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Poly[ethylenediammonium [cuprate(II)-μ_4-benzene-1,2,4,5-tetracarboxylato-$\kappa^4O:O':O'':O'''$] 2.5-hydrate]

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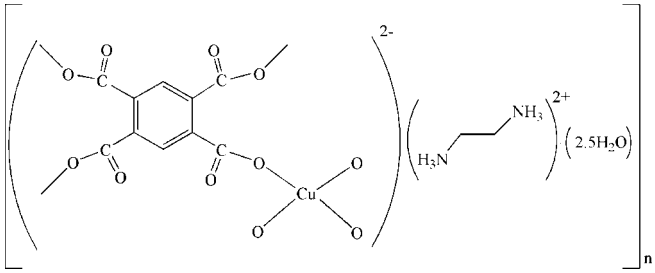
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; some non-H atoms missing; disorder in solvent or counterion; R factor = 0.037; wR factor = 0.100; data-to-parameter ratio = 22.6.

The asymmetric unit of the title compound, $\{(C_2H_{10}N_2)[Cu(C_{10}H_2O_8)]\cdot 2.5H_2O\}_n$, contains one cuprate(II)-μ_4-benzene-1,2,4,5-tetracarboxylate anion, one ethylenediammonium cation and two and a half water molecules. The Cu atom is four-coordinated by four O atoms from four benzene-1,2,4,5-tetracarboxylate anions. Intra- and intermolecular O—H···O and N—H···O hydrogen bonds in the formation of a supramolecular structure. One of the water molecules is disordered equally over two sites.

Related literature

For general backgroud, see: Hu *et al.* (2004, 2001); Fu *et al.* (2004); Cheng *et al.* (2002); Hou *et al.* (2004); Chu *et al.* (2001); Rochon & Massarweh (2000); Cao *et al.* (2002); Daiguebonne *et al.* (2003); Rafizadeh *et al.* (2006). For related literature, see: Cheng *et al.* (2003); Day & Luehrs (1988); Kim *et al.* (2003); Yuan *et al.* (2005); Hao *et al.* (2004).



Experimental

Crystal data

$(C_2H_{10}N_2)[Cu(C_{10}H_2O_8)]\cdot 2.5H_2O$
M_r = 420.82
Monoclinic, $P2_1/c$
a = 7.3937 (5) Å
b = 18.4414 (11) Å
c = 11.3607 (7) Å
β = 94.783 (1)°
V = 1543.64 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.48 mm^{-1}
T = 100 (2) K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.744, T_{max} = 0.751
22717 measured reflections
5364 independent reflections
4304 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.01
5364 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.9456 (12)	Cu1—O7	1.9500 (12)
Cu1—O1	1.9466 (12)	Cu1—O5	1.9514 (12)
O3—Cu1—O1	91.96 (5)	O3—Cu1—O5	169.55 (6)
O3—Cu1—O7	88.55 (5)	O1—Cu1—O5	88.69 (5)
O1—Cu1—O7	170.20 (6)	O7—Cu1—O5	92.59 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1′—H1′*C*···O2^{i}	0.91	2.18	2.921 (2)	138
N1′—H1′*C*···O5^{i}	0.91	2.30	2.993 (2)	132
N1′—H1′*D*···O4^{ii}	0.91	2.11	2.810 (2)	133
N1′—H1′*E*···O6^{iii}	0.91	1.92	2.799 (2)	161
N2′—H2′*C*···O6	0.91	2.14	2.902 (2)	141
N2′—H2′*D*···O2^{ii}	0.91	1.92	2.807 (2)	164
N2′—H2′*E*···O8^{iii}	0.91	2.09	2.810 (2)	135
O1*W*—H1*WA*···O2*W*^{iv}	0.85	2.32	3.116 (2)	157
O1*W*—H1*WB*···O3^{v}	0.85	2.16	2.9784 (19)	162
O2*W*—H2*WA*···O1*W*	0.85	1.99	2.813 (2)	164
O2*W*—H2*WB*···O7	0.85	2.18	2.987 (2)	159

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: HK2258).

