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Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)	Zhong, Zeng, Yang & Luo (2007*a*)	10.1107/S1600536807017461	ITCPCO01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)	Zhong, Zeng, Yang & Luo (2007*b*)	10.1107/S160053680701879X	AVUJEG02
Tetrakis(nitrato-κ^2O,O')bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^2N,N')tetrakis(nitrato-κ^2O,O')cerium(IV)	Zhong, Zeng, Yang & Luo (2007*d*)	10.1107/S1600536807021502	YIDNEF
(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)	Zhong, Yang, Luo & Xu (2007*a*)	10.1107/S1600536807028061	EDUTUT
(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)	Zhong, Yang, Luo & Xu (2007*b*)	10.1107/S1600536807028693	RIGQEE
(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)	Zhong, Yang, Luo & Xu (2007*g*)	10.1107/S1600536807035350	TIGFEV
2-Fluoro-3,5-dinitrobenzamide monohydrate	Zhong, Yang, Xie & Luo (2007*j*)	10.1107/S1600536807038676	VIKGAY
2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*k*)	10.1107/S1600536807039724	KILKIA
1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate	Zhong, Yang, Xie & Luo (2007*l*)	10.1107/S1600536807040779	AFETAH
N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*m*)	10.1107/S160053680704086X	AFINAF
catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*a*)	10.1107/S1600536807043528	PILDAQ
2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate	Zhong, Yang, Xie & Luo (2007*n*)	10.1107/S1600536807045199	XILWIZ
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*b*)	10.1107/S1600536807048489	WIMWEV
Hexaaquacopper(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*c*)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*d*)	10.1107/S1600536807051240	GIMZEI
Hexaaquachromium(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*e*)	10.1107/S1600536807051227	GIMZIM
Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*f*)	10.1107/S1600536807052051	QUKQES01
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*g*)	10.1107/S1600536807053494	NIQLAB
Hexaaquanickel(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*a*)	10.1107/S1600536807054372	HIPZOW
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*h*)	10.1107/S160053680705622X	XIRGOV
Hexaaquazinc(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*b*)	10.1107/S1600536807056498	XIRJEO
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*i*)	10.1107/S1600536807058540	HIQJOH
Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
catena-Poly[[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-κ^2N,N')-praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-di-μ-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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Hexaaquacopper(II) bis(4-methylbenzenesulfonate)

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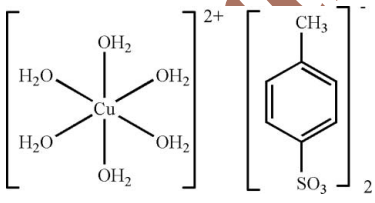
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.108; data-to-parameter ratio = 14.9.

The asymmetric unit of the title compound, $[Cu(H_2O)_6](C_7H_7O_3S)_2$, contains one half-cation and one anion; the Cu atom lies on an inversion centre. In the crystal structure, intermolecular O—H···O and O—H···S hydrogen bonds result in the formation of a supramolecular network structure; an intramolecular C—H···O hydrogen bond is also present.

Related literature

For general background, see: Desiraju (1995, 1997); Braga *et al.* (1998); Zaworotko (1997); Braga & Grepioni (2000); Moulton & Zaworotko (2001); Pan *et al.* (2001); Ma *et al.* (2001); Prior & Rosseinsky (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Cu(H_2O)_6](C_7H_7O_3S)_2$
M_r = 514.01
Monoclinic, $P2_1/n$
a = 6.9472 (4) Å
b = 6.2891 (3) Å
c = 25.1581 (14) Å
β = 91.565 (1)°
V = 1098.79 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 273 (2) K
0.48 × 0.37 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.588, T_{max} = 0.794
7237 measured reflections
2349 independent reflections
2004 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.108
S = 1.03
2349 reflections
158 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O4	2.045 (2)	Cu1—O6	2.046 (2)
Cu1—O5	2.0182 (19)		
O4^i—Cu1—O4	180	O5—Cu1—O5^i	180
O4—Cu1—O5^i	89.29 (9)	O5—Cu1—O6^i	89.29 (9)
O4—Cu1—O5	90.71 (9)	O5—Cu1—O6	90.71 (9)
O4—Cu1—O6	91.41 (12)	O6^i—Cu1—O6	180
O4—Cu1—O6^i	88.59 (12)		

