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catena-Poly[[aquacopper(II)]-μ-[(*S*)-*N*-(2-hydroxybenzyl)-L-aspartato]]

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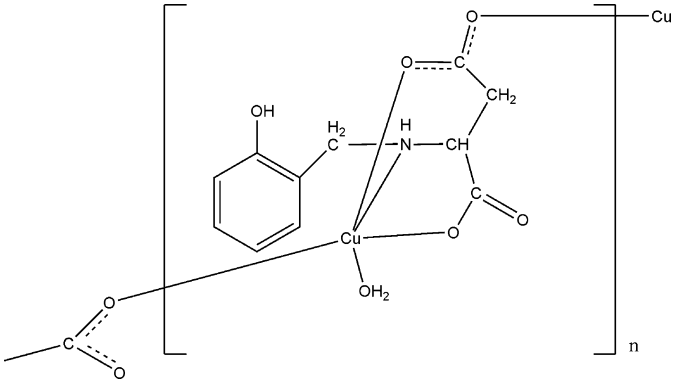
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.079; data-to-parameter ratio = 17.1.

The title compound, $[Cu(C_{11}H_{11}NO_5)(H_2O)]_n$, was obtained by the reaction of $Cu(NO_3)_2$ and the homochiral organic ligand (*S*)-*N*-(2-hydroxybenzyl)-L-aspartic acid (*S*-H_3sasp). The Cu^{II} ion has a distorted square-pyramidal geometry and is coordinated by one N atom and three O atoms from the organic ligand and one O atom from a water molecule. The carboxyl O atoms of the ligands bridge the Cu atoms to form an infinite one-dimensional zigzag chain. Intermolecular hydrogen bonds link these chains into a two-dimensional arrangement.

Related literature

For related literature, see: Yang *et al.* (2004); Lü *et al.* (2005); Sreenivasulu & Vittal (2004); Sreenivasulu *et al.* (2005); Wang *et al.* (2006).



Experimental

Crystal data

$[Cu(C_{11}H_{11}NO_5)(H_2O)]$
M_r = 318.77
Monoclinic, $P2_1$
a = 5.9107 (13) Å
b = 8.826 (2) Å
c = 11.903 (3) Å
β = 93.787 (19)°
V = 619.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.79 mm^{-1}
T = 293 (2) K
0.2 × 0.2 × 0.2 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.690, T_{max} = 0.703
6500 measured reflections
2934 independent reflections
2532 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.079
S = 0.99
2934 reflections
172 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Absolute structure: Flack (1983), 1355 Friedel pairs
Flack parameter: 0.064 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2^{i}	0.82	1.91	2.688 (3)	158
O1W—H1WB···O4^{ii}	0.84	2.30	2.913 (4)	129
N1—H1B···O3^{i}	0.96	1.93	2.843 (4)	158
O1—H1A···O5^{iii}	0.82	2.02	2.837 (4)	178

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1999); 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: PK2047).

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supplementary materials

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catena-Poly[[aquacopper(II)]-μ-[(*S*)-*N*-(2-hydroxybenzyl)-L-aspartato]]

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Comment

In the past several years, considerable attention has been paid to the design and construction of chiral supramolecular architecture owing to their potential applications in enantioselective synthesis, asymmetric catalysis, magnetism and nonlinear optical materials (Lü *et al.*, 2005). Among these supramolecular structures, one-dimensional coordination polymers appear to dominate the literature, involving linear, zigzag and helical polymers (Wang *et al.*, 2006). In addition, the one-dimensional polymers can further assemble *via* hydrogen bonds or other non-covalent interactions to give two-dimensional or three-dimensional coordination polymeric structures (Yang *et al.*, 2004).

We have focused on the synthesis of multi-dimensional network structures from a flexible chiral multi-dentate ligand, namely the reduced Schiff base formed between salicylaldehyde and *L*-aspartic acid (Sreenivasulu *et al.*, 2005). Here we report the synthesis and crystal structure of the title compound.

As shown in Fig. 1, there exists a chiral center C8 in the organic ligand *S*-H_3sasp which induces the title compound to crystallize in a chiral space group $P2_1$. In the title compound, the central Cu atom is five- coordinated and adopts a distorted square-pyramidal geometry. The coordination environment is defined by one N atom and three O atoms from the *S*-H_3sasp ligand, and one O atom from the water molecule. The carboxyl O of the ligands bridge the Cu atoms to form an infinite one-dimensional zigzag chain.