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supplementary materials

Acta Cryst. (2007). E**63**, m1841-m1842 [**doi:10.1107/S1600536807025834**]

Poly[ethylenediammonium [cuprate(II)-μ_4-benzene-1,2,4,5-tetracarboxylato-$\kappa^4O:O':O'':O'''$] 2.5-hydrate\]

M. Rafizadeh, V. Amani, L. Dehghan, F. Azadbakht and E. Sahlolbei

Comment

The self-assembly of metal ions with aromatic carboxylates is a rapidly developing research field of modern coordination chemistry, because of the aggregation of metal ions and these carboxylate ligands in versatile binding modes, such as monodentate, chelating bidentate, bridging bidentate and bridging tridentate. Hereby, benzene-1,2,4,5-tetracarboxylic acid (H_4BTC) is a good bridging ligand, and numerous complexes with H_4BTC anions have been prepared, such as those of cobalt (Hu *et al.*, 2004; Fu *et al.*, 2004; Cheng *et al.*, 2002), nickel (Kim *et al.*, 2003; Cheng *et al.*, 2003), thallium (Day & Luehrs, 1988), copper (Kim *et al.*, 2003; Yuan *et al.*, 2005; Hao *et al.*, 2004), zinc (Hou *et al.*, 2004), iron (Chu *et al.*, 2001) and manganese (Rochon & Massarweh, 2000; Hu *et al.*, 2001). There are also compounds of the rare earth elements reported (Cao *et al.*, 2002; Daiguebonne *et al.*, 2003). The complex of benzene-1,2,4,5-tetracarboxylate containing organic ammonium cations are rare and may have interesting polymeric chemistry. Recently, we have reported the syntheses and crystal structure of a proton transfer system using (H_4BTC), with ethylenediamine (en), $(BTC)(H_2en)_2{\cdot}2H_2O$, (Rafizadeh *et al.*, 2006). We herein report the synthesis and crystal structure of the title compound, (I), which was synthesized by reaction of $Cu(NO_3)_2{\cdot}3H_2O$ and $(BTC)(H_2en)_2{\cdot}2H_2O$.

The asymmetric unit of (I) contains one $[Cu(C_{10}H_2O_8)]$ anion, one ($N_2C_2H_{10}$) cation and two and a half water molecules. The Cu atom is four-coordinated by four O atoms from four benzene-1,2,4,5-tetracarboxylate (btc) anions (Fig. 1). The Cu—O bond lengths and angles (Table 1) are within normal ranges (Kim *et al.*, 2003; Yuan *et al.*, 2005; Hao *et al.*, 2004).

The intra- and intermolecular O—H—O and N—H···O hydrogen bonds (Table 2) seem to be effective in the stabilization of the crystal structure, resulting in the formation of a supramolecular structure (Fig. 2). Dipol-dipol and van der Waals interactions are also effective in the molecular packing.

Experimental

For the preparation of the title compound, (I), a solution of $(BTC)(H_2en)_2{\cdot}2H_2O$, (0.30 g, 0.73 mmol) in water (100 ml) was added to a solution of $Cu(NO_3)_2{\cdot}3H_2O$ (0.09 g, 0.365 mmol) in water (10 ml) and the resulting blue solution was stirred for 5 min at room temperature. Then, it was left to evaporate slowly at room temperature. After one week, blue prismatic crystals of (I) were isolated (yield; 0.13 g, 84.6%; decompose <562 K).

Figures

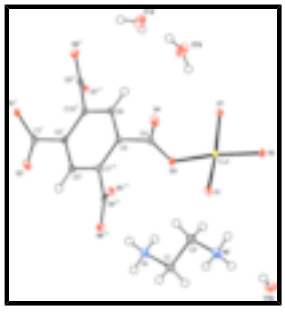

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (i) 2 − *x*, *y* − 1/2, 2.5 − *z*, (ii) 2 − *x*, 1 − *y*, 2 − *z*, (iii) 2 − *x*, *y* − 1/2, 2.5 − *z*].

