)	171 (3)
O7—H7*A*···O6^{v}	0.867 (17)	1.94 (2)	2.767 (3)	159 (3)
O7—H7*B*···O2^{vi}	0.852 (17)	1.892 (18)	2.741 (3)	174 (3)
O8—H8*A*···O2^{vii}	0.881 (17)	1.869 (18)	2.745 (3)	174 (3)
O8—H8*B*···O3*W*^{viii}	0.889 (17)	1.899 (18)	2.786 (3)	175 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalMaker* (Palmer, 2005); software used to prepare material for publication: *SHELXL97*.

The authors gratefully acknowledge Michigan State University for funding of this work and Mr B. King for experimental assistance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2260).

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  doi:10.1107/S1600536807034253

supplementary materials

Acta Cryst. (2007). E**63**, m2166 [**doi:10.1107/S1600536807034253**]

Diaqua[(*Z*)-4,4'-ethylenedipyridine *N*,*N*'-dioxide-κO](malonato-$\kappa^2 O$:*O*)copper(II) trihydrate

M. R. Montney and R. L. LaDuca

Comment

The title compound was prepared during an attempt to synthesize a copper malonate coordination polymer incorporating *Z*-1,2-di-4-pyridylethylene-*bis*-*N*-oxide (bpeno), inspired by a report of the ferromagnetically coupled two-dimensional material [Cu_2(malonate)$_2$(H_2O)$_2$(4,4'-bipyridine)] (Rodriguez-Martin *et al.*, 2001). Its asymmetric unit consists of a single [Cu(malonate)(bpeno)(H_2O)$_2$] molecule along with three water molecules of crystallization (Figure 1). The bond distances about the Cu atom are consistent with a "4 + 1" Jahn-Teller distorted square pyramidal coordination sphere (Table 1). The ligated water molecules are oriented in a *cis* fashion with respect to each other; one (O8) lies in the axial position of the square pyramid while the other (O7) rests in the equatorial plane. The oxygen donor atom belonging to the pendant, monodentate bpeno is oriented *cis* to both aqua ligands. The malonate ligand serves only as a chelating ligand to a single Cu atom.

Individual [Cu(malonate)(bpeno)(H_2O)$_2$] molecules aggregate into pairs through O—H···O hydrogen bonding between aqua ligands (O8) and the unligated oxygen atom of the monodentate bpeno ligands (O2) as well as π-π stacking between bpeno pyridyl rings. In turn, these form one-dimensional supramolecular chains through O—H···O hydrogen bonding between aquo ligands (O7) and unligated malonate oxygen atoms (O6). These further aggregate into *pseudo* two-dimensional layers (Figure 2) that course parallel to the *bc* crystallographic planes, through hydrogen bonding between the water molecules of crystallization and aquo ligands (O8) and unligated malonate oxygen atoms (O6). The water molecules of crystallization form discrete trimeric units. The *pseudo* two-dimensional layers stack into the three-dimensional crystal structure of I through additional hydrogen bonding patterns. Metrical parameters for the supramolecular interactions are given in Table 2.

Experimental

Copper malonate (Li *et al.*, 1997) and *Z*-1,2-dipyridylethylene-*bis*-*N*-oxide were prepared *via* published procedures (Simpson *et al.*, 1963). Copper malonate (202 mg, 1.0 mmol) was dissolved in 30 ml H_2O. To this solution was added a solution of *Z*-1,2-dipyridylethylene-*bis*-*N*-oxide (107 mg, 0.5 mmol) in 10 ml e thanol. The mixture was then heated under autogenous pressure at 373 K for 5 min. Large green blocks of the title compound were isolated after cooling and standing for 7 d.

Refinement

All H atoms bound to C atoms were placed in calculated positions, with C—H = 0.95 (2) Å and refined in riding mode with U_{iso} = 1.2U_{eq}(C). All H atoms bound to O atoms were placed in calculated positions. The H atoms bound to O were found *via* Fourier difference map, restrained with O—H = 0.89 (2) Å, and refined with U_{iso} = 1.2U_{eq}(N).