The intermolecular hydrogen bonds, O1W—H1WA···O2, O1W—H1WB···O4, O1—H1A···O5, N1—H1B···O3 and other non-covalent interactions link the coordination polymer into a two-dimensional network (Table 2 and Fig. 2).

Experimental

The homochiral reduced Schiff-base ligand *S*-*N*-(2-hydroxybenzyl)-*L*-aspartic acid was synthesized by the reaction of salicylaldehyde and *L*-aspartic acid according to the published procedure described in the literature (Sreenivasulu & Vittal, 2004). A mixture of *S*-*N*-(2-hydroxybenzyl)-*L*-aspartic acid (23.9 mg, 0.1 mmol) and $Cu(NO_3)_2.3H_2O$ (24.2 mg, 0.1 mmol) were dissolved in water and methanol. Blue crystals suitable for X-ray analysis were obtained by slow evaporation at room temperature over several days.

Refinement

The water H atoms bonded to O1W were located in a difference map and refined with distance restraints of O1W—H = 0.83 (2) but were subsequently fixed. Other H atoms were calculated geometrically and were allowed to ride on the atoms to which they are bonded. U_{iso}(H) values were 1.5Ueq(O) and 1.2Ueq(C or N).

Figures

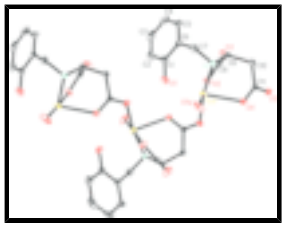

Fig. 1. The molecular structure of the compound with the atomic numbering scheme. Displacement ellipsoids are at the 30% probability level and all hydrogen atoms are omitted for clarity.

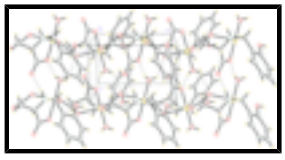

Fig. 2. A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[Cu(C_{11}H_{11}NO_5)(H_2O)]$	F_{000} = 326
M_r = 318.77	D_x = 1.709 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 1876 reflections
a = 5.9107 (13) Å	θ = 3.4–27.5º
b = 8.826 (2) Å	μ = 1.79 mm^{-1}
c = 11.903 (3) Å	T = 293 (2) K
β = 93.787 (19)º	Prism, colourless
V = 619.6 (3) Å^3	0.2 × 0.2 × 0.2 mm
Z = 2	

Data collection

Rigaku Mercury2 (2x2 bin mode) diffractometer	2934 independent reflections
Radiation source: fine-focus sealed tube	2532 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 27.9º
T = 293(2) K	θ_{min} = 2.9º
ω scans	h = −7→7
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −11→11
T_{min} = 0.690, T_{max} = 0.703	l = −15→15
6500 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.079$

$S = 0.99$

2934 reflections

172 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0135P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.48$ e Å^{-3}

$\Delta\rho_{min} = -0.41$ e Å^{-3}

Extinction correction: none

Absolute structure: Flack (1983), 1355 Friedel pairs

Flack parameter: 0.064 (16)

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 $F^2 > 2\sigma(F^2)$ 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	0.10776 (6)	0.12114 (6)	0.91119 (3)	0.02344 (12)
O2	−0.2062 (4)	0.0614 (3)	0.8604 (2)	0.0281 (6)
O1W	0.4293 (4)	0.1802 (3)	0.9514 (2)	0.0474 (9)
H1WA	0.5139	0.1301	0.9141	0.071*
H1WB	0.4689	0.2697	0.9684	0.071*
N1	0.1790 (5)	0.0507 (3)	0.7580 (2)	0.0202 (6)
H1B	0.3241	0.0025	0.7702	0.024*
O1	0.0408 (5)	0.3744 (3)	0.8257 (2)	0.0410 (7)
H1A	0.0157	0.4558	0.8557	0.061*
C8	0.0087 (6)	−0.0670 (4)	0.7261 (3)	0.0212 (8)
H8A	−0.0121	−0.0715	0.6438	0.025*
O3	−0.3920 (4)	−0.0856 (3)	0.7316 (3)	0.0415 (8)
C6	−0.0171 (7)	0.2611 (4)	0.6464 (3)	0.0285 (9)
C9	−0.2184 (6)	−0.0274 (4)	0.7737 (3)	0.0226 (8)
C1	−0.0879 (7)	0.3633 (5)	0.7264 (3)	0.0309 (9)
C2	−0.2846 (7)	0.4502 (5)	0.7032 (4)	0.0408 (11)
H2A	−0.3337	0.5172	0.7568	0.049*
C5	−0.1454 (8)	0.2473 (5)	0.5451 (3)	0.0393 (12)
H5A	−0.1014	0.1782	0.4918	0.047*
C7	0.1977 (7)	0.1710 (4)	0.6726 (3)	0.0312 (9)
H7A	0.2426	0.1250	0.6035	0.037*