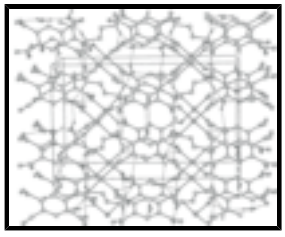

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

Poly[ethylenediammonium [copper(II)-μ$_4$-benzene-1,2,4,5-tetracarboxylato-κ^4*O*:*O*':*O*'':*O*'''] 2.5-hydrate]

Crystal data

$(C_2H_{10}N_2)[Cu(C_{10}H_2O_8)]\cdot 2.5H_2O$	F_{000} = 864
M_r = 420.82	D_x = 1.811 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5022 reflections
a = 7.3937 (5) Å	θ = 2.8–34.7º
b = 18.4414 (11) Å	μ = 1.48 mm^{-1}
c = 11.3607 (7) Å	*T* = 100 (2) K
β = 94.783 (1)º	Cube, blue
V = 1543.64 (17) Å^3	0.20 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker APEX II CCD area-detector diffractometer	5364 independent reflections
Radiation source: fine-focus sealed tube	4304 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 100(2) K	θ_{max} = 32.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (APEX2; Bruker, 2005)	*h* = −11→11
T_{min} = 0.744, T_{max} = 0.751	*k* = −27→27
22717 measured reflections	*l* = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 1.6005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
5364 reflections	$\Delta\rho_{max} = 0.95$ e Å^{-3}
237 parameters	$\Delta\rho_{min} = -0.70$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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}	Occ. (<1)
Cu1	0.98260 (3)	0.743122 (11)	0.999045 (17)	0.00747 (7)	
O1	1.00080 (18)	0.81812 (7)	1.12002 (11)	0.0109 (2)	
O2	0.72149 (18)	0.85964 (7)	1.06384 (11)	0.0129 (2)	
O3	1.04758 (17)	0.66759 (6)	1.11446 (11)	0.0096 (2)	
O4	0.74826 (18)	0.65069 (7)	1.11395 (12)	0.0137 (3)	
O5	0.96462 (18)	0.81928 (7)	0.87939 (11)	0.0107 (2)	
O6	1.24867 (18)	0.85345 (7)	0.93744 (11)	0.0125 (2)	
O7	0.92059 (17)	0.66741 (6)	0.88281 (11)	0.0092 (2)	
O8	1.22206 (18)	0.65801 (7)	0.88507 (12)	0.0127 (3)	
C1	0.8752 (2)	0.86592 (9)	1.11718 (14)	0.0085 (3)	
C2	0.9277 (2)	0.93511 (9)	1.18051 (14)	0.0075 (3)	
C3	0.8811 (2)	1.00135 (9)	1.12768 (15)	0.0085 (3)	
H3A	0.8076	1.0025	1.0550	0.010*	
C4	0.9066 (2)	0.63317 (9)	1.14322 (15)	0.0085 (3)	
C5	0.9522 (2)	0.56440 (9)	1.21098 (14)	0.0070 (3)	
C6	0.9048 (2)	0.49801 (9)	1.15800 (15)	0.0080 (3)	
H6A	0.8307	0.4968	1.0856	0.010*	
C7	1.0580 (2)	0.93391 (9)	0.81899 (14)	0.0078 (3)	
C8	1.0975 (2)	0.86364 (9)	0.88280 (14)	0.0084 (3)	