Figures

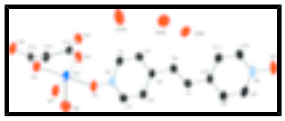

Fig. 1. Asymmetric unit of the title compound, showing 50% probability ellipsoids and atom numbering scheme. Most hydrogen atoms have been omitted for clarity.

Fig. 2. A *pseudo* two-dimensional layer in (I), viewed slightly offset from the *a* crystal direction. Color codes: light-blue N, red O within ligands, orange O within water molecules, black C, dark blue Cu.

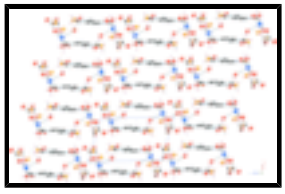

Fig. 3. Packing diagram illustrating the stacking of the *pseudo* layers to form the three-dimensional crystal structure of (I).

Diaqua[(*Z*)-4,4'-ethylenedipyridine N,*N*'-dioxide-κ*O*](malonato-κ^2*O*:*O*)copper(II) trihydrate

Crystal data

$[Cu(C_3H_2O_4)(C_{12}H_{10}N_2O_2)(H_2O)_2]\cdot 3H_2O$	$Z = 2$
$M_r = 469.89$	$F_{000} = 486$
Triclinic, $P\overline{1}$	$D_x = 1.623$ Mg m^{-3}
$a = 7.526$ (3) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 11.781$ (4) Å	Cell parameters from 10713 reflections
$c = 12.723$ (5) Å	$\theta = 1.8$–28.2°
$\alpha = 111.701$ (6)°	$\mu = 1.20$ mm^{-1}
$\beta = 99.270$ (6)°	$T = 293$ (2) K
$\gamma = 106.219$ (6)°	Block, green
$V = 961.2$ (6) Å^3	0.75 × 0.12 × 0.12 mm

Data collection

Bruker SMART 1 K diffractometer	4273 independent reflections
Radiation source: fine-focus sealed tube	3606 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
$T = 293$(2) K	$\theta_{max} = 28.2^\circ$
ω scans	$\theta_{min} = 1.8^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{min} = 0.635$, $T_{max} = 0.866$	$k = -15 \rightarrow 14$
10713 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.106$	$w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 0.2918P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
4273 reflections	$\Delta\rho_{max} = 0.57$ e Å^{-3}
292 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
15 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}
Cu1	0.08675 (4)	−0.18865 (2)	0.66333 (2)	0.03131 (11)
O1	0.2763 (2)	−0.02081 (15)	0.78449 (16)	0.0368 (4)
O1W	0.7376 (3)	0.1511 (2)	0.5214 (3)	0.0659 (7)
H1WA	0.617 (3)	0.139 (4)	0.510 (4)	0.079*
H1WB	0.755 (5)	0.085 (3)	0.525 (4)	0.079*
O2	0.3440 (3)	1.08288 (16)	1.16265 (19)	0.0479 (5)
O2W	0.8976 (4)	0.4226 (2)	0.6538 (2)	0.0615 (6)
H2WB	0.952 (5)	0.455 (3)	0.612 (3)	0.074*
H2WA	0.862 (6)	0.3382 (18)	0.615 (3)	0.074*
O3	−0.0695 (3)	−0.10789 (16)	0.60478 (17)	0.0387 (4)
O3W	0.6847 (3)	0.5529 (2)	0.76154 (17)	0.0512 (5)
H3WB	0.573 (3)	0.539 (3)	0.718 (3)	0.061*
H3WA	0.742 (4)	0.503 (3)	0.724 (3)	0.061*
O4	−0.3436 (3)	−0.10490 (17)	0.51713 (16)	0.0405 (4)
O5	−0.0721 (2)	−0.36467 (15)	0.54332 (15)	0.0346 (4)
O6	−0.3333 (3)	−0.50656 (16)	0.39468 (16)	0.0425 (4)

