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Pentaaqua(1*H*-benzimidazole-5,6-dicarboxylato-κN^3)copper(II) pentahydrate

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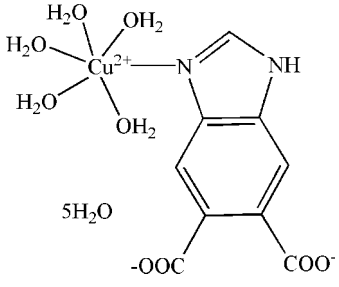
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.093; data-to-parameter ratio = 10.7.

The title compound, $[Cu(C_9H_4N_2O_4)(H_2O)_5]\cdot 5H_2O$, contains one crystallographically independent Cu^{II} atom and one 1*H*-benzimidazole-5,6-dicarboxylate (bdc) ligand, along with five coordinated and five uncoordinated water molecules. The Cu^{II} atom is six-coordinated by one N atom from the bdc ligand and five O atoms from water molecules, giving an octahedral coordination geometry. Hydrogen bonds link the mononuclear complex and uncoordinated water molecules into a three-dimensional network.

Related literature

For related literature, see: Lemos *et al.* (2004); Park *et al.* (2006); Zhang *et al.* (2007).



Experimental

Crystal data

$[Cu(C_9H_4N_2O_4)(H_2O)_5]\cdot 5H_2O$
M_r = 447.84
Triclinic, $P\overline{1}$
a = 6.8449 (5) Å
b = 11.4381 (8) Å
c = 12.3549 (9) Å
α = 78.1549 (1)°
β = 78.6224 (1)°
γ = 74.8804 (1)°
V = 903.29 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.28 mm^{-1}
T = 296 (2) K
0.24 × 0.24 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.748, T_{max} = 0.748
4648 measured reflections
3164 independent reflections
2774 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.05
3164 reflections
295 parameters
20 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O10*W*—H10*A*···O1*W*^{i}	0.80 (3)	2.09 (3)	2.855 (3)	160 (4)
O10*W*—H10*B*···O3^{ii}	0.81 (3)	2.05 (3)	2.802 (3)	155 (4)
O9*W*—H9*B*···O4^{iii}	0.81 (3)	1.94 (3)	2.739 (3)	174 (4)
O7*W*—H7*B*···O6*W*	0.83 (3)	1.95 (3)	2.758 (4)	166 (4)
O7*W*—H7*A*···O3	0.81 (3)	1.94 (3)	2.735 (3)	165 (4)
O6*W*—H6*C*···O2	0.79 (3)	2.03 (3)	2.773 (3)	156 (5)
O6*W*—H6*B*···O1^{iv}	0.84 (3)	1.96 (3)	2.772 (4)	162 (5)
O5*W*—H5*A*···O2^{v}	0.78 (2)	1.84 (3)	2.611 (3)	170 (4)
O5*W*—H5*B*···O10*W*	0.80 (2)	2.01 (3)	2.793 (3)	169 (4)
O4*W*—H4*A*···O10*W*^{vi}	0.81 (3)	1.96 (3)	2.760 (3)	168 (5)
O4*W*—H4*B*···O7*W*^{ii}	0.79 (3)	1.97 (3)	2.723 (4)	160 (5)
O3*W*—H3*C*···O9*W*^{i}	0.78 (2)	2.05 (3)	2.820 (3)	172 (4)
O3*W*—H3*B*···O3^{ii}	0.81 (2)	2.00 (3)	2.800 (3)	170 (4)
O2*W*—H2*A*···O4^{vii}	0.82 (3)	1.93 (3)	2.709 (3)	160 (4)
O2*W*—H2*B*···O9*W*	0.80 (3)	1.94 (3)	2.735 (3)	172 (4)
O1*W*—H1*D*···O1^{v}	0.78 (2)	1.85 (3)	2.621 (3)	170 (4)
N1—H1*A*···O7*W*^{iii}	0.86	1.97	2.805 (3)	163

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2082).