C9	1.0668 (2)	0.63647 (9)	0.85520 (14)	0.0081 (3)	
C10	1.0338 (2)	0.56645 (9)	0.78862 (14)	0.0076 (3)	
N1'	1.5660 (2)	0.65943 (8)	1.32091 (14)	0.0127 (3)	
H1'C	1.6629	0.6490	1.3729	0.019*	
H1'D	1.5774	0.6356	1.2518	0.019*	
H1'E	1.4621	0.6450	1.3518	0.019*	
N2'	1.4052 (2)	0.83478 (9)	1.17836 (14)	0.0137 (3)	
H2'C	1.3108	0.8450	1.1243	0.021*	
H2'D	1.5107	0.8500	1.1506	0.021*	
H2'E	1.3887	0.8580	1.2473	0.021*	
C1'	1.5587 (3)	0.73907 (10)	1.29853 (17)	0.0134 (3)	
H1'A	1.6781	0.7563	1.2764	0.016*	
H1'B	1.5303	0.7649	1.3711	0.016*	
C2'	1.4139 (3)	0.75515 (10)	1.19949 (17)	0.0138 (3)	
H2'A	1.4432	0.7299	1.1266	0.017*	
H2'B	1.2948	0.7374	1.2211	0.017*	
O1W	0.6201 (2)	0.42273 (8)	0.89555 (14)	0.0216 (3)	
H1WA	0.5629	0.4100	0.9540	0.032*	
H1WB	0.7244	0.4053	0.8861	0.032*	
O2W	0.5892 (2)	0.57443 (9)	0.87753 (16)	0.0262 (4)	
H2WA	0.5758	0.5287	0.8801	0.039*	
H2WB	0.6951	0.5922	0.8909	0.039*	
O3W	1.4335 (4)	0.99565 (15)	1.1305 (3)	0.0217 (6)	0.50
H3WA	1.3268	1.0023	1.1510	0.033*	0.50
H3WB	1.4755	1.0113	1.0679	0.033*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01489 (11)	0.00322 (10)	0.00438 (10)	0.00031 (7)	0.00120 (7)	0.00017 (7)
O1	0.0199 (6)	0.0058 (5)	0.0068 (5)	0.0024 (4)	0.0001 (4)	−0.0008 (4)
O2	0.0136 (6)	0.0148 (6)	0.0103 (6)	−0.0050 (5)	0.0009 (4)	−0.0029 (5)
O3	0.0151 (6)	0.0059 (5)	0.0078 (6)	−0.0009 (4)	0.0014 (4)	0.0014 (4)
O4	0.0139 (6)	0.0149 (6)	0.0123 (6)	0.0060 (5)	0.0020 (5)	0.0034 (5)
O5	0.0181 (6)	0.0062 (5)	0.0077 (6)	−0.0025 (4)	0.0012 (4)	0.0015 (4)
O6	0.0152 (6)	0.0114 (6)	0.0107 (6)	0.0033 (5)	0.0008 (5)	0.0023 (5)
O7	0.0135 (6)	0.0069 (5)	0.0073 (5)	0.0017 (4)	0.0015 (4)	−0.0014 (4)
O8	0.0140 (6)	0.0120 (6)	0.0123 (6)	−0.0046 (5)	0.0021 (5)	−0.0014 (5)
C1	0.0139 (8)	0.0068 (7)	0.0053 (7)	−0.0017 (5)	0.0040 (5)	0.0005 (5)
C2	0.0113 (7)	0.0046 (7)	0.0067 (7)	0.0003 (5)	0.0015 (5)	−0.0008 (5)
C3	0.0125 (8)	0.0062 (7)	0.0067 (7)	0.0005 (5)	0.0007 (5)	−0.0001 (6)
C4	0.0135 (8)	0.0057 (7)	0.0065 (7)	0.0014 (5)	0.0022 (5)	−0.0008 (5)
C5	0.0102 (7)	0.0058 (7)	0.0052 (7)	0.0002 (5)	0.0015 (5)	0.0007 (5)
C6	0.0107 (7)	0.0069 (7)	0.0066 (7)	0.0000 (5)	0.0012 (5)	0.0001 (6)
C7	0.0131 (7)	0.0048 (7)	0.0057 (7)	0.0004 (5)	0.0024 (5)	0.0012 (5)
C8	0.0155 (8)	0.0042 (7)	0.0060 (7)	0.0008 (5)	0.0032 (5)	−0.0004 (5)
C9	0.0144 (8)	0.0047 (7)	0.0054 (7)	−0.0005 (5)	0.0014 (5)	0.0002 (5)
C10	0.0109 (7)	0.0052 (7)	0.0067 (7)	−0.0005 (5)	0.0017 (5)	−0.0008 (5)

