

Table 2. Selected geometric parameters (Å, °)

Pb—O	2.372 (9)	S—C	1.667 (14)
Pb—O <sup>i</sup>	2.453 (5)	C—N	1.16 (2)
Pb—N	2.629 (13)	O—H	0.76 (14)
N—Pb—O	106.5 (4)	Pb—O—Pb <sup>i</sup>	108.4 (2)
N—Pb—O <sup>i</sup>	71.4 (2)	Pb—O <sup>i</sup> —Pb <sup>i</sup>	108.4 (2)
O—Pb—O <sup>i</sup>	71.6 (2)	Pb—N—C	179.9 (12)
O <sup>i</sup> —Pb—O <sup>ii</sup>	115.8 (4)	S—C—N	178.5 (13)

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

The Pb(OH)(NCS) crystals were described in the *Pbmm* non-standard setting of the *Pnma* (No. 62) space group; the transformation matrix is (001/100/010) and the coordinates of the equivalent positions are:  $x, y, z$ ;  $x + \frac{1}{2}, -y + \frac{1}{2}, -z$ ;  $x - \frac{1}{2}, -y - \frac{1}{2}, z - \frac{1}{2}$ ;  $x, y, -z - \frac{1}{2}$ ; together with those related by a centre of symmetry at 0,0,0. The integrated intensities were obtained by a modified version (Belletti, Uguzzoli, Cantoni & Pasquinelli, 1979) of the Lehmann & Larsen (1974) peak-profile analysis procedure. All reflections were corrected for Lorentz and polarization effects, absorption correction was for a cylindrical sample ( $\mu R = 2.2$ ) and coefficients were taken from *International Tables for Crystallography* (1992, Vol. C, Table 6.3.3.2, p. 523).

The structure was solved by the Patterson method and refined by anisotropic full-matrix least squares on  $F^2$  using *SHELXL93* (Sheldrick, 1993). Refinement on  $F^2$  involved all reflections except for one probably affected by systematic errors. Two residual peaks of 2.68 and 2.35 e Å<sup>-3</sup> were found in the final difference map at *ca* 1 Å from Pb.

Calculations were carried out on the ENCORE91 and GOULD-POWERNODE 6040 computers of the Centro di Studio per la Strutturistica Diffraattometrica del CNR, Parma, and on a COMPAQ 486c portable computer.

Data collection: local programs. Cell refinement: *LQPARM* (Nardelli & Mangia, 1984). Data reduction: local programs. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93*. Molecular graphics: *PLATON* (Spek, 1990); *PLUTO* (Motherwell & Clegg, 1976). Software used to prepare material for publication: *PARST* (Nardelli, 1983); *PARSTCIF* (Nardelli, 1991).

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Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: HA1124). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## A Novel Structure of (L-Aspartato)(1,10-phenanthroline)copper(II) Hydrate

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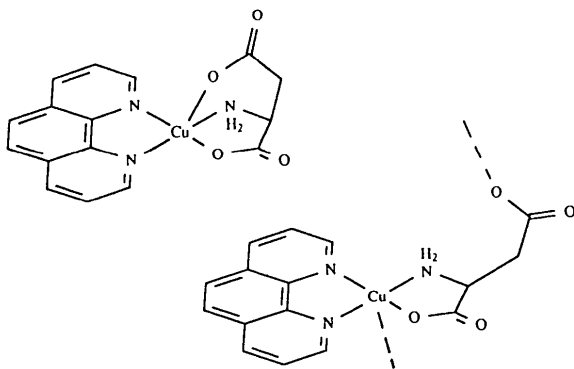
## Abstract

The title compound, [Cu(C<sub>4</sub>H<sub>5</sub>NO<sub>4</sub>)(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)]·3.5H<sub>2</sub>O, consists of two types of different pentacoordinate copper complex: one monomeric, with the aspartate group acting as a tridentate ligand, and the other polymeric, with the aspartate group bridging two different copper centers. The whole structure is held together by a complex hydrogen-bonding scheme involving the water molecules of solvation.