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supplementary materials

Acta Cryst. (2008). E**64**, m928 [**doi:10.1107/S1600536808017595**]

Pentaaqua(1*H*-benzimidazole-5,6-dicarboxylato-κN^3)copper(II) pentahydrate

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Comment

Several coordination polymers formed by the ligand 1H-benzoimidazole-5,6-dicarboxylic acid have been reported recently: μ^2-2,2'-Bibenzimidazolato-N',N'',N''')tetrakis (triphenylphosphine)-di-copper(I) dichloromethane solvate (Lemos et al., 2004), catena-poly [tetrakis(μ^2Benzimidazolato-N,N')-di-Co(II) unknown clathrate hydrate] (Park et al., 2006), and catena-poly [bis (μ^5Benzotriazole-5-carboxylate) -bis(μ^2-hydroxo)-tri-Co(II)] (Zhang et al., 2007) The first complex is a binuclear structure and the latter two are 3D porous metal-organic frameworks. However, up to now, the Cu^{II} complex of the 1H-benzoimidazole-5,6-dicarboxylic acid ligand (H_2L), has not been reported.

As shown in Figure 1, the title compound has a mononuclear structure, in which there exists only one crystallographically independent Cu (II) atom and only one 1H-benzoimidazole-5,6-dicarboxylate ligand, along with five coordinated and five uncoordinated water. Each Cu (II) is six-coordinated with one N atom from the ligand, and five O atoms from water molecules, giving an octahedral coordination geometry. Hydrogen bonds link the mononuclear complex and uncoordinated water molecules into a three-dimensional network.

Experimental

The title complex was synthesized by carefully layering a solution of $Cu(NO_3)_2.3H_2O$ (24 mg, 0.1 mmol) in MeOH (10 ml) on top of a solution of H_2L (27 mg, 0.1 mmol) and LiOH (8.4 mg, 0.2 mmol) in H_2O (10 ml) in a test-tube. After about several months at room temperature, green block-shaped single crystals suitable for X-ray investigation appeared at the boundary between MeOH and H_2O with a yield of 25%.

Refinement

H atoms of C were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C,*N*). The H atoms of the water molecules were located in Fourier difference maps and refined with isotropic displacement parameters set at 1.5 times those of the parent O atoms.

Figures

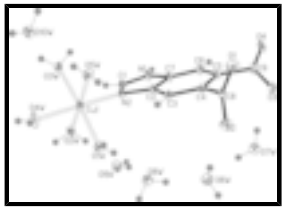


Fig. 1. Structure of the title complex, showing displacement ellipsoids at the 30% probability level.