N1'	0.0127 (7)	0.0150 (7)	0.0105 (7)	0.0026 (5)	0.0006 (5)	0.0012 (5)
N2'	0.0142 (7)	0.0153 (7)	0.0116 (7)	0.0032 (5)	0.0008 (5)	0.0016 (6)
C1'	0.0142 (8)	0.0122 (8)	0.0132 (8)	0.0020 (6)	−0.0015 (6)	0.0016 (6)
C2'	0.0130 (8)	0.0147 (8)	0.0134 (8)	0.0016 (6)	−0.0013 (6)	0.0009 (6)
O1W	0.0207 (7)	0.0168 (7)	0.0282 (8)	−0.0001 (5)	0.0085 (6)	−0.0002 (6)
O2W	0.0165 (7)	0.0189 (7)	0.0429 (10)	0.0002 (5)	0.0012 (6)	0.0094 (7)
O3W	0.0218 (15)	0.0176 (14)	0.0245 (16)	−0.0036 (10)	−0.0049 (12)	0.0016 (12)

Geometric parameters (Å, °)

Cu1—O3	1.9456 (12)	C7—C8	1.502 (2)
Cu1—O1	1.9466 (12)	C9—C10	1.506 (2)
Cu1—O7	1.9500 (12)	C10—C6^{iii}	1.393 (2)
Cu1—O5	1.9514 (12)	C10—C2^{iv}	1.402 (2)
O1—C1	1.279 (2)	N1'—C1'	1.491 (2)
O2—C1	1.248 (2)	N1'—H1'C	0.9100
O3—C4	1.285 (2)	N1'—H1'D	0.9100
O4—C4	1.233 (2)	N1'—H1'E	0.9100
O5—C8	1.276 (2)	N2'—C2'	1.489 (2)
O6—C8	1.247 (2)	N2'—H2'C	0.9100
O7—C9	1.284 (2)	N2'—H2'D	0.9100
O8—C9	1.235 (2)	N2'—H2'E	0.9100
C1—C2	1.500 (2)	C1'—C2'	1.516 (3)
C2—C3	1.392 (2)	C1'—H1'A	0.9900
C2—C10^{i}	1.402 (2)	C1'—H1'B	0.9900
C3—C7^{ii}	1.396 (2)	C2'—H2'A	0.9900
C3—H3A	0.9500	C2'—H2'B	0.9900
C4—C5	1.507 (2)	O1W—H1WA	0.8499
C5—C6	1.396 (2)	O1W—H1WB	0.8500
C5—C7^{i}	1.399 (2)	O2W—H2WA	0.8501
C6—C10^{iii}	1.393 (2)	O2W—H2WB	0.8500
C6—H6A	0.9500	O3W—H3WA	0.8500
C7—C3^{ii}	1.396 (2)	O3W—H3WB	0.8499
C7—C5^{iv}	1.399 (2)		
O3—Cu1—O1	91.96 (5)	O8—C9—O7	124.89 (16)
O3—Cu1—O7	88.55 (5)	O8—C9—C10	121.42 (15)
O1—Cu1—O7	170.20 (6)	O7—C9—C10	113.55 (14)
O3—Cu1—O5	169.55 (6)	C6^{iii}—C10—C2^{iv}	120.14 (15)
O1—Cu1—O5	88.69 (5)	C6^{iii}—C10—C9	118.68 (14)
O7—Cu1—O5	92.59 (5)	C2^{iv}—C10—C9	120.87 (14)
C1—O1—Cu1	117.69 (11)	C1'—N1'—H1'C	109.5
C4—O3—Cu1	111.40 (11)	C1'—N1'—H1'D	109.5
C8—O5—Cu1	115.63 (11)	H1'C—N1'—H1'D	109.5
C9—O7—Cu1	109.17 (11)	C1'—N1'—H1'E	109.5
O2—C1—O1	125.32 (16)	H1'C—N1'—H1'E	109.5
O2—C1—C2	120.03 (15)	H1'D—N1'—H1'E	109.5
O1—C1—C2	114.60 (15)	C2'—N2'—H2'C	109.5