### Comment

As part of systematic studies on the magneto-structural properties of copper(II) complexes, we prepared the mixed-ligand complex [Cu(asp)(phen)], where asp is L-aspartate and phen is 1,10-phenanthroline. Although the technique used was the one described by Antolini *et al.* (1986) for the synthesis of [Cu(asp)(phen)].4H<sub>2</sub>O, the structure determination of the single crystals obtained for use in electron spin resonance (ESR) studies showed a different hydration number than that reported previously for [Cu(asp)(phen)].4H<sub>2</sub>O, as well as a different mode of aspartate ligand binding. In this paper, we provide a description of this new structure.

The title structure consists of two different kinds of copper complex which coexist in the crystal (see scheme below and Fig. 1), along with seven water molecules of solvation per asymmetric unit.



The first type of complex exists as discrete molecules in which the aspartate ligand is tridentate and the phenanthroline ligand behaves in the usual bidentate manner. The geometry around the copper center is square pyramidal. The basal plane is formed by Cu(2)—N(5) [2.002 (5) Å] and Cu(2)—N(6) [2.011 (5) Å], provided by the phenanthroline group, and Cu(2)—N(4) [1.992 (5) Å] and Cu(2)—O(6) [1.959 (5) Å], provided by the aspartate moiety. The pyramid is completed by the apical bond Cu(2)—O(7) [2.226 (5) Å] from the same aspartate group. Atoms N(4), O(6), N(5) and N(6) deviate from the best mean basal plane by 0.0047, -0.0052, 0.0052 and -0.0047 Å, respectively, with the Cu atom and the apical O(7) atom being 0.1529 and 2.3512 Å, respectively, from the plane. All the distances in the structure are comparable with the corresponding ones in the structure of [Cu(asp)(phen)].4H<sub>2</sub>O, the only exception being the apical Cu(2)—O(7) bond [2.226 (5) Å], which is somewhat shorter than its analogue (2.344 Å).

The coordinated water molecules lie along the *b* axis and are linked by two types of hydrogen bond, namely, O(5)··H(4A)—N(4) and O(8)··H(4B)—N(4) (see Fig. 2).

The second type of copper complex is polymeric in nature and the aspartate ligand links two differ-

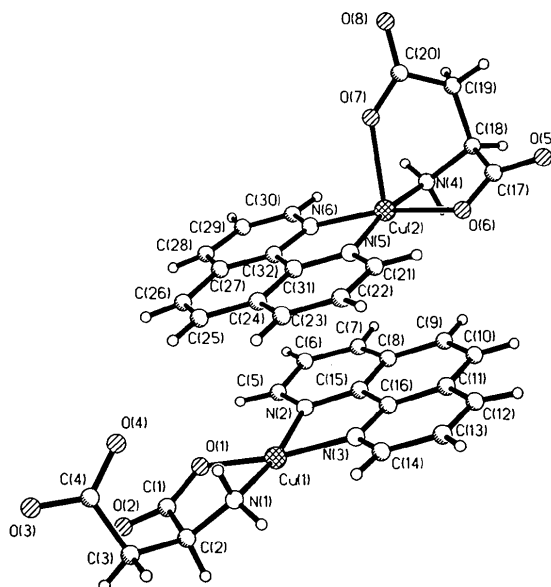


Fig. 1. The molecular structure and numbering scheme of the title complexes.

