

Aqua(L-aspartato- κ^2N,O)(2,2'-bipyridine- κ^2N,N)copper(II) pentahydrateHong-Jian Zhao,^a Ming-Xing Li,^{a*}
Min Shao^b and Hong-Jiang Liu^a^aDepartment of Chemistry, College of Science, Shanghai University, Shanghai 200444, People's Republic of China, and ^bResearch Center of Analysis and Measurement, Shanghai University, Shanghai 200444, People's Republic of ChinaCorrespondence e-mail:
mx_li@mail.shu.edu.cn

Key indicators

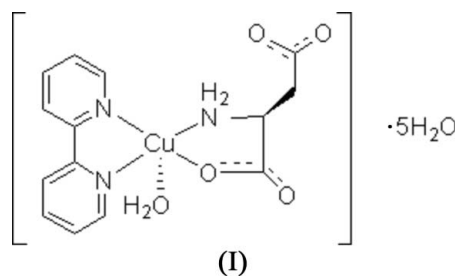
Single-crystal X-ray study
 $T = 273\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.023
 wR factor = 0.063
Data-to-parameter ratio = 9.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $[\text{Cu}(\text{C}_4\text{H}_5\text{NO}_4)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot 5\text{H}_2\text{O}$, the Cu^{II} atom is coordinated by an N,O -bidentate L-aspartate dianion, a bipyridine ligand and a water molecule in a distorted square-pyramidal geometry. Intermolecular hydrogen bonds involving the non-coordinated water molecules help to consolidate the crystal packing.

Received 24 February 2006
Accepted 30 March 2006

Comment

There is great interest in the ability of amino acids to coordinate to metal ions containing hydrogen bonds in their complexes (Hu *et al.*, 2004). As a binary amino acid, aspartic acid is especially important from both a biological and a simple coordination point of view (Casellato *et al.*, 1991; Ma *et al.*, 2004). By hydrothermal synthesis, an L-aspartate–copper complex $[\text{Cu}(\text{L-asp})(\text{bipy})(\text{H}_2\text{O})] \cdot 5\text{H}_2\text{O}$ (L-asp is L-aspartate and bipy is 2,2'-bipyridine), (I), was prepared and its crystal structure is presented here. The asymmetric unit of (I) consists of a Cu^{II} ion, an L-aspartate dianion, a bipyridine ligand, a coordinated water and five uncoordinated water molecules.



The molecular structure of (I) is shown in Fig. 1. The coordination geometry around the Cu^{II} atom is five-coordinate distorted square-pyramidal. The L-aspartate dianion (O1/N3) and bipyridine ligand (N1/N2) lie on the basal plane and coordinate to the Cu^{II} ion, forming two five-membered chelate rings. The apical position is occupied by a coordinated water molecule (O5), with a $\text{Cu1}-\text{O5}$ distance of 2.2840 (15) \AA (Table 1), slightly shorter than the coordinated water bond length (2.368 \AA) of the analogous complex $[\text{Cu}(\text{L-asp})(\text{bipy})(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O}$ (Brondino *et al.*, 1995; Antolini *et al.*, 1983).

An intramolecular hydrogen bond exists between O3 and N3 (Table 2), which causes the uncoordinated carboxylate group to bend markedly towards the amino group. The uncoordinated carboxylate O2 atom links to an uncoordinated water molecule, while the other uncoordinated carboxylate O atom (O4) links to a neighboring L-aspartate ligand *via* an $\text{N3}-\text{H12} \cdots \text{O4}$ hydrogen bond (Fig. 2).

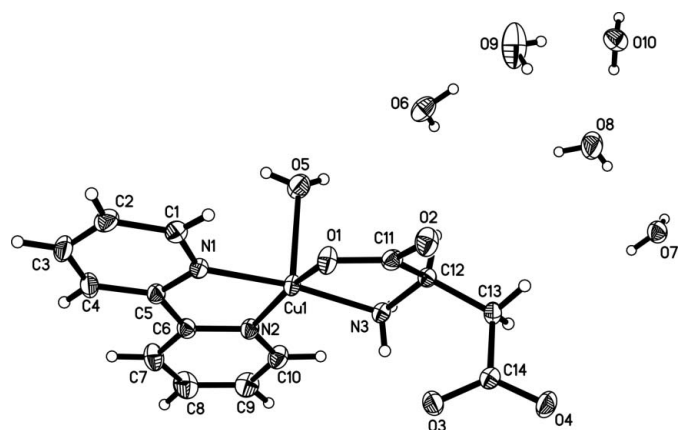


Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

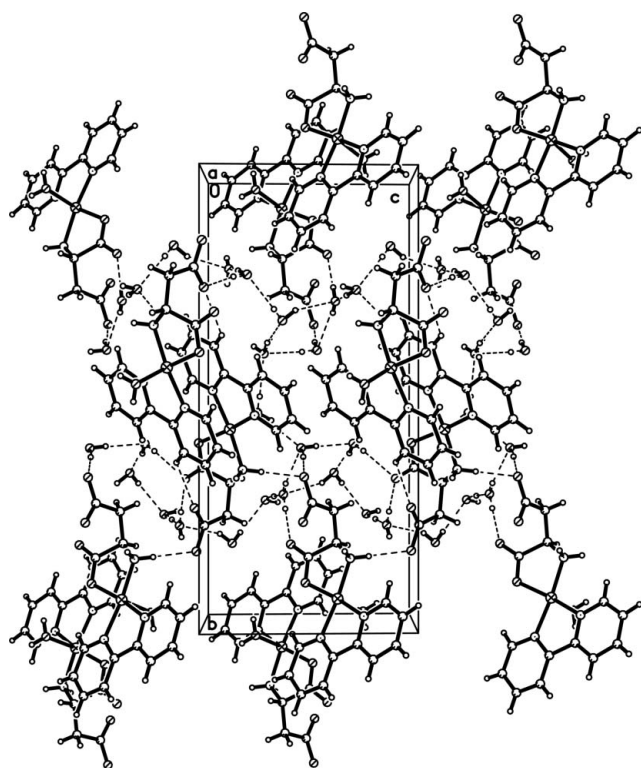


Figure 2
A crystal packing diagram of (I), with intermolecular hydrogen bonds involving the uncoordinated water molecules shown as dashed lines.