O7	0.2857 (3)	−0.25608 (17)	0.70707 (17)	0.0394 (4)
H7A	0.288 (4)	−0.330 (2)	0.659 (2)	0.047*
H7B	0.399 (3)	−0.198 (2)	0.746 (2)	0.047*
O8	−0.0726 (3)	−0.1970 (2)	0.80628 (19)	0.0457 (5)
H8A	−0.153 (4)	−0.155 (3)	0.817 (3)	0.055*
H8B	−0.153 (4)	−0.275 (2)	0.795 (3)	0.055*
N1	0.2473 (3)	0.09267 (17)	0.80976 (17)	0.0297 (4)
N2	0.3096 (3)	0.95500 (18)	1.1263 (2)	0.0359 (5)
C1	0.2451 (4)	0.1434 (2)	0.7312 (2)	0.0381 (6)
H1	0.2506	0.0948	0.6541	0.046*
C2	0.2349 (4)	0.2655 (2)	0.7624 (2)	0.0396 (6)
H2	0.2323	0.3003	0.7059	0.047*
C3	0.2283 (4)	0.3391 (2)	0.8746 (2)	0.0312 (5)
C4	0.2247 (4)	0.2804 (2)	0.9519 (2)	0.0356 (5)
H4	0.2161	0.3259	1.0289	0.043*
C5	0.2334 (4)	0.1579 (2)	0.9179 (2)	0.0356 (5)
H5	0.2296	0.1188	0.9712	0.043*
C6	0.2314 (4)	0.4725 (2)	0.9081 (2)	0.0357 (5)
H6	0.2235	0.5019	0.8479	0.043*
C7	0.2444 (4)	0.5558 (2)	1.0156 (2)	0.0328 (5)
H7	0.2447	0.5246	1.0746	0.039*
C8	0.2975 (4)	0.9014 (2)	1.2024 (2)	0.0426 (6)
H8	0.3059	0.9539	1.2818	0.051*
C9	0.2728 (4)	0.7710 (2)	1.1669 (2)	0.0383 (6)
H9	0.2656	0.7348	1.2223	0.046*
C10	0.2583 (3)	0.6916 (2)	1.0509 (2)	0.0302 (5)
C11	0.2640 (4)	0.7503 (2)	0.9737 (2)	0.0388 (6)
H11	0.2491	0.6991	0.8928	0.047*
C12	0.2907 (4)	0.8806 (2)	1.0125 (2)	0.0401 (6)
H12	0.2959	0.9188	0.9585	0.048*
C13	−0.2471 (3)	−0.1632 (2)	0.54898 (19)	0.0283 (5)
C14	−0.3532 (3)	−0.3063 (2)	0.5211 (2)	0.0339 (5)
H14A	−0.3874	−0.3089	0.5924	0.041*
H14B	−0.4760	−0.3409	0.4575	0.041*
C15	−0.2454 (3)	−0.3987 (2)	0.4829 (2)	0.0290 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03120 (17)	0.01942 (15)	0.03551 (18)	0.01190 (11)	0.00088 (12)	0.00577 (12)
O1	0.0372 (9)	0.0175 (7)	0.0463 (10)	0.0139 (7)	0.0017 (7)	0.0057 (7)
O1W	0.0503 (13)	0.0477 (13)	0.1030 (19)	0.0219 (11)	0.0188 (13)	0.0354 (13)
O2	0.0389 (10)	0.0188 (8)	0.0728 (13)	0.0125 (7)	0.0051 (9)	0.0096 (9)
O2W	0.0680 (15)	0.0591 (14)	0.0599 (14)	0.0263 (13)	0.0297 (12)	0.0219 (12)
O3	0.0340 (9)	0.0234 (8)	0.0532 (11)	0.0110 (7)	0.0022 (8)	0.0151 (8)
O3W	0.0559 (13)	0.0497 (12)	0.0379 (11)	0.0215 (10)	0.0057 (9)	0.0106 (9)
O4	0.0445 (10)	0.0365 (9)	0.0466 (10)	0.0237 (8)	0.0083 (8)	0.0202 (8)
O5	0.0316 (9)	0.0234 (8)	0.0413 (9)	0.0136 (7)	0.0029 (7)	0.0071 (7)