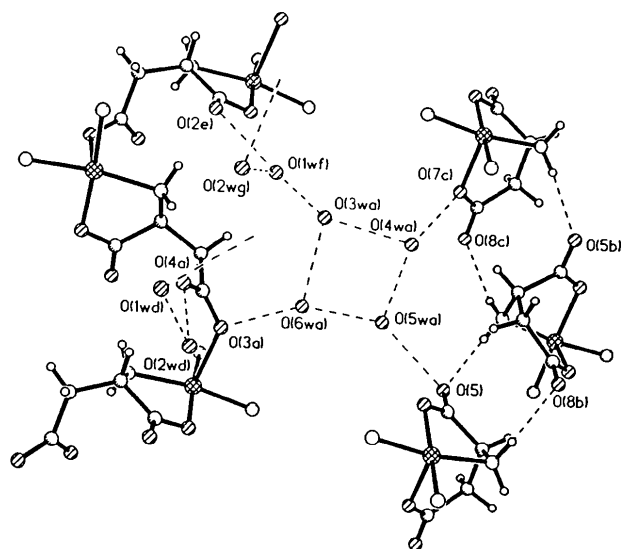


Fig. 2. Diagram showing intermolecular contacts. [Symmetry codes: (a)  $1-x, y-\frac{3}{2}, 1+z$ ; (b)  $1-x, -\frac{1}{2}-y, -z$ ; (c)  $x, y-1, z$ ; (d)  $1+x, y, z$ ; (e)  $1+x, y-1, z$ ; (f)  $-x, 1-y, 1-z$ ; (g)  $-x, y-\frac{1}{2}, 1-z$ .]

ent copper centers giving rise to a chain along the *b* axis similar to that in the previous case (Antolini *et al.*, 1986). The geometry around the copper ion is also described as square pyramidal; in this case the basal plane is formed by Cu(1)—N(2) [1.998 (5) Å] and Cu(1)—N(3) [2.027 (6) Å], provided by the phenanthroline ligand, and Cu(1)—N(1) [2.002 (5) Å] and Cu(1)—O(1) [1.949 (4) Å], provided by one aspartate ligand. However, the apical Cu(1)—O(3)( $-x, y-\frac{1}{2}, 1-z$ ) bond

[2.344 (5) Å] is now provided by a different aspartate moiety. Atoms N(1), O(1), N(2) and N(3) deviate from the best mean basal plane by 0.0314, -0.0339, 0.0337 and -0.0312 Å, respectively. The Cu and apical O(3)(-x, y- $\frac{1}{2}$ , 1-z) atoms deviate by -0.1394 and -2.4822 Å, respectively. Thus, the geometries of these two different coordination modes are quite similar.

The polymeric chains link through direct hydrogen bonding, N(1)—H(1B)··O(2), as well as through some complex contacts mediated by O(1W) and O(2W). Inspection of Fig. 2 reveals the complex linkage between the monomeric and polymeric chain types through hydrogen bonds involving atoms O(1W), O(3W), O(4W), O(5W) and O(6W). The last water molecule of solvation, O(7W), does not participate in any hydrogen bonding.

## Experimental

### Crystal data

[Cu(C <sub>4</sub> H <sub>5</sub> NO <sub>4</sub> )(C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> )]· 3.5H <sub>2</sub> O	Mo K $\alpha$ radiation
$M_r = 436.9$	$\lambda = 0.71073$ Å
Monoclinic	Cell parameters from 25 reflections
$P2_1$	$\theta = 15\text{--}25^\circ$
$a = 8.497$ (3) Å	$\mu = 1.285$ mm <sup>-1</sup>
$b = 9.902$ (3) Å	$T = 293$ K
$c = 21.030$ (5) Å	Irregular block
$\beta = 92.14$ (1)°	0.55 × 0.18 × 0.18 mm
$V = 1768.2$ (9) Å <sup>3</sup>	Deep blue
$Z = 4$	
$D_x = 1.641$ Mg m <sup>-3</sup>	

### Data collection

Siemens R3m diffractometer	$R_{\text{int}} = 0.0179$
$\theta$ - $2\theta$ scans (speed 4.19– 29.3° min <sup>-1</sup> )	$\theta_{\text{max}} = 22.5^\circ$
Absorption correction: none	$h = -9 \rightarrow 9$
2552 measured reflections	$k = 0 \rightarrow 10$
2476 independent reflections	$l = 0 \rightarrow 22$
2168 observed reflections	2 standard reflections
$[F > 4\sigma(F)]$	monitored every 98 reflections
	intensity decay: none

