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Aqua(2,2′-bipyridine-κ²N,N′)(L-cysteato-κ²N,O)-copper(II) dihydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.028
wR factor = 0.078
Data-to-parameter ratio = 9.7

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

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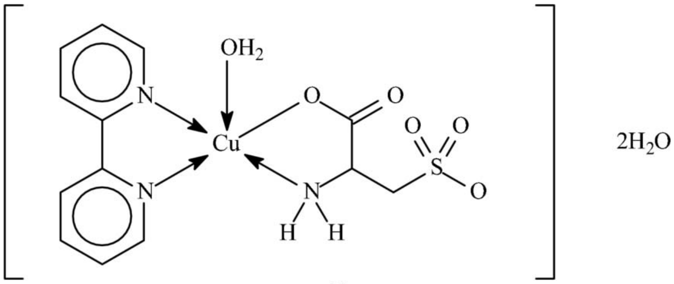
The Cu atom in the title compound, $[Cu(C_3H_5NO_5S)(C_{10}H_8N_2)(H_2O)]\cdot 2H_2O$, exists in a square-pyramidal environment. The two independent mononuclear complex molecules and the four uncoordinated water molecules in the asymmetric unit are engaged in extensive hydrogen-bonding interactions, forming a three-dimensional network.

Comment

Although the Cambridge Structural Database (Version 5.27; Allen, 2002) contains a large number of transition metal derivatives of amino acids, it does not list any metal derivative of cysteic acid, an amino acid having a sulfonate substituent. The crystal structure of L-cysteic acid monohydrate has been determined by X-ray diffraction (Hendrickson & Karle, 1971) and neutron diffraction (Ramanadham *et al.*, 1973) data. The structure of DL-cysteic acid was been reported a long time ago (Clarke & Steward, 1971); a strontium complex of this has recently been reported (Liu *et al.*, 2005).



(I)

The asymmetric unit consists of two complex molecules and four solvent molecules. The cysteate dianion in the title copper complex (I) behaves in a manner typical of amino acids in that it chelates through the amino and carboxylate ends only, leaving the sulfonate end free. The *N*-heterocycle also functions in a chelating mode, and the square-pyramidal geometry is completed by a water molecule. The two independent mononuclear molecules interact with the four uncoordinated water molecules through hydrogen bonds (Table 2), forming a three-dimensional network.

Experimental

L-Cysteic acid (0.094 g, 0.5 mmol) and potassium hydroxide (0.06 g, 1 mmol) dissolved in water (10 ml) were added to a 1:1 methanol–water (10 ml) solution of copper(II) chloride dihydrate (0.085 g, 0.5 mmol). To this mixture was added a solution of 2,2′-bipyridine (0.078 g, 0.5 mmol) in methanol (4 ml). The blue solution was set aside for two weeks for the growth of blue prismatic crystals.

Crystal data

$[Cu(C_3H_5NO_5S)(C_{10}H_8N_2)(H_2O)]\cdot 2H_2O$
$M_r = 440.91$
Triclinic, $P1$
$a = 7.7463$ (2) Å
$b = 10.3041$ (2) Å
$c = 11.7022$ (2) Å
$\alpha = 74.585$ (8)°
$\beta = 78.996$ (8)°
$\gamma = 74.596$ (8)°
$V = 860.81$ (3) Å^3
$Z = 2$
$D_x = 1.701$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.44$ mm^{-1}
$T = 293$ (2) K
Prism, blue
0.45 × 0.32 × 0.22 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min} = 0.564$, $T_{max} = 0.743$
6541 measured reflections
5011 independent reflections
4643 reflections with $I > 2\sigma(I)$
$R_{int} = 0.009$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.078$
$S = 1.02$
5011 reflections
517 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Absolute structure: Flack (1983), 1171 Friedel pairs
Flack parameter: 0.01 (1)