Symmetry code: (i) $-x+1, -y, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2	0.93	2.59	2.938 (4)	103
O4—H4A···O1^{ii}	0.785 (17)	1.997 (19)	2.765 (3)	166 (3)
O6—H6A···O3^{iii}	0.796 (17)	1.984 (18)	2.772 (3)	171 (4)
O5—H5A···O1^{iv}	0.813 (17)	1.950 (18)	2.761 (3)	175 (3)
O5—H5A···S1^{iv}	0.813 (17)	3.055 (18)	3.839 (2)	163 (3)
O4—H4B···O2^{iv}	0.833 (17)	1.98 (2)	2.803 (3)	167 (4)
O5—H5B···O3^{v}	0.786 (17)	1.958 (17)	2.742 (3)	176 (3)
O6—H6B···O2^{v}	0.832 (17)	1.98 (2)	2.791 (3)	166 (4)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); 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: HK2341).

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supplementary materials

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Hexaaquacopper(II) bis(4-methylbenzenesulfonate)

H. Zhong, X.-M. Yang, H.-L. Xie and C.-J. Luo

Comment

In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Due to hydrogen-bonding interactions are of critical importance in biological systems, organic materials and coordination chemistry, hydrogen-bonding is currently the best tool in achieving this goal (Zaworotko, 1997; Braga & Grepioni, 2000). Supramolecular architectures are of considerable contemporary interest by virtue of their potential applications in various fields (Moulton & Zaworotko, 2001; Pan *et al.*, 2001; Ma *et al.*, 2001; Prior & Rosseinsky, 2001). We originally attempted to synthesize complexes featuring La and Cu metals chains by reaction of the lanthanum(III) and copper(II) ions with 4-methylbenzenesulfonic acid ligand. Unfortunately, we obtained only the title compound, (I), and we report herein its crystal structure.

The asymmetric unit of the title compound, (I), (Fig. 1) contains one half cation and one anion, in which the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).

In the crystal structure, intermolecular O—H···O and O—H···S hydrogen bonds (Table 1, Fig. 2) result in the formation of a supramolecular network structure; an intramolecular C—H···O hydrogen bond is also present.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Lanthanum (III) nitrate hexahydrate (216.4 mg, 0.5 mmol), copper nitrate hexahydrate (295.6 mg, 1 mmol), 4-methylbenzene- sulfonic acid (344.4 mg, 2 mmol), ammonia (0.5 mol/l, 4 ml) and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 443 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small blue crystals. These crystals were washed with distilled water followed by ethanol and allowed to air-dry at room temperature.

Refinement

H atoms (for H_2O) were located in difference syntheses and refined isotropically [O—H = 0.785 (17)–0.833 (17) Å and U_{iso}(H) = 0.058 (9) −0.080 (12) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å, for aromatic and methyl H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for aromatic H atoms.

Figures

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): 3/2 − x, 1/2 − y, 1/2 − z].

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

Hexaaquacopper(II) bis(4-methylbenzenesulfonate)

Crystal data

$[Cu(H_2O)_6](C_7H_7O_3S)_2$	$F_{000} = 534$
$M_r = 514.01$	$D_x = 1.554$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 5117 reflections
$a = 6.9472$ (4) Å	$\theta = 2.4$–28.3°
$b = 6.2891$ (3) Å	$\mu = 1.24$ mm^{-1}
$c = 25.1581$ (14) Å	$T = 273$ (2) K
$\beta = 91.565$ (1)°	Prism, blue
$V = 1098.79$ (10) Å^3	0.48 × 0.37 × 0.20 mm
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	2349 independent reflections
Radiation source: fine-focus sealed tube	2004 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 273(2)$ K	$\theta_{max} = 27.0^\circ$
φ and ω scans	$\theta_{min} = 3.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8\rightarrow8$
$T_{min} = 0.588$, $T_{max} = 0.794$	$k = -7\rightarrow7$
7237 measured reflections	$l = -32\rightarrow31$

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
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.4823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2349 reflections	$\Delta\rho_{max} = 0.35$ e Å^{-3}
158 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}