O6	0.0404 (10)	0.0225 (8)	0.0453 (10)	0.0125 (7)	−0.0002 (8)	−0.0003 (8)
O7	0.0346 (9)	0.0238 (8)	0.0479 (10)	0.0148 (7)	0.0008 (8)	0.0051 (8)
O8	0.0414 (11)	0.0498 (12)	0.0553 (12)	0.0237 (9)	0.0181 (9)	0.0262 (10)
N1	0.0293 (10)	0.0178 (8)	0.0357 (10)	0.0092 (7)	0.0043 (8)	0.0070 (8)
N2	0.0310 (10)	0.0189 (9)	0.0484 (12)	0.0107 (8)	0.0044 (9)	0.0070 (9)
C1	0.0545 (16)	0.0245 (11)	0.0309 (12)	0.0141 (11)	0.0143 (11)	0.0074 (10)
C2	0.0603 (17)	0.0276 (12)	0.0327 (12)	0.0153 (12)	0.0151 (12)	0.0154 (10)
C3	0.0382 (13)	0.0204 (10)	0.0315 (12)	0.0116 (9)	0.0074 (10)	0.0082 (9)
C4	0.0528 (15)	0.0268 (12)	0.0304 (12)	0.0200 (11)	0.0136 (11)	0.0117 (10)
C5	0.0471 (15)	0.0287 (12)	0.0334 (12)	0.0163 (11)	0.0096 (11)	0.0152 (10)
C6	0.0472 (15)	0.0251 (11)	0.0364 (13)	0.0154 (10)	0.0098 (11)	0.0146 (10)
C7	0.0442 (14)	0.0223 (11)	0.0336 (12)	0.0135 (10)	0.0097 (10)	0.0140 (10)
C8	0.0516 (16)	0.0280 (12)	0.0391 (14)	0.0154 (11)	0.0129 (12)	0.0050 (11)
C9	0.0510 (16)	0.0257 (12)	0.0368 (13)	0.0142 (11)	0.0146 (11)	0.0116 (10)
C10	0.0306 (12)	0.0228 (11)	0.0343 (12)	0.0103 (9)	0.0074 (9)	0.0102 (9)
C11	0.0554 (16)	0.0270 (12)	0.0322 (12)	0.0185 (11)	0.0086 (11)	0.0106 (10)
C12	0.0488 (15)	0.0287 (12)	0.0429 (14)	0.0155 (11)	0.0058 (12)	0.0182 (11)
C13	0.0372 (13)	0.0255 (11)	0.0249 (10)	0.0171 (9)	0.0111 (9)	0.0092 (9)
C14	0.0299 (12)	0.0257 (11)	0.0417 (13)	0.0127 (9)	0.0088 (10)	0.0093 (10)
C15	0.0340 (12)	0.0204 (10)	0.0344 (12)	0.0118 (9)	0.0101 (10)	0.0125 (9)

Geometric parameters (Å, °)

Cu1—O3	1.9263 (17)	C1—C2	1.372 (3)
Cu1—O5	1.9357 (17)	C1—H1	0.9500
Cu1—O1	1.9450 (17)	C2—C3	1.387 (3)
Cu1—O7	1.9766 (18)	C2—H2	0.9500
Cu1—O8	2.350 (2)	C3—C4	1.395 (3)
O1—N1	1.344 (2)	C3—C6	1.461 (3)
O1W—H1WA	0.857 (18)	C4—C5	1.369 (3)
O1W—H1WB	0.842 (18)	C4—H4	0.9500
O2—N2	1.334 (2)	C5—H5	0.9500
O2W—H2WB	0.850 (18)	C6—C7	1.324 (3)
O2W—H2WA	0.866 (18)	C6—H6	0.9500
O3—C13	1.257 (3)	C7—C10	1.460 (3)
O3W—H3WB	0.861 (18)	C7—H7	0.9500
O3W—H3WA	0.871 (17)	C8—C9	1.379 (3)
O4—C13	1.246 (3)	C8—H8	0.9500
O5—C15	1.268 (3)	C9—C10	1.391 (3)
O6—C15	1.245 (3)	C9—H9	0.9500
O7—H7A	0.867 (17)	C10—C11	1.395 (3)
O7—H7B	0.852 (17)	C11—C12	1.369 (3)
O8—H8A	0.881 (17)	C11—H11	0.9500
O8—H8B	0.889 (17)	C12—H12	0.9500
N1—C1	1.341 (3)	C13—C14	1.524 (3)
N1—C5	1.343 (3)	C14—C15	1.519 (3)
N2—C8	1.339 (4)	C14—H14A	0.9900
N2—C12	1.346 (3)	C14—H14B	0.9900
O3—Cu1—O5	93.99 (8)	C5—C4—H4	119.7