Pentaaqua(1*H*-benzimidazole-5,6-dicarboxylato-κN^3)copper(II) pentahydrate

Crystal data

$[Cu(C_9H_4N_2O_4)(H_2O)_5]\cdot 5H_2O$	$Z = 2$
$M_r = 447.84$	$F_{000} = 466$
Triclinic, $P\overline{1}$	$D_x = 1.647$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.8449$ (5) Å	Cell parameters from 2164 reflections
$b = 11.4381$ (8) Å	$\theta = 2.7$–27.7º
$c = 12.3549$ (9) Å	$\mu = 1.28$ mm^{-1}
$\alpha = 78.1549$ (1)º	$T = 296$ (2) K
$\beta = 78.6224$ (1)º	Block, green
$\gamma = 74.8804$ (1)º	0.24 × 0.24 × 0.24 mm
$V = 903.29$ (11) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3164 independent reflections
Radiation source: fine-focus sealed tube	2774 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.018$
$T = 296(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -8\rightarrow 7$
$T_{min} = 0.748$, $T_{max} = 0.748$	$k = -13\rightarrow 9$
4648 measured reflections	$l = -14\rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 1.2855P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
3164 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
295 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
20 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}
Cu2	0.40064 (5)	0.90276 (3)	0.25900 (3)	0.01956 (13)
C1	0.5610 (5)	0.7927 (3)	0.0504 (2)	0.0208 (6)
H1B	0.5372	0.8719	0.0100	0.025*
C2	0.5701 (4)	0.6408 (2)	0.1857 (2)	0.0155 (6)
C3	0.5523 (4)	0.5625 (2)	0.2878 (2)	0.0164 (6)
H3A	0.4908	0.5933	0.3535	0.020*
C4	0.6288 (4)	0.4374 (2)	0.2891 (2)	0.0164 (6)
C5	0.7248 (4)	0.3904 (3)	0.1890 (2)	0.0174 (6)
C6	0.7410 (5)	0.4686 (3)	0.0879 (2)	0.0209 (6)
H6A	0.8036	0.4385	0.0220	0.025*
C7	0.6613 (4)	0.5927 (3)	0.0878 (2)	0.0188 (6)
C8	0.6183 (4)	0.3556 (2)	0.4017 (2)	0.0181 (6)
C9	0.7972 (5)	0.2539 (3)	0.1890 (2)	0.0200 (6)
N1	0.6497 (4)	0.6937 (2)	0.0032 (2)	0.0232 (6)
H1A	0.6921	0.6925	−0.0670	0.028*
N2	0.5095 (4)	0.7684 (2)	0.16013 (19)	0.0178 (5)
O1	0.7832 (3)	0.3070 (2)	0.43846 (19)	0.0333 (6)
O1W	0.1811 (3)	0.8182 (2)	0.36057 (18)	0.0231 (5)
H1D	0.206 (6)	0.780 (3)	0.418 (2)	0.035*
H1C	0.145 (6)	0.774 (3)	0.331 (3)	0.035*
O2	0.4460 (3)	0.3461 (2)	0.45410 (18)	0.0296 (5)
O2W	0.2065 (4)	0.9916 (2)	0.14521 (19)	0.0267 (5)
H2B	0.151 (6)	0.950 (3)	0.122 (3)	0.040*
H2A	0.119 (5)	1.055 (3)	0.154 (3)	0.040*
O3	0.6926 (3)	0.18604 (18)	0.25581 (18)	0.0281 (5)
O3W	0.6198 (3)	0.9979 (2)	0.16683 (18)	0.0236 (5)
H3B	0.652 (6)	1.045 (3)	0.196 (3)	0.035*
H3C	0.719 (5)	0.957 (3)	0.139 (3)	0.035*
O4	0.9510 (3)	0.21717 (19)	0.12100 (18)	0.0296 (5)
O4W	0.2824 (5)	1.0432 (2)	0.3484 (2)	0.0410 (7)
H4B	0.255 (7)	1.113 (3)	0.320 (4)	0.061*
H4A	0.275 (7)	1.030 (4)	0.416 (2)	0.061*
O5W	0.6079 (3)	0.8194 (2)	0.36953 (18)	0.0241 (5)