### Refinement

Refinement on $F$	$(\Delta/\sigma)_{\text{max}} = 0.024$
$R = 0.0322$	$\Delta\rho_{\text{max}} = 0.53$ e Å <sup>-3</sup>
$wR = 0.0424$	$\Delta\rho_{\text{min}} = -0.42$ e Å <sup>-3</sup>
$S = 1.12$	Atomic scattering factors from <i>International Tables</i> for <i>X-ray Crystallography</i> (1974, Vol. IV)
2168 reflections	
496 parameters	
$w = 1/[\sigma^2(F) + 0.001F^2]$	

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>)

$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^*$				
	x	y	z	$U_{\text{eq}}$
Cu(1)	0.0693 (1)	0.8314	0.3776 (1)	0.028 (1)
C(1)	-0.0950 (8)	0.9844 (7)	0.4606 (3)	0.030 (2)
C(2)	0.0050 (8)	0.8898 (7)	0.5040 (3)	0.026 (2)

C(3)	0.0495 (8)	0.9568 (7)	0.5679 (3)	0.035 (2)
C(4)	0.1438 (8)	1.0861 (7)	0.5630 (3)	0.032 (2)
N(1)	0.1389 (6)	0.8381 (6)	0.4695 (2)	0.031 (2)
O(1)	-0.0691 (5)	0.9786 (4)	0.4011 (2)	0.035 (2)
O(2)	-0.1984 (5)	1.0532 (5)	0.4835 (2)	0.040 (2)
O(3)	0.1304 (5)	1.1729 (5)	0.6065 (2)	0.038 (2)
O(4)	0.2265 (6)	1.1016 (5)	0.5154 (2)	0.048 (2)
C(5)	-0.0768 (7)	0.9452 (8)	0.2568 (3)	0.039 (2)
C(6)	-0.1026 (8)	0.9454 (10)	0.1896 (3)	0.051 (3)
C(7)	-0.0256 (9)	0.8504 (10)	0.1543 (3)	0.054 (3)
C(8)	0.0821 (8)	0.7602 (8)	0.1819 (3)	0.040 (2)
C(9)	0.1742 (9)	0.6657 (10)	0.1482 (3)	0.052 (3)
C(10)	0.2753 (9)	0.5793 (9)	0.1791 (3)	0.050 (3)
C(11)	0.3001 (8)	0.5888 (7)	0.2467 (3)	0.040 (2)
C(12)	0.4093 (9)	0.5099 (8)	0.2816 (4)	0.052 (3)
C(13)	0.4250 (9)	0.5260 (8)	0.3465 (3)	0.050 (3)
C(14)	0.3312 (9)	0.6202 (8)	0.3767 (3)	0.043 (3)
C(15)	0.1009 (8)	0.7676 (7)	0.2485 (3)	0.036 (2)
C(16)	0.2097 (7)	0.6801 (7)	0.2808 (3)	0.029 (2)
N(2)	0.0204 (6)	0.8559 (5)	0.2846 (2)	0.030 (2)
N(3)	0.2255 (6)	0.6954 (6)	0.3452 (2)	0.033 (2)
Cu(2)	0.4212 (1)	0.9361 (1)	0.1213 (1)	0.031 (1)
C(17)	0.5931 (8)	0.7626 (7)	0.0554 (3)	0.036 (2)
C(18)	0.5213 (8)	0.8536 (7)	0.0041 (3)	0.032 (2)
C(19)	0.6333 (8)	0.9653 (7)	-0.0137 (3)	0.035 (2)
C(20)	0.6840 (8)	1.0718 (7)	0.0362 (3)	0.034 (2)
N(4)	0.3717 (6)	0.9106 (5)	0.0288 (2)	0.030 (2)
O(5)	0.6953 (6)	0.6792 (5)	0.0392 (2)	0.045 (2)
O(6)	0.5490 (5)	0.7733 (5)	0.1114 (2)	0.039 (2)
O(7)	0.6164 (5)	1.0678 (5)	0.0905 (2)	0.037 (2)
O(8)	0.7803 (5)	1.1561 (5)	0.0209 (2)	0.046 (2)
C(21)	0.5538 (7)	0.8502 (7)	0.2504 (3)	0.037 (2)
C(22)	0.5699 (8)	0.8615 (8)	0.3168 (3)	0.042 (3)
C(23)	0.4800 (8)	0.9545 (9)	0.3473 (3)	0.045 (3)
C(24)	0.3737 (8)	1.0379 (8)	0.3126 (3)	0.037 (2)
C(25)	0.2717 (8)	1.1374 (9)	0.3401 (3)	0.044 (3)
C(26)	0.1751 (9)	1.2143 (9)	0.3031 (3)	0.051 (3)
C(27)	0.1712 (8)	1.2024 (7)	0.2346 (3)	0.038 (2)
C(28)	0.0719 (8)	1.2792 (8)	0.1926 (3)	0.045 (3)
C(29)	0.0736 (9)	1.2546 (8)	0.1291 (3)	0.050 (3)
C(30)	0.1719 (8)	1.1572 (8)	0.1062 (3)	0.040 (2)
C(31)	0.3702 (7)	1.0236 (7)	0.2467 (3)	0.029 (2)
C(32)	0.2662 (7)	1.1043 (7)	0.2075 (3)	0.031 (2)
N(5)	0.4565 (6)	0.9301 (6)	0.2160 (2)	0.031 (2)
N(6)	0.2679 (6)	1.0818 (6)	0.1437 (2)	0.033 (2)
O(1W)	-0.6267 (6)	0.7311 (6)	0.5939 (3)	0.054 (1)
O(2W)	-0.4293 (6)	0.8150 (7)	0.4984 (3)	0.061 (1)
O(3W)	0.2537 (7)	1.7707 (7)	0.7135 (3)	0.070 (2)
O(4W)	0.4053 (7)	1.7951 (7)	0.8329 (3)	0.066 (2)
O(5W)	0.2103 (7)	2.0133 (8)	0.8566 (3)	0.079 (2)
O(6W)	0.1554 (8)	2.0371 (8)	0.7263 (3)	0.085 (2)
O(7W)	1.0312 (10)	0.9841 (10)	-0.0167 (4)	0.131 (3)

