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μ-4,4′-Bipyridine-bis[aqua(*N*-salicylideneaspartato)copper(II)]

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Key indicators

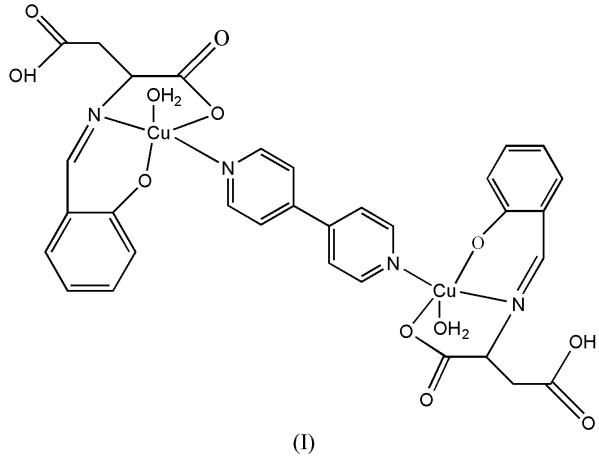
Single-crystal X-ray study
T = 130 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.113
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title complex has a binuclear structure, formulated as $[Cu_2(C_{11}H_9NO_3)_2(C_{10}H_8N_2)(H_2O)_2]$. It is a centrosymmetric molecule with both D- and L-sasp ligands (sasp is the *N*-salicylideneaspartic acid anion) coordinated to the Cu^{II} centers which are bridged by 4,4′-bipyridine. Intermolecular hydrogen bonds give rise to a three-dimensional supramolecular structure.

Comment

Copper(II)–amino acid complexes and their derivatives have attracted considerable attention due to their biochemical and pharmacological properties (Sarkar, 1999; Deschamps *et al.*, 2003). Whilst investigating the preparation of Schiff base copper complexes with amino acid ligands, the title binuclear compound, (I), was obtained.



(I)

The title compound has a centrosymmetric binuclear molecule in which the sasp (sasp is *N*-salicylideneaspartate) anion acts as a tridentate ligand chelating the Cu^{II} atom

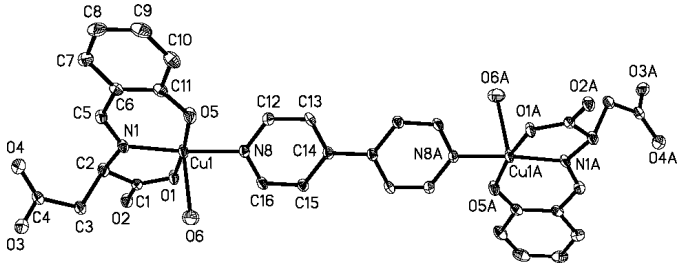


Figure 1
The structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level. The suffix A indicates the symmetry code $(2-x, 1-y, 1-z)$.

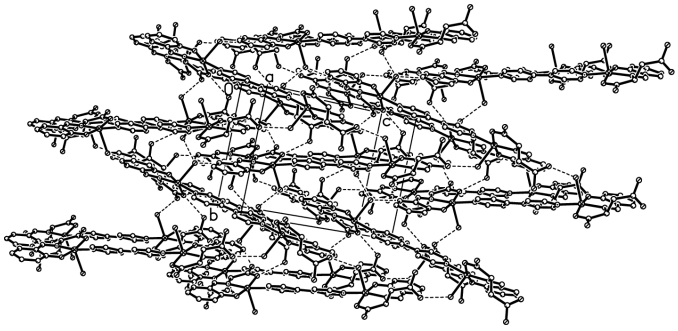


Figure 2
The three-dimensional packing of the complex. Dashed lines indicate hydrogen bonds.

through the phenolate O atom, an N atom and a carboxylic acid O atom. 4,4′-Bipyridine bridges two Cu^{II} centers and apical water molecules complete the nearly square-pyramidal geometry of the Cu^{II} centers. The binuclear structure is shown Fig. 1 and selected distances and angles are listed in Table 1.

The binuclear molecules interact through intermolecular hydrogen bonds (Table 2), giving a three-dimensional supramolecular structure, as shown in Fig. 2.

Experimental

To an aqueous solution (10 ml) of D,L-aspartic acid (0.067 g, 0.50 mmol) and NaOH (0.040 g, 1.00 mmol), salicylaldehyde (0.061 g, 0.50 mmol) in ethanol (5 ml) was added slowly. The solution was stirred for 30 min and then $Cu(NO_3)_2{\cdot}2H_2O$ (0.120 g, 0.50 mmol) in water (5 ml) was added. To the resulting solution, 4,4′-bipyridine (0.040 g, 0.25 mmol) in ethanol (5 ml) was added slowly. After filtration, the solution was allowed to stand in air and after several days, blue crystals were obtained in 40% yield.

Crystal data

$[Cu_2(C_{11}H_9NO_3)_2(C_{10}H_8N_2)(H_2O)_2]$
M_r = 789.68
Monoclinic, $P2_1/n$
a = 10.2015 (17) Å
b = 10.6210 (13) Å
c = 14.872 (2) Å
β = 106.838 (8)°
V = 1542.3 (4) Å^3
Z = 2
D_x = 1.700 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3383 reflections
θ = 3.4–27.5°
μ = 1.45 mm^{-1}
T = 130 (2) K
Prism, blue
0.25 × 0.15 × 0.08 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.611, T_{max} = 0.890
11 473 measured reflections
3516 independent reflections
3004 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°
$h = -11 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -19 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.113
S = 1.09
3516 reflections
236 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 1.5366P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O5	1.900 (2)	Cu1—O1	2.014 (2)
Cu1—N1	1.938 (2)	Cu1—O6	2.335 (3)
Cu1—N8	1.997 (2)		
O5—Cu1—N1	93.85 (9)	N8—Cu1—O1	91.20 (9)
O5—Cu1—N8	90.84 (9)	O5—Cu1—O6	99.55 (10)
N1—Cu1—N8	168.76 (10)	N1—Cu1—O6	100.69 (10)
O5—Cu1—O1	169.16 (9)	N8—Cu1—O6	88.58 (10)
N1—Cu1—O1	82.34 (9)	O1—Cu1—O6	91.15 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1^{i}	0.84	1.86	2.661 (3)	160
O6—H6A···O2^{i}	0.67 (4)	2.09 (4)	2.760 (3)	173 (5)
O6—H6B···O4^{ii}	0.94 (5)	1.90 (5)	2.812 (3)	160 (4)

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

The H atoms of water molecules and the H atom bound to C5 were located in difference Fourier maps; the former were refined freely. Other H atoms were positioned geometrically and, together with H5, were constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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