H5B	0.647 (6)	0.873 (3)	0.385 (3)	0.036*
H5A	0.579 (6)	0.775 (3)	0.424 (2)	0.036*
O6W	0.0815 (4)	0.4415 (2)	0.3683 (2)	0.0397 (6)
H6B	−0.005 (6)	0.402 (4)	0.403 (4)	0.060*
H6C	0.164 (6)	0.421 (4)	0.410 (3)	0.060*
O7W	0.2891 (4)	0.2718 (2)	0.2314 (2)	0.0330 (5)
H7A	0.406 (4)	0.257 (4)	0.244 (4)	0.050*
H7B	0.224 (6)	0.331 (3)	0.262 (3)	0.050*
O8W	0.9900 (4)	0.6813 (2)	0.2776 (2)	0.0353 (6)
H8B	0.874 (4)	0.710 (4)	0.303 (3)	0.053*
H8A	1.008 (7)	0.609 (3)	0.303 (4)	0.053*
O9W	−0.0044 (4)	0.8476 (2)	0.0862 (2)	0.0339 (6)
H9B	0.018 (7)	0.825 (4)	0.027 (3)	0.051*
H9A	0.013 (7)	0.789 (3)	0.133 (3)	0.051*
O10W	0.8011 (4)	0.9835 (2)	0.4212 (2)	0.0312 (5)
H10B	0.779 (6)	1.053 (3)	0.387 (3)	0.047*
H10A	0.919 (4)	0.953 (4)	0.402 (3)	0.047*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu2	0.0244 (2)	0.0145 (2)	0.0180 (2)	−0.00297 (14)	−0.00237 (14)	−0.00150 (14)
C1	0.0287 (16)	0.0122 (14)	0.0197 (15)	−0.0042 (12)	−0.0049 (12)	0.0018 (11)
C2	0.0185 (14)	0.0112 (13)	0.0165 (14)	−0.0022 (11)	−0.0039 (11)	−0.0021 (11)
C3	0.0208 (15)	0.0161 (14)	0.0120 (13)	−0.0041 (11)	−0.0004 (11)	−0.0040 (11)
C4	0.0193 (14)	0.0141 (14)	0.0159 (14)	−0.0041 (11)	−0.0056 (11)	0.0005 (11)
C5	0.0193 (14)	0.0140 (14)	0.0183 (14)	−0.0022 (11)	−0.0033 (11)	−0.0031 (11)
C6	0.0280 (16)	0.0184 (15)	0.0141 (14)	−0.0040 (12)	0.0024 (12)	−0.0046 (11)
C7	0.0242 (15)	0.0157 (14)	0.0146 (14)	−0.0038 (12)	−0.0028 (11)	0.0010 (11)
C8	0.0270 (16)	0.0118 (14)	0.0153 (14)	−0.0054 (12)	−0.0039 (12)	0.0000 (11)
C9	0.0253 (16)	0.0148 (14)	0.0203 (15)	−0.0010 (12)	−0.0084 (12)	−0.0037 (12)
N1	0.0372 (15)	0.0161 (13)	0.0117 (12)	−0.0040 (11)	0.0002 (11)	0.0016 (10)
N2	0.0240 (13)	0.0106 (12)	0.0168 (12)	−0.0022 (10)	−0.0031 (10)	−0.0002 (9)
O1	0.0296 (13)	0.0388 (14)	0.0270 (12)	−0.0103 (10)	−0.0113 (10)	0.0145 (10)
O1W	0.0278 (12)	0.0234 (12)	0.0173 (11)	−0.0090 (9)	−0.0051 (9)	0.0038 (9)
O2	0.0263 (12)	0.0315 (13)	0.0239 (12)	−0.0079 (10)	−0.0016 (9)	0.0111 (10)
O2W	0.0290 (13)	0.0182 (12)	0.0315 (12)	0.0036 (9)	−0.0134 (10)	−0.0038 (10)
O3	0.0342 (13)	0.0142 (11)	0.0338 (13)	−0.0069 (9)	−0.0013 (10)	−0.0013 (9)
O3W	0.0270 (12)	0.0193 (11)	0.0253 (12)	−0.0088 (9)	0.0003 (9)	−0.0050 (9)
O4	0.0333 (13)	0.0177 (11)	0.0302 (12)	0.0044 (9)	0.0016 (10)	−0.0061 (9)
O4W	0.0744 (19)	0.0175 (12)	0.0255 (13)	−0.0081 (12)	0.0065 (13)	−0.0079 (11)
O5W	0.0322 (12)	0.0231 (12)	0.0182 (11)	−0.0122 (10)	−0.0075 (9)	0.0053 (9)
O6W	0.0334 (15)	0.0358 (15)	0.0475 (17)	−0.0081 (12)	−0.0107 (12)	0.0035 (12)
O7W	0.0357 (14)	0.0362 (14)	0.0265 (12)	−0.0074 (12)	−0.0041 (11)	−0.0054 (10)
O8W	0.0307 (13)	0.0291 (13)	0.0446 (15)	−0.0055 (11)	−0.0069 (11)	−0.0029 (11)
O9W	0.0407 (14)	0.0334 (14)	0.0280 (13)	−0.0050 (11)	−0.0076 (11)	−0.0080 (11)
O10W	0.0313 (13)	0.0268 (13)	0.0305 (13)	−0.0033 (11)	−0.0033 (11)	0.0007 (10)