O3—Cu1—O1	93.20 (8)	C3—C4—H4	119.7
O5—Cu1—O1	171.90 (7)	N1—C5—C4	120.4 (2)
O3—Cu1—O7	167.73 (8)	N1—C5—H5	119.8
O5—Cu1—O7	89.06 (8)	C4—C5—H5	119.8
O1—Cu1—O7	83.14 (8)	C7—C6—C3	125.2 (2)
O3—Cu1—O8	92.76 (8)	C7—C6—H6	117.4
O5—Cu1—O8	95.96 (8)	C3—C6—H6	117.4
O1—Cu1—O8	87.42 (8)	C6—C7—C10	125.4 (2)
O7—Cu1—O8	98.75 (8)	C6—C7—H7	117.3
N1—O1—Cu1	122.35 (13)	C10—C7—H7	117.3
H1WA—O1W—H1WB	109 (3)	N2—C8—C9	120.8 (2)
H2WB—O2W—H2WA	106 (3)	N2—C8—H8	119.6
C13—O3—Cu1	125.26 (15)	C9—C8—H8	119.6
H3WB—O3W—H3WA	113 (3)	C8—C9—C10	120.8 (2)
C15—O5—Cu1	124.50 (14)	C8—C9—H9	119.6
Cu1—O7—H7A	121 (2)	C10—C9—H9	119.6
Cu1—O7—H7B	115 (2)	C9—C10—C11	116.4 (2)
H7A—O7—H7B	113 (3)	C9—C10—C7	120.6 (2)
Cu1—O8—H8A	117 (2)	C11—C10—C7	123.0 (2)
Cu1—O8—H8B	118 (2)	C12—C11—C10	121.1 (2)
H8A—O8—H8B	98 (2)	C12—C11—H11	119.4
C1—N1—C5	121.0 (2)	C10—C11—H11	119.4
C1—N1—O1	120.4 (2)	N2—C12—C11	120.6 (2)
C5—N1—O1	118.5 (2)	N2—C12—H12	119.7
O2—N2—C8	120.5 (2)	C11—C12—H12	119.7
O2—N2—C12	119.2 (2)	O4—C13—O3	122.8 (2)
C8—N2—C12	120.2 (2)	O4—C13—C14	117.6 (2)
N1—C1—C2	119.9 (2)	O3—C13—C14	119.6 (2)
N1—C1—H1	120.1	C15—C14—C13	116.6 (2)
C2—C1—H1	120.1	C15—C14—H14A	108.1
C1—C2—C3	121.3 (2)	C13—C14—H14A	108.1
C1—C2—H2	119.3	C15—C14—H14B	108.1
C3—C2—H2	119.3	C13—C14—H14B	108.1
C2—C3—C4	116.6 (2)	H14A—C14—H14B	107.3
C2—C3—C6	120.1 (2)	O6—C15—O5	122.7 (2)
C4—C3—C6	123.2 (2)	O6—C15—C14	118.2 (2)
C5—C4—C3	120.7 (2)	O5—C15—C14	119.1 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O4^{i}	0.857 (18)	1.929 (19)	2.786 (3)	178 (4)
O1W—H1WB···O4^{ii}	0.842 (18)	2.11 (2)	2.883 (3)	152 (3)
O2W—H2WB···O5^{iii}	0.850 (18)	2.33 (3)	2.963 (3)	131 (3)
O2W—H2WB···O5^{iv}	0.850 (18)	2.62 (3)	3.271 (3)	134 (3)
O2W—H2WA···O1W	0.866 (18)	1.923 (19)	2.780 (4)	170 (4)
O3W—H3WB···O6^{i}	0.861 (18)	1.960 (19)	2.818 (3)	174 (3)
O3W—H3WA···O2W	0.871 (17)	1.845 (18)	2.707 (3)	171 (3)