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.924 (3)	Cu2—O6	1.929 (3)
Cu1—O1w	2.329 (4)	Cu2—O4*W*	2.303 (4)
Cu1—N1	2.001 (4)	Cu2—N4	2.012 (4)
Cu1—N2	2.011 (4)	Cu2—N5	2.005 (4)
Cu1—N3	1.990 (4)	Cu2—N6	1.982 (4)
O1—Cu1—O1w	100.3 (1)	O6—Cu2—O4w	99.6 (2)
O1—Cu1—N1	83.8 (2)	O6—Cu2—N4	84.5 (2)
O1—Cu1—N2	165.9 (2)	O6—Cu2—N5	168.0 (2)
O1—Cu1—N3	91.3 (1)	O6—Cu2—N6	91.4 (2)
O1w—Cu1—N1	92.5 (2)	O4w—Cu2—N4	95.9 (2)
O1w—Cu1—N2	92.4 (1)	O4w—Cu2—N5	91.1 (1)
O1w—Cu1—N3	94.8 (1)	O4w—Cu2—N6	96.4 (2)
N1—Cu1—N2	101.8 (2)	N4—Cu2—N5	99.9 (2)
N1—Cu1—N3	171.8 (2)	N4—Cu2—N6	167.6 (2)
N3—Cu1—N2	81.6 (2)	N5—Cu2—N6	81.9 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O7	0.85 (1)	2.03 (3)	2.758 (5)	144 (4)
O1*w*—H1*w*2···O2*w*	0.85 (1)	1.95 (2)	2.746 (6)	154 (5)
O2*w*—H2*w*1···O8^{i}	0.86 (1)	1.96 (2)	2.809 (6)	167 (5)
O2*w*—H2*w*2···O3*w*	0.85 (1)	2.04 (3)	2.780 (6)	145 (5)
O3*w*—H3*w*1···O5	0.86 (1)	2.05 (2)	2.888 (7)	168 (6)
O3*w*—H3*w*2···O7	0.86 (1)	2.04 (2)	2.863 (6)	160 (6)
O4*w*—H4*w*1···O2	0.85 (1)	1.98 (3)	2.727 (4)	147 (4)
O4*w*—H4*w*2···O5*w*	0.85 (1)	1.91 (1)	2.757 (6)	178 (4)
O5*w*—H5*w*1···O3^{ii}	0.85 (1)	1.89 (1)	2.739 (6)	174 (6)
O5*w*—H5*w*2···O6*w*	0.85 (1)	2.05 (4)	2.757 (7)	140 (5)
N1—H1N1···O8^{iii}	0.85 (1)	2.49 (2)	3.305 (7)	161 (3)
N1—H1N2···O2*w*	0.85 (1)	2.25 (1)	3.075 (7)	164 (4)
N4—H4N1···O4^{iv}	0.85 (1)	2.29 (1)	3.134 (5)	170 (3)
N4—H4N2···O5*w*	0.85 (1)	2.23 (2)	3.020 (6)	155 (4)

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

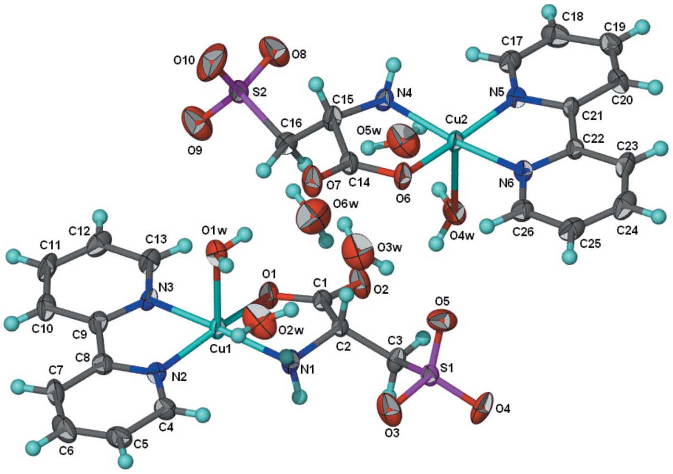


Figure 1
The asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Carbon-bound H atoms were placed at calculated positions (C—H = 0.93–0.97 Å), and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The amino and water H atoms were located in a difference Fourier map, and were refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å, and with $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *CrystalClear* (Rigaku, 2000); 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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

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