C3—C2—C10^{i}	119.76 (15)	C2'—N2'—H2'D	109.5
C3—C2—C1	119.68 (15)	H2'C—N2'—H2'D	109.5
C10^{i}—C2—C1	120.42 (14)	C2'—N2'—H2'E	109.5
C2—C3—C7^{ii}	120.27 (15)	H2'C—N2'—H2'E	109.5
C2—C3—H3A	119.9	H2'D—N2'—H2'E	109.5
C7^{ii}—C3—H3A	119.9	N1'—C1'—C2'	109.42 (15)
O4—C4—O3	125.01 (16)	N1'—C1'—H1'A	109.8
O4—C4—C5	121.65 (15)	C2'—C1'—H1'A	109.8
O3—C4—C5	113.21 (14)	N1'—C1'—H1'B	109.8
C6—C5—C7^{i}	119.96 (15)	C2'—C1'—H1'B	109.8
C6—C5—C4	118.72 (14)	H1'A—C1'—H1'B	108.2
C7^{i}—C5—C4	120.92 (14)	N2'—C2'—C1'	109.34 (15)
C10^{iii}—C6—C5	119.99 (15)	N2'—C2'—H2'A	109.8
C10^{iii}—C6—H6A	120.0	C1'—C2'—H2'A	109.8
C5—C6—H6A	120.0	N2'—C2'—H2'B	109.8
C3^{ii}—C7—C5^{iv}	119.86 (15)	C1'—C2'—H2'B	109.8
C3^{ii}—C7—C8	119.05 (15)	H2'A—C2'—H2'B	108.3
C5^{iv}—C7—C8	120.96 (14)	H1WA—O1W—H1WB	120.7
O6—C8—O5	125.05 (16)	H2WA—O2W—H2WB	118.9
O6—C8—C7	120.04 (15)	H3WA—O3W—H3WB	126.4
O5—C8—C7	114.85 (15)		
O3—Cu1—O1—C1	−135.64 (12)	Cu1—O3—C4—C5	167.38 (10)
O7—Cu1—O1—C1	−42.8 (4)	O4—C4—C5—C6	63.2 (2)
O5—Cu1—O1—C1	54.80 (12)	O3—C4—C5—C6	−112.90 (17)
O1—Cu1—O3—C4	100.44 (11)	O4—C4—C5—C7^{i}	−124.12 (19)
O7—Cu1—O3—C4	−69.76 (11)	O3—C4—C5—C7^{i}	59.8 (2)
O5—Cu1—O3—C4	−166.2 (3)	C7^{i}—C5—C6—C10^{iii}	−1.4 (3)
O3—Cu1—O5—C8	−35.5 (3)	C4—C5—C6—C10^{iii}	171.39 (15)
O1—Cu1—O5—C8	58.23 (12)	Cu1—O5—C8—O6	15.9 (2)
O7—Cu1—O5—C8	−131.50 (12)	Cu1—O5—C8—C7	−161.28 (11)
O3—Cu1—O7—C9	−70.78 (11)	C3^{ii}—C7—C8—O6	−40.7 (2)
O1—Cu1—O7—C9	−163.9 (3)	C5^{iv}—C7—C8—O6	143.24 (17)
O5—Cu1—O7—C9	98.82 (11)	C3^{ii}—C7—C8—O5	136.63 (17)
Cu1—O1—C1—O2	18.8 (2)	C5^{iv}—C7—C8—O5	−39.4 (2)
Cu1—O1—C1—C2	−158.60 (11)	Cu1—O7—C9—O8	−9.2 (2)
O2—C1—C2—C3	−42.1 (2)	Cu1—O7—C9—C10	166.48 (11)
O1—C1—C2—C3	135.45 (17)	O8—C9—C10—C6^{iii}	61.5 (2)
O2—C1—C2—C10^{i}	142.31 (17)	O7—C9—C10—C6^{iii}	−114.33 (17)
O1—C1—C2—C10^{i}	−40.1 (2)	O8—C9—C10—C2^{iv}	−124.93 (19)
C10^{i}—C2—C3—C7^{ii}	1.0 (3)	O7—C9—C10—C2^{iv}	59.2 (2)
C1—C2—C3—C7^{ii}	−174.62 (15)	N1'—C1'—C2'—N2'	179.25 (14)
Cu1—O3—C4—O4	−8.5 (2)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1'—H1'C···O2^{v}	0.91	2.18	2.921 (2)	138
N1'—H1'C···O5^{v}	0.91	2.30	2.993 (2)	132
N1'—H1'D···O4^{vi}	0.91	2.11	2.810 (2)	133
N1'—H1'E···O6^{i}	0.91	1.92	2.799 (2)	161
N2'—H2'C···O6	0.91	2.14	2.902 (2)	141
N2'—H2'D···O2^{vi}	0.91	1.92	2.807 (2)	164
N2'—H2'E···O8^{i}	0.91	2.09	2.810 (2)	135
O1W—H1WA···O2W^{vii}	0.85	2.32	3.116 (2)	157
O1W—H1WB···O3^{iii}	0.85	2.16	2.9784 (19)	162
O2W—H2WA···O1W	0.85	1.99	2.813 (2)	164
O2W—H2WB···O7	0.85	2.18	2.987 (2)	159