Geometric parameters (Å, °)

Cu2—O4W	2.037 (2)	C9—O4	1.248 (4)
Cu2—O2W	2.055 (2)	C9—O3	1.261 (4)
Cu2—N2	2.055 (2)	N1—H1A	0.8600
Cu2—O1W	2.070 (2)	O1W—H1D	0.78 (2)
Cu2—O5W	2.076 (2)	O1W—H1C	0.80 (2)
Cu2—O3W	2.097 (2)	O2W—H2B	0.80 (3)
C1—N2	1.322 (4)	O2W—H2A	0.82 (3)
C1—N1	1.328 (4)	O3W—H3B	0.81 (2)
C1—H1B	0.9300	O3W—H3C	0.78 (2)
C2—C3	1.393 (4)	O4W—H4B	0.79 (3)
C2—N2	1.396 (3)	O4W—H4A	0.81 (3)
C2—C7	1.397 (4)	O5W—H5B	0.80 (2)
C3—C4	1.387 (4)	O5W—H5A	0.78 (2)
C3—H3A	0.9300	O6W—H6B	0.84 (3)
C4—C5	1.420 (4)	O6W—H6C	0.79 (3)
C4—C8	1.510 (4)	O7W—H7A	0.81 (3)
C5—C6	1.382 (4)	O7W—H7B	0.83 (3)
C5—C9	1.510 (4)	O8W—H8B	0.80 (3)
C6—C7	1.381 (4)	O8W—H8A	0.81 (3)
C6—H6A	0.9300	O9W—H9B	0.81 (3)
C7—N1	1.387 (4)	O9W—H9A	0.79 (3)
C8—O2	1.248 (4)	O10W—H10B	0.81 (3)
C8—O1	1.249 (4)	O10W—H10A	0.80 (3)
O4W—Cu2—O2W	88.82 (10)	C6—C7—C2	122.3 (3)
O4W—Cu2—N2	176.07 (10)	N1—C7—C2	105.0 (2)
O2W—Cu2—N2	87.32 (9)	O2—C8—O1	124.5 (3)
O4W—Cu2—O1W	86.06 (10)	O2—C8—C4	118.2 (2)
O2W—Cu2—O1W	92.49 (9)	O1—C8—C4	117.3 (3)
N2—Cu2—O1W	94.83 (9)	O4—C9—O3	125.0 (3)
O4W—Cu2—O5W	90.71 (11)	O4—C9—C5	117.9 (3)
O2W—Cu2—O5W	176.77 (9)	O3—C9—C5	117.0 (3)
N2—Cu2—O5W	93.11 (9)	C1—N1—C7	107.4 (2)
O1W—Cu2—O5W	90.66 (9)	C1—N1—H1A	126.3
O4W—Cu2—O3W	89.28 (10)	C7—N1—H1A	126.3
O2W—Cu2—O3W	89.14 (9)	C1—N2—C2	104.4 (2)
N2—Cu2—O3W	89.94 (9)	C1—N2—Cu2	122.93 (19)
O1W—Cu2—O3W	175.03 (9)	C2—N2—Cu2	132.25 (19)
O5W—Cu2—O3W	87.67 (9)	Cu2—O1W—H1D	118 (3)
N2—C1—N1	113.8 (2)	Cu2—O1W—H1C	113 (3)
N2—C1—H1B	123.1	H1D—O1W—H1C	106 (4)
N1—C1—H1B	123.1	Cu2—O2W—H2B	117 (3)
C3—C2—N2	130.6 (3)	Cu2—O2W—H2A	123 (3)
C3—C2—C7	120.0 (3)	H2B—O2W—H2A	105 (4)
N2—C2—C7	109.4 (2)	Cu2—O3W—H3B	118 (3)
C4—C3—C2	118.3 (3)	Cu2—O3W—H3C	115 (3)
C4—C3—H3A	120.8	H3B—O3W—H3C	109 (4)