9 restraints
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 $F^2 > 2\mathrm{sigma}(F^2)$ 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	0.5000	0.0000	0.0000	0.04199 (16)
S1	−0.01464 (9)	0.60839 (10)	0.90519 (3)	0.04218 (18)
O1	0.1552 (3)	0.5134 (3)	0.93086 (9)	0.0539 (5)
O2	−0.0141 (3)	0.8398 (3)	0.90896 (8)	0.0533 (5)
O3	−0.1925 (3)	0.5162 (3)	0.92401 (9)	0.0544 (5)
O4	0.7237 (3)	−0.1026 (4)	0.04791 (11)	0.0726 (7)
O5	0.5088 (3)	0.2886 (3)	0.03508 (9)	0.0549 (5)
O6	0.3032 (4)	−0.1034 (4)	0.05323 (11)	0.0727 (7)
C1	−0.0452 (5)	0.6350 (7)	0.74521 (14)	0.0754 (10)
H1	−0.0789	0.7348	0.7193	0.090*
C2	−0.0544 (5)	0.6913 (6)	0.79850 (13)	0.0639 (8)
H2	−0.0946	0.8267	0.8081	0.077*
C3	−0.0035 (4)	0.5452 (5)	0.83688 (11)	0.0462 (6)
C4	0.0521 (5)	0.3430 (5)	0.82212 (12)	0.0606 (7)
H4	0.0841	0.2424	0.8480	0.073*
C5	0.0601 (5)	0.2907 (6)	0.76879 (13)	0.0702 (9)
H5	0.0985	0.1547	0.7592	0.084*
C6	0.0123 (5)	0.4356 (7)	0.72983 (13)	0.0694 (9)
C7	0.0308 (6)	0.3770 (9)	0.67186 (14)	0.0989 (15)
H7B	0.1610	0.3353	0.6655	0.148*
H7A	−0.0025	0.4975	0.6501	0.148*
H7C	−0.0545	0.2611	0.6633	0.148*
H4A	0.763 (4)	−0.220 (3)	0.0485 (12)	0.059 (10)*
H5A	0.610 (3)	0.340 (5)	0.0462 (12)	0.058 (9)*
H6A	0.261 (5)	−0.220 (3)	0.0575 (15)	0.080 (12)*
H4B	0.814 (4)	−0.020 (4)	0.0558 (15)	0.069 (11)*
H5B	0.419 (3)	0.342 (5)	0.0480 (12)	0.059 (10)*
H6B	0.216 (4)	−0.017 (4)	0.0593 (14)	0.065 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0394 (2)	0.0311 (3)	0.0555 (3)	0.00069 (16)	0.00176 (18)	0.00152 (17)
S1	0.0414 (3)	0.0320 (3)	0.0532 (4)	0.0005 (2)	0.0027 (2)	−0.0004 (3)
O1	0.0559 (11)	0.0410 (11)	0.0641 (12)	0.0056 (8)	−0.0113 (10)	−0.0018 (8)
O2	0.0529 (10)	0.0318 (10)	0.0754 (13)	0.0002 (8)	0.0044 (9)	−0.0022 (9)
O3	0.0536 (11)	0.0405 (11)	0.0701 (13)	−0.0043 (8)	0.0171 (10)	−0.0020 (8)
O4	0.0691 (14)	0.0359 (12)	0.1105 (19)	0.0052 (11)	−0.0400 (13)	0.0005 (12)
O5	0.0451 (11)	0.0380 (11)	0.0816 (14)	−0.0005 (9)	0.0052 (10)	−0.0146 (9)
O6	0.0746 (15)	0.0363 (12)	0.1095 (19)	−0.0008 (11)	0.0460 (14)	0.0054 (12)
C1	0.067 (2)	0.098 (3)	0.0618 (19)	0.007 (2)	−0.0002 (16)	0.0239 (19)
C2	0.0637 (18)	0.059 (2)	0.0689 (19)	0.0101 (15)	0.0047 (14)	0.0124 (15)
C3	0.0392 (12)	0.0463 (15)	0.0532 (15)	0.0002 (11)	0.0015 (11)	0.0022 (11)
C4	0.074 (2)	0.0507 (18)	0.0575 (16)	0.0096 (14)	−0.0003 (14)	−0.0018 (14)
C5	0.080 (2)	0.069 (2)	0.0618 (19)	0.0039 (18)	0.0046 (16)	−0.0145 (16)
C6	0.0511 (17)	0.099 (3)	0.0579 (18)	−0.0072 (18)	0.0023 (14)	−0.0035 (18)
C7	0.085 (3)	0.156 (5)	0.056 (2)	−0.005 (3)	0.0067 (18)	−0.008 (2)

Geometric parameters (Å, °)