H7B	0.3173	0.2403	0.6987	0.037*
C3	−0.4050 (8)	0.4350 (6)	0.6000 (4)	0.0506 (13)
H3A	−0.5334	0.4938	0.5835	0.061*
C10	0.0854 (6)	−0.2238 (4)	0.7707 (3)	0.0239 (8)
H10A	−0.0131	−0.3008	0.7358	0.029*
H10B	0.2382	−0.2434	0.7493	0.029*
C11	0.0808 (6)	−0.2362 (4)	0.8979 (3)	0.0238 (8)
C4	−0.3354 (9)	0.3333 (6)	0.5220 (4)	0.0505 (13)
H4A	−0.4177	0.3229	0.4531	0.061*
O5	−0.0374 (4)	−0.3461 (3)	0.9343 (2)	0.0297 (7)
O4	0.1842 (5)	−0.1414 (3)	0.9602 (2)	0.0350 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01864 (19)	0.0292 (2)	0.0225 (2)	−0.0011 (2)	0.00118 (15)	−0.0045 (2)
O2	0.0185 (13)	0.0362 (14)	0.0302 (14)	−0.0005 (11)	0.0067 (11)	−0.0075 (12)
O1W	0.0204 (15)	0.061 (2)	0.060 (2)	−0.0040 (13)	0.0016 (14)	−0.0351 (17)
N1	0.0182 (15)	0.0212 (14)	0.0213 (15)	−0.0010 (12)	0.0014 (12)	−0.0015 (13)
O1	0.0457 (18)	0.0356 (16)	0.0408 (17)	0.0072 (14)	−0.0029 (15)	−0.0119 (14)
C8	0.0221 (19)	0.0250 (18)	0.0167 (17)	−0.0038 (16)	0.0027 (15)	−0.0007 (15)
O3	0.0161 (14)	0.054 (2)	0.0540 (19)	−0.0037 (13)	−0.0015 (13)	−0.0196 (15)
C6	0.039 (2)	0.0231 (19)	0.024 (2)	−0.0066 (17)	0.0083 (18)	0.0059 (16)
C9	0.0185 (18)	0.028 (2)	0.0207 (18)	0.0008 (15)	−0.0036 (15)	0.0019 (15)
C1	0.034 (2)	0.024 (2)	0.034 (2)	−0.0066 (18)	0.0044 (19)	0.0021 (18)
C2	0.038 (2)	0.027 (2)	0.057 (3)	−0.002 (2)	0.003 (2)	0.001 (2)
C5	0.060 (3)	0.038 (3)	0.020 (2)	−0.010 (2)	0.002 (2)	0.0048 (19)
C7	0.036 (2)	0.026 (2)	0.033 (2)	−0.0079 (16)	0.0151 (18)	0.0016 (15)
C3	0.036 (3)	0.039 (2)	0.077 (4)	−0.006 (2)	0.000 (3)	0.028 (3)
C10	0.024 (2)	0.0228 (18)	0.0253 (19)	−0.0027 (16)	0.0057 (16)	−0.0012 (16)
C11	0.027 (2)	0.0228 (18)	0.0220 (19)	0.0082 (16)	0.0042 (17)	0.0037 (15)
C4	0.059 (3)	0.055 (3)	0.035 (3)	−0.018 (3)	−0.014 (2)	0.024 (2)
O5	0.0316 (14)	0.0326 (19)	0.0252 (13)	−0.0070 (12)	0.0045 (11)	0.0059 (11)
O4	0.0492 (18)	0.0286 (15)	0.0255 (14)	−0.0088 (15)	−0.0093 (13)	0.0005 (12)

Geometric parameters (Å, °)