Experimental

The title complex was synthesized by a hydrothermal synthesis method from a mixture of L-aspartic acid (0.399 g, 3.0 mmol), CuCO_3 (0.240 g, 2.0 mmol), 2,2'-bipyridine (0.156 g, 1.0 mmol) and water (30 ml) in a 40 ml Teflon-lined stainless steel reactor. The mixture was heated at 393 K for 2 d. After cooling to room temperature, dark-blue single crystals of (I) were obtained.

Crystal data

$[\text{Cu}(\text{C}_4\text{H}_5\text{NO}_4)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot 5\text{H}_2\text{O}$
 $M_r = 458.91$
 Monoclinic, $P2_1/c$
 $a = 9.0194(3) \text{ \AA}$
 $b = 21.4430(6) \text{ \AA}$
 $c = 10.0189(3) \text{ \AA}$
 $\beta = 93.088(1)^\circ$

$V = 1934.9(1) \text{ \AA}^3$
 $Z = 4$
 $D_x = 1.575 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 1.19 \text{ mm}^{-1}$
 $T = 273(2) \text{ K}$
 Block, blue
 $0.20 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.797$, $T_{\max} = 0.911$

21692 measured reflections
 3404 independent reflections
 3100 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.063$
 $S = 1.06$
 3404 reflections
 353 parameters
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.7615P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

C11—O2	1.237 (2)	Cu1—O1	1.9484 (12)
C11—O1	1.274 (2)	Cu1—N3	1.9722 (15)
C12—N3	1.478 (2)	Cu1—N1	1.9856 (14)
C14—O3	1.242 (2)	Cu1—N2	2.0130 (14)
C14—O4	1.259 (2)	Cu1—O5	2.2840 (15)
O2—C11—O1	123.55 (16)	N3—Cu1—N2	98.88 (6)
O1—Cu1—N3	83.98 (6)	N1—Cu1—N2	81.30 (6)
O1—Cu1—N1	93.66 (5)	O1—Cu1—O5	96.40 (6)
N3—Cu1—N1	171.65 (6)	C12—N3—Cu1	108.31 (10)
O1—Cu1—N2	164.41 (6)	C11—O1—Cu1	115.18 (11)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
N3—H12 \cdots O4 ⁱ	0.87 (2)	2.02 (2)	2.890 (2)	176.1 (19)
O7—H24 \cdots O6 ⁱ	0.82 (3)	1.98 (4)	2.799 (3)	173 (3)
O7—H25 \cdots O4 ⁱⁱ	0.77 (3)	1.89 (3)	2.652 (2)	173 (3)
O10—H23 \cdots O8	0.84 (3)	1.96 (3)	2.762 (3)	159 (3)
O10—H22 \cdots O3 ⁱⁱⁱ	0.79 (3)	1.95 (3)	2.738 (2)	170 (3)
O8—H21 \cdots O7	0.63 (3)	2.21 (3)	2.836 (3)	170 (4)
O8—H20 \cdots O2 ⁱⁱ	0.82 (4)	1.99 (4)	2.814 (3)	178 (4)
O9—H19 \cdots O10	0.73 (4)	2.05 (4)	2.779 (3)	172 (4)
O9—H18 \cdots O8 ^{iv}	0.85 (1)	2.51 (4)	3.287 (5)	153 (7)
O6—H17 \cdots O9	0.87 (5)	1.93 (5)	2.789 (4)	166 (5)
O6—H16 \cdots O2 ⁱⁱ	0.67 (3)	2.14 (3)	2.799 (2)	170 (3)
N3—H11 \cdots O10 ^v	0.81 (2)	2.52 (2)	3.111 (2)	131.0 (17)
N3—H11 \cdots O3	0.81 (2)	2.35 (2)	2.917 (2)	127.4 (17)
O5—H10 \cdots O7 ^{iv}	0.79 (3)	2.01 (3)	2.784 (2)	166 (2)
O5—H9 \cdots O6 ^{vi}	0.80 (3)	2.02 (3)	2.815 (3)	177 (3)

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

The H atoms were identified in difference Fourier syntheses and refined freely.

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

The project was supported by the Development Foundation of Shanghai Municipal Education Commission, China.

References

- Antolini, L., Marcotriggiano, G., Menabue, L. & Pellacani, G. C. (1983). *Inorg. Chem.* **22**, 141–145.
- Brondino, C. D., Calvo, R., Atria, A. M., Spodine, E. & Pena, O. (1995). *Inorg. Chim. Acta*, **228**, 261–266.
- Bruker (2000). *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Casellato, U., Graziani, R., Bonomo, R. P. & Dibilio, A. J. (1991). *J. Chem. Soc. Dalton Trans.* pp. 23–31.
- Hu, Z. Q., Xu, D. J., Xu, Y. Z., Wu, J. Y. & Chang, M. Y. (2004). *Chin. J. Struct. Chem.* **23**, 38–40.
- Ma, L. F., Liang, F. P., Qin, H. C., Hu, R. X., Zhang, M. B. & Yu, K. B. (2004). *Chin. J. Inorg. Chem.* **20**, 1429–1432.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (2000). *SHELXTL*. Version 6.1. Bruker AXS Inc., Madison, Wisconsin, USA.