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

Fig. 1

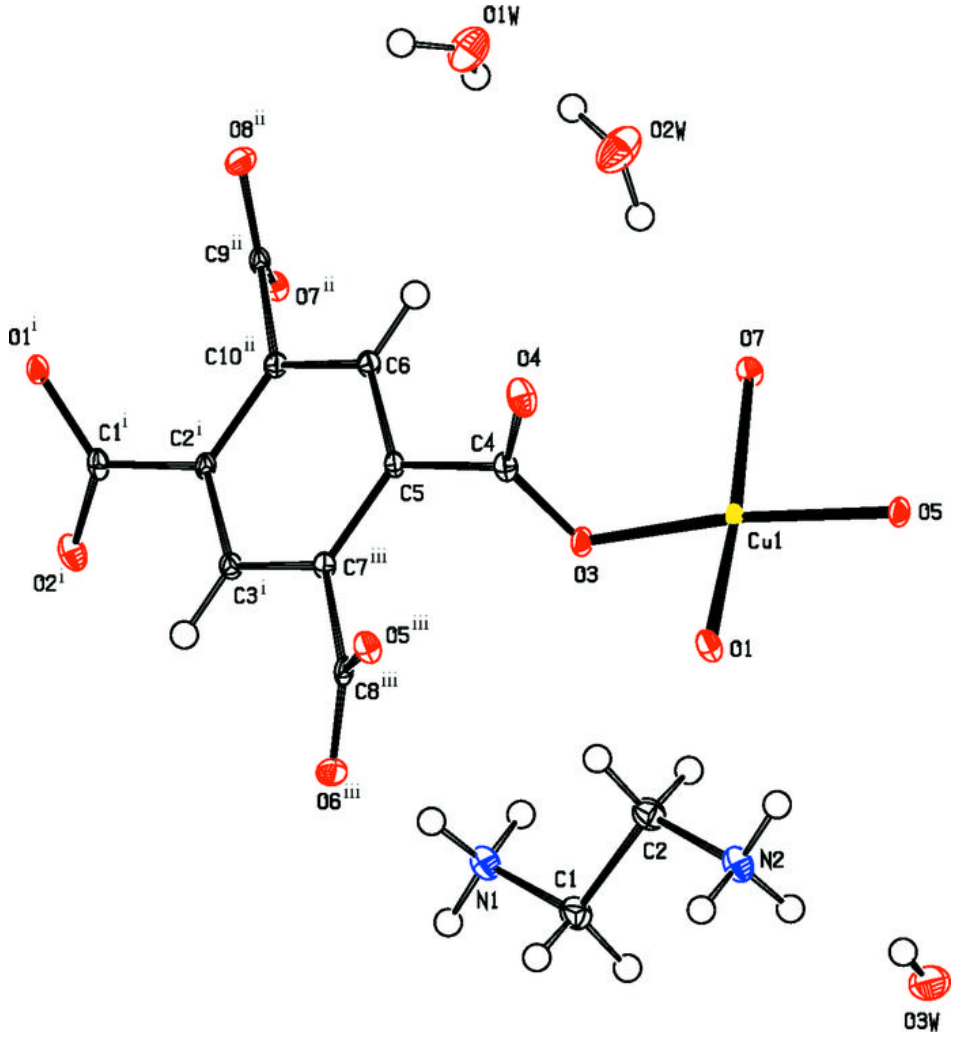
O1W
O2W
O8ii
C9ii
O7ii
O1i
C10ii
C6
O4
O7
C1i
C2i
C4
C5
O5
O2i
C7iii
Cu1
O3
C3i
O5iii
O1
C8iii
O6iii
C2
N2
C1
N1
O3W

Fig. 2