Cu1—O5^{i}	1.934 (2)	C6—C1	1.395 (6)
Cu1—O2	1.985 (3)	C6—C7	1.513 (5)
Cu1—N1	1.998 (3)	C1—C2	1.405 (6)
Cu1—O1W	1.998 (3)	C2—C3	1.385 (6)
Cu1—O4	2.424 (3)	C2—H2A	0.9300
O2—C9	1.294 (4)	C5—C4	1.368 (7)
O1W—H1WA	0.8200	C5—H5A	0.9300
O1W—H1WB	0.8442	C7—H7A	0.9700
N1—C8	1.479 (4)	C7—H7B	0.9700
N1—C7	1.479 (4)	C3—C4	1.374 (7)
N1—H1B	0.9600	C3—H3A	0.9300

O1—C1	1.366 (4)	C10—C11	1.520 (5)
O1—H1A	0.8200	C10—H10A	0.9700
C8—C9	1.532 (5)	C10—H10B	0.9700
C8—C10	1.540 (5)	C11—O4	1.250 (5)
C8—H8A	0.9800	C11—O5	1.287 (4)
O3—C9	1.225 (4)	C4—H4A	0.9300
C6—C5	1.387 (6)	O5—Cu1^{ii}	1.934 (2)
O5^{i}—Cu1—O2	94.24 (11)	O1—C1—C6	117.5 (4)
O5^{i}—Cu1—N1	170.47 (11)	O1—C1—C2	122.5 (4)
O2—Cu1—N1	83.59 (12)	C6—C1—C2	120.1 (4)
O5^{i}—Cu1—O1W	89.66 (11)	C3—C2—C1	119.4 (4)
O2—Cu1—O1W	176.09 (11)	C3—C2—H2A	120.3
N1—Cu1—O1W	92.61 (12)	C1—C2—H2A	120.3
O5^{i}—Cu1—O4	87.84 (10)	C4—C5—C6	121.4 (4)
O2—Cu1—O4	88.57 (10)	C4—C5—H5A	119.3
N1—Cu1—O4	82.84 (11)	C6—C5—H5A	119.3
O1W—Cu1—O4	91.87 (11)	N1—C7—C6	114.7 (3)
C9—O2—Cu1	113.9 (2)	N1—C7—H7A	108.6
Cu1—O1W—H1WA	109.5	C6—C7—H7A	108.6
Cu1—O1W—H1WB	123.1	N1—C7—H7B	108.6
H1WA—O1W—H1WB	117.7	C6—C7—H7B	108.6
C8—N1—C7	114.1 (3)	H7A—C7—H7B	107.6
C8—N1—Cu1	105.8 (2)	C4—C3—C2	120.2 (4)
C7—N1—Cu1	115.7 (2)	C4—C3—H3A	119.9
C8—N1—H1B	108.3	C2—C3—H3A	119.9
C7—N1—H1B	108.4	C11—C10—C8	112.6 (3)
Cu1—N1—H1B	103.9	C11—C10—H10A	109.1
C1—O1—H1A	109.5	C8—C10—H10A	109.1
N1—C8—C9	110.1 (3)	C11—C10—H10B	109.1
N1—C8—C10	111.3 (3)	C8—C10—H10B	109.1
C9—C8—C10	108.8 (3)	H10A—C10—H10B	107.8
N1—C8—H8A	108.9	O4—C11—O5	124.0 (3)
C9—C8—H8A	108.9	O4—C11—C10	120.2 (3)
C10—C8—H8A	108.9	O5—C11—C10	115.8 (3)
C5—C6—C1	118.6 (4)	C5—C4—C3	120.3 (4)
C5—C6—C7	122.4 (4)	C5—C4—H4A	119.8
C1—C6—C7	119.0 (4)	C3—C4—H4A	119.8
O3—C9—O2	125.6 (3)	C11—O5—Cu1^{ii}	126.0 (2)
O3—C9—C8	118.9 (3)	C11—O4—Cu1	114.9 (2)
O2—C9—C8	115.4 (3)		
O5^{i}—Cu1—O2—C9	−153.3 (2)	O1—C1—C2—C3	179.0 (4)
N1—Cu1—O2—C9	17.3 (2)	C6—C1—C2—C3	−1.0 (6)
O4—Cu1—O2—C9	−65.6 (2)	C1—C6—C5—C4	1.2 (6)
O2—Cu1—N1—C8	−28.4 (2)	C7—C6—C5—C4	−178.0 (4)
O1W—Cu1—N1—C8	152.5 (2)	C8—N1—C7—C6	60.9 (4)
O4—Cu1—N1—C8	61.0 (2)	Cu1—N1—C7—C6	−62.2 (4)
O2—Cu1—N1—C7	99.0 (3)	C5—C6—C7—N1	−108.9 (4)