Table 2. Selected geometric parameters (Å, °)

Cu(1)—N(1)	2.002 (5)	C(32)—N(6)	1.362 (8)
Cu(1)—N(2)	1.998 (5)	Cu(1)—O(1)	1.949 (4)
Cu(1)—O(3')	2.344 (5)	Cu(1)—N(3)	2.027 (6)
C(1)—O(1)	1.278 (8)	C(1)—C(2)	1.542 (9)
C(2)—C(3)	1.533 (9)	C(1)—O(2)	1.225 (8)
C(3)—C(4)	1.516 (10)	C(2)—N(1)	1.465 (8)
C(4)—O(4)	1.253 (8)	C(4)—O(3)	1.264 (8)
C(5)—C(6)	1.422 (10)	O(3)—Cu(1')	2.344 (5)
C(6)—C(7)	1.378 (12)	C(5)—N(2)	1.330 (9)
C(8)—C(9)	1.425 (11)	C(7)—C(8)	1.390 (11)
C(9)—C(10)	1.360 (11)	C(8)—C(15)	1.406 (9)
C(11)—C(12)	1.400 (10)	C(10)—C(11)	1.432 (10)
C(12)—C(13)	1.374 (11)	C(11)—C(16)	1.401 (9)
C(14)—N(3)	1.325 (9)	C(13)—C(14)	1.396 (11)
C(15)—N(2)	1.359 (9)	C(15)—C(16)	1.422 (9)
Cu(2)—N(4)	1.992 (5)	C(16)—N(3)	1.364 (8)
Cu(2)—O(7)	2.226 (5)	Cu(2)—O(6)	1.959 (5)
Cu(2)—O(7)	2.226 (5)	Cu(2)—N(5)	2.002 (5)
Cu(2)—N(6)	2.011 (5)	C(17)—C(18)	1.515 (9)
C(17)—O(5)	1.255 (9)	C(17)—O(6)	1.254 (8)
C(18)—C(19)	1.515 (9)	C(18)—N(4)	1.501 (8)