Cu1—O4^{i}	2.045 (2)	O6—H6B	0.832 (17)
Cu1—O4	2.045 (2)	C1—C6	1.375 (6)
Cu1—O5	2.0182 (19)	C1—C2	1.390 (5)
Cu1—O5^{i}	2.0182 (19)	C1—H1	0.9300
Cu1—O6^{i}	2.046 (2)	C2—C3	1.372 (4)
Cu1—O6	2.046 (2)	C2—H2	0.9300
S1—O3	1.456 (2)	C3—C4	1.382 (4)
S1—O1	1.458 (2)	C4—C5	1.384 (4)
S1—O2	1.458 (2)	C4—H4	0.9300
S1—C3	1.768 (3)	C5—C6	1.373 (5)
O4—H4A	0.785 (17)	C5—H5	0.9300
O4—H4B	0.833 (17)	C6—C7	1.513 (5)
O5—H5A	0.813 (17)	C7—H7B	0.9600
O5—H5B	0.786 (17)	C7—H7A	0.9600
O6—H6A	0.796 (17)	C7—H7C	0.9600
O4^{i}—Cu1—O4	180.00 (18)	Cu1—O6—H6A	129 (3)
O4—Cu1—O5^{i}	89.29 (9)	Cu1—O6—H6B	115 (2)
O4^{i}—Cu1—O5^{i}	90.71 (9)	H6A—O6—H6B	107 (2)
O4—Cu1—O5	90.71 (9)	C6—C1—C2	121.7 (3)
O4^{i}—Cu1—O5	89.29 (9)	C6—C1—H1	119.2
O4^{i}—Cu1—O6	88.59 (12)	C2—C1—H1	119.2
O4—Cu1—O6	91.41 (12)	C3—C2—C1	119.4 (3)
O4^{i}—Cu1—O6^{i}	91.41 (12)	C3—C2—H2	120.3
O4—Cu1—O6^{i}	88.59 (12)	C1—C2—H2	120.3

O5—Cu1—O5^{i}	180.00 (12)	C2—C3—C4	119.7 (3)
O5—Cu1—O6^{i}	89.29 (9)	C2—C3—S1	121.1 (2)
O5^{i}—Cu1—O6^{i}	90.71 (9)	C4—C3—S1	119.2 (2)
O5—Cu1—O6	90.71 (9)	C3—C4—C5	119.9 (3)
O5^{i}—Cu1—O6	89.29 (9)	C3—C4—H4	120.1
O6^{i}—Cu1—O6	180.00 (12)	C5—C4—H4	120.1
O3—S1—O1	112.13 (13)	C6—C5—C4	121.3 (3)
O3—S1—O2	112.14 (11)	C6—C5—H5	119.4
O1—S1—O2	112.30 (12)	C4—C5—H5	119.4
O3—S1—C3	106.67 (13)	C5—C6—C1	118.1 (3)
O1—S1—C3	106.39 (12)	C5—C6—C7	120.1 (4)
O2—S1—C3	106.72 (13)	C1—C6—C7	121.8 (4)
Cu1—O4—H4A	124 (2)	C6—C7—H7B	109.5
Cu1—O4—H4B	120 (2)	C6—C7—H7A	109.5
H4A—O4—H4B	109 (2)	H7B—C7—H7A	109.5
Cu1—O5—H5A	122 (2)	C6—C7—H7C	109.5
Cu1—O5—H5B	124 (2)	H7B—C7—H7C	109.5
H5A—O5—H5B	112 (3)	H7A—C7—H7C	109.5

Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2	0.93	2.59	2.938 (4)	103
O4—H4A···O1^{ii}	0.785 (17)	1.997 (19)	2.765 (3)	166 (3)
O6—H6A···O3^{iii}	0.796 (17)	1.984 (18)	2.772 (3)	171 (4)
O5—H5A···O1^{iv}	0.813 (17)	1.950 (18)	2.761 (3)	175 (3)
O5—H5A···S1^{iv}	0.813 (17)	3.055 (18)	3.839 (2)	163 (3)
O4—H4B···O2^{iv}	0.833 (17)	1.98 (2)	2.803 (3)	167 (4)
O5—H5B···O3^{v}	0.786 (17)	1.958 (17)	2.742 (3)	176 (3)
O6—H6B···O2^{v}	0.832 (17)	1.98 (2)	2.791 (3)	166 (4)

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

Fig. 1

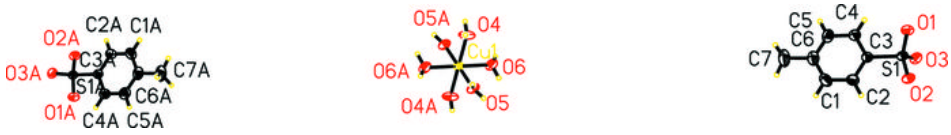

Fig. 2