C2—C3—H3A	120.8	Cu2—O4W—H4B	123 (3)
C3—C4—C5	120.9 (3)	Cu2—O4W—H4A	120 (3)
C3—C4—C8	117.1 (2)	H4B—O4W—H4A	116 (5)
C5—C4—C8	121.9 (2)	Cu2—O5W—H5B	107 (3)
C6—C5—C4	120.5 (3)	Cu2—O5W—H5A	122 (3)
C6—C5—C9	118.4 (3)	H5B—O5W—H5A	109 (4)
C4—C5—C9	121.0 (3)	H6B—O6W—H6C	100 (5)
C7—C6—C5	117.9 (3)	H7A—O7W—H7B	107 (4)
C7—C6—H6A	121.0	H8B—O8W—H8A	104 (5)
C5—C6—H6A	121.0	H9B—O9W—H9A	108 (4)
C6—C7—N1	132.7 (3)	H10B—O10W—H10A	107 (4)
N2—C2—C3—C4	−179.4 (3)	C4—C5—C9—O4	−148.5 (3)
C7—C2—C3—C4	0.6 (4)	C6—C5—C9—O3	−141.7 (3)
C2—C3—C4—C5	0.7 (4)	C4—C5—C9—O3	33.8 (4)
C2—C3—C4—C8	176.6 (3)	N2—C1—N1—C7	−0.4 (4)
C3—C4—C5—C6	−1.1 (4)	C6—C7—N1—C1	−178.6 (3)
C8—C4—C5—C6	−176.7 (3)	C2—C7—N1—C1	1.0 (3)
C3—C4—C5—C9	−176.4 (3)	N1—C1—N2—C2	−0.5 (3)
C8—C4—C5—C9	7.9 (4)	N1—C1—N2—Cu2	172.7 (2)
C4—C5—C6—C7	0.1 (4)	C3—C2—N2—C1	−178.9 (3)
C9—C5—C6—C7	175.5 (3)	C7—C2—N2—C1	1.1 (3)
C5—C6—C7—N1	−179.2 (3)	C3—C2—N2—Cu2	8.8 (5)
C5—C6—C7—C2	1.3 (5)	C7—C2—N2—Cu2	−171.1 (2)
C3—C2—C7—C6	−1.6 (5)	O2W—Cu2—N2—C1	47.3 (2)
N2—C2—C7—C6	178.3 (3)	O1W—Cu2—N2—C1	139.6 (2)
C3—C2—C7—N1	178.7 (3)	O5W—Cu2—N2—C1	−129.5 (2)
N2—C2—C7—N1	−1.3 (3)	O3W—Cu2—N2—C1	−41.8 (2)
C3—C4—C8—O2	67.2 (4)	O2W—Cu2—N2—C2	−141.6 (3)
C5—C4—C8—O2	−116.9 (3)	O1W—Cu2—N2—C2	−49.4 (3)
C3—C4—C8—O1	−109.2 (3)	O5W—Cu2—N2—C2	41.6 (3)
C5—C4—C8—O1	66.7 (4)	O3W—Cu2—N2—C2	129.2 (3)
C6—C5—C9—O4	36.1 (4)		