O1W—Cu1—N1—C7	−80.0 (3)	C1—C6—C7—N1	71.9 (4)
O4—Cu1—N1—C7	−171.6 (3)	C1—C2—C3—C4	1.5 (6)
C7—N1—C8—C9	−93.8 (3)	N1—C8—C10—C11	70.4 (4)
Cu1—N1—C8—C9	34.5 (3)	C9—C8—C10—C11	−51.0 (4)
C7—N1—C8—C10	145.4 (3)	C8—C10—C11—O4	−54.0 (5)
Cu1—N1—C8—C10	−86.2 (3)	C8—C10—C11—O5	124.7 (3)
Cu1—O2—C9—O3	175.6 (3)	C6—C5—C4—C3	−0.7 (6)
Cu1—O2—C9—C8	−1.0 (4)	C2—C3—C4—C5	−0.6 (6)
N1—C8—C9—O3	159.8 (3)	O4—C11—O5—Cu1^{ii}	6.6 (5)
C10—C8—C9—O3	−78.0 (4)	C10—C11—O5—Cu1^{ii}	−172.1 (2)
N1—C8—C9—O2	−23.4 (4)	O5—C11—O4—Cu1	−128.6 (3)
C10—C8—C9—O2	98.9 (3)	C10—C11—O4—Cu1	50.0 (4)
C5—C6—C1—O1	179.7 (3)	O5^{i}—Cu1—O4—C11	127.5 (3)
C7—C6—C1—O1	−1.1 (5)	O2—Cu1—O4—C11	33.2 (3)
C5—C6—C1—C2	−0.3 (6)	N1—Cu1—O4—C11	−50.5 (3)
C7—C6—C1—C2	178.9 (3)	O1W—Cu1—O4—C11	−142.9 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O2^{iii}	0.82	1.91	2.688 (3)	158
O1W—H1WB···O4^{iv}	0.84	2.30	2.913 (4)	129
N1—H1B···O3^{iii}	0.96	1.93	2.843 (4)	158
O1—H1A···O5^{v}	0.82	2.02	2.837 (4)	178

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

Fig. 1

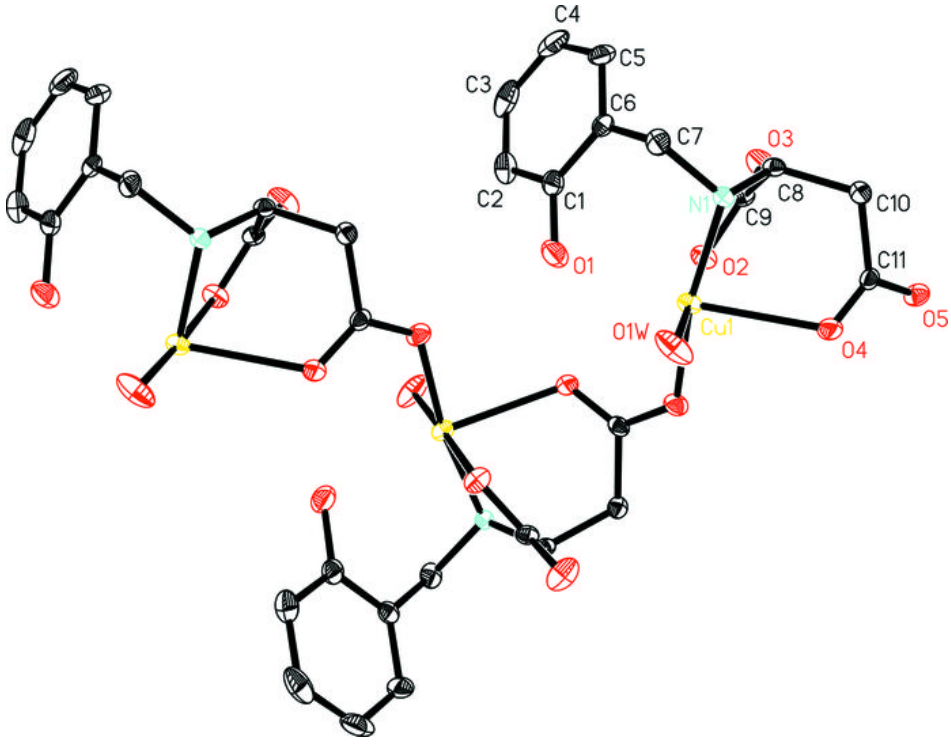

Fig. 2