O7—H7A···O6^{v}	0.867 (17)	1.94 (2)	2.767 (3)	159 (3)
O7—H7B···O2^{vi}	0.852 (17)	1.892 (18)	2.741 (3)	174 (3)
O8—H8A···O2^{vii}	0.881 (17)	1.869 (18)	2.745 (3)	174 (3)
O8—H8B···O3W^{viii}	0.889 (17)	1.899 (18)	2.786 (3)	175 (3)

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

Fig. 1

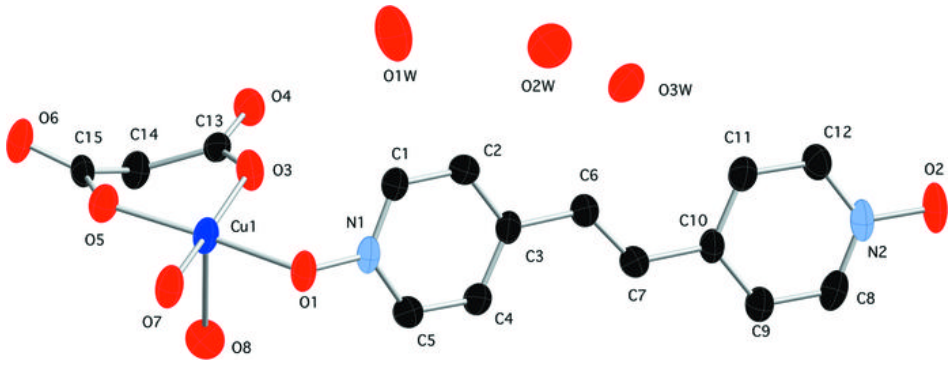
O1W
O2W
O3W
O4
O6
C15
C14
C13
O3
C1
C2
C6
C11
C12
O2
O5
Cu1
N1
C3
C10
N2
O1
C7
C8
O7
C4
C9
O8
C5

Fig. 2

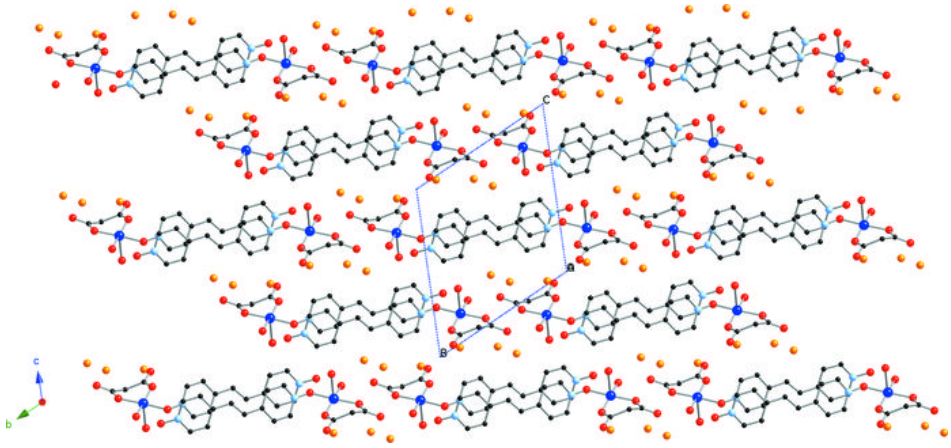

Fig. 3