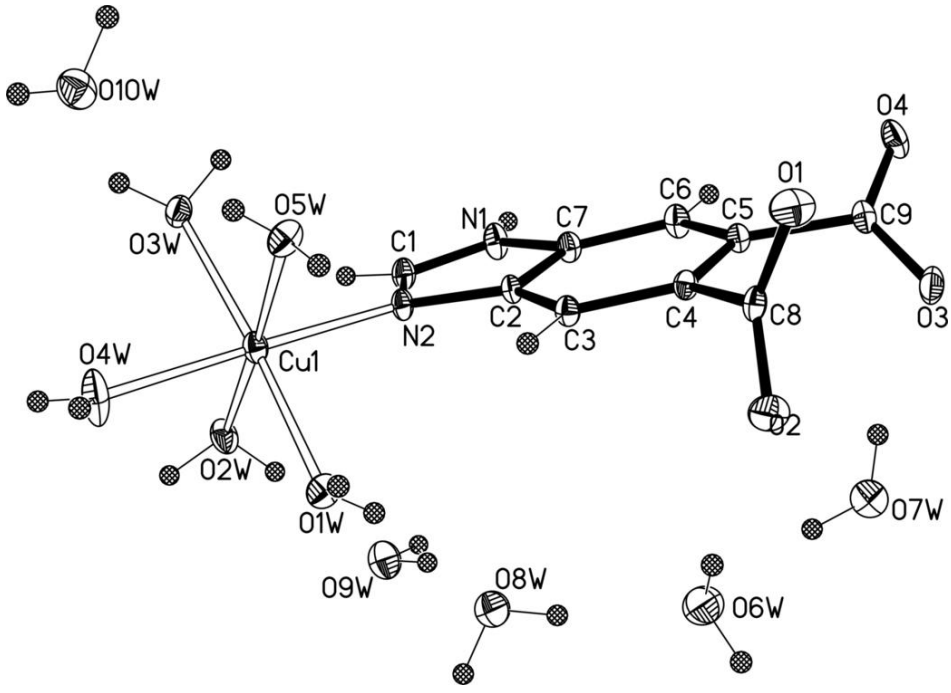
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O10W—H10A···O1W^{i}	0.80 (3)	2.09 (3)	2.855 (3)	160 (4)
O10W—H10B···O3^{ii}	0.81 (3)	2.05 (3)	2.802 (3)	155 (4)
O9W—H9B···O4^{iii}	0.81 (3)	1.94 (3)	2.739 (3)	174 (4)
O7W—H7B···O6W	0.83 (3)	1.95 (3)	2.758 (4)	166 (4)
O7W—H7A···O3	0.81 (3)	1.94 (3)	2.735 (3)	165 (4)
O6W—H6C···O2	0.79 (3)	2.03 (3)	2.773 (3)	156 (5)
O6W—H6B···O1^{iv}	0.84 (3)	1.96 (3)	2.772 (4)	162 (5)
O5W—H5A···O2^{v}	0.78 (2)	1.84 (3)	2.611 (3)	170 (4)
O5W—H5B···O10W	0.80 (2)	2.01 (3)	2.793 (3)	169 (4)
O4W—H4A···O10W^{vi}	0.81 (3)	1.96 (3)	2.760 (3)	168 (5)
O4W—H4B···O7W^{ii}	0.79 (3)	1.97 (3)	2.723 (4)	160 (5)

O3W—H3C···O9W^{i}	0.78 (2)	2.05 (3)	2.820 (3)	172 (4)
O3W—H3B···O3^{ii}	0.81 (2)	2.00 (3)	2.800 (3)	170 (4)
O2W—H2A···O4^{vii}	0.82 (3)	1.93 (3)	2.709 (3)	160 (4)
O2W—H2B···O9W	0.80 (3)	1.94 (3)	2.735 (3)	172 (4)
O1W—H1D···O1^{v}	0.78 (2)	1.85 (3)	2.621 (3)	170 (4)
N1—H1A···O7W^{iii}	0.86	1.97	2.805 (3)	163

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

Fig. 1


O10W
O4
O1
C6
C5
C9
O5W
N1
C7
O3W
C1
O3
C2
C4
C8
N2
C3
O4W
Cu1
O2
O2W
O7W
O1W
O9W
O8W
O6W