C(19)—C(20)	1.537 (9)	C(20)—O(7)	1.298 (8)
C(20)—O(8)	1.220 (8)	C(21)—C(22)	1.402 (9)
C(21)—N(5)	1.337 (8)	C(22)—C(23)	1.371 (10)
C(23)—C(24)	1.408 (10)	C(24)—C(25)	1.446 (11)
C(24)—C(31)	1.393 (9)	C(25)—C(26)	1.345 (11)
C(26)—C(27)	1.445 (10)	C(27)—C(28)	1.420 (10)
C(27)—C(32)	1.398 (9)	C(28)—C(29)	1.356 (10)
C(29)—C(30)	1.376 (11)	C(30)—N(6)	1.341 (9)
C(31)—C(32)	1.429 (9)	C(31)—N(5)	1.359 (8)
N(1)—Cu(1)—O(1)	83.6 (2)	N(4)—Cu(2)—O(6)	83.6 (2)
O(1)—Cu(1)—N(2)	93.0 (2)	O(6)—Cu(2)—O(7)	91.7 (2)
O(1)—Cu(1)—N(3)	172.6 (2)	O(6)—Cu(2)—N(5)	91.1 (2)
N(1)—Cu(1)—O(3')	94.3 (2)	N(4)—Cu(2)—N(6)	101.8 (2)
N(2)—Cu(1)—O(3')	95.5 (2)	O(7)—Cu(2)—N(6)	98.3 (2)
C(2)—C(1)—O(1)	116.2 (6)	C(18)—C(17)—O(5)	117.6 (6)
O(1)—C(1)—O(2)	124.2 (6)	O(5)—C(17)—O(6)	123.0 (6)
C(1)—C(2)—N(1)	109.8 (5)	C(17)—C(18)—N(4)	107.5 (5)
C(2)—C(3)—C(4)	114.8 (5)	C(18)—C(19)—C(20)	119.7 (5)
C(3)—C(4)—O(4)	118.1 (6)	C(19)—C(20)—O(8)	117.5 (6)
C(6)—C(5)—N(2)	120.5 (7)	C(22)—C(21)—N(5)	121.8 (6)
C(6)—C(7)—C(8)	122.2 (6)	C(22)—C(23)—C(24)	120.6 (6)
C(7)—C(8)—C(15)	115.5 (7)	C(23)—C(24)—C(31)	116.5 (6)
C(8)—C(9)—C(10)	121.6 (7)	C(24)—C(25)—C(26)	121.1 (7)
C(10)—C(11)—C(12)	123.7 (7)	C(26)—C(27)—C(28)	124.6 (7)
C(12)—C(11)—C(16)	117.1 (6)	O(5)—C(17)—C(32)	117.2 (6)
C(12)—C(13)—C(14)	119.6 (7)	C(28)—C(29)—C(30)	120.0 (7)
C(8)—C(15)—C(16)	119.4 (6)	C(24)—C(31)—C(32)	120.4 (6)
C(16)—C(15)—N(2)	117.2 (5)	C(32)—C(31)—N(5)	116.1 (5)
C(11)—C(16)—N(3)	123.0 (6)	C(27)—C(32)—N(6)	122.9 (6)
C(5)—N(2)—C(15)	119.9 (5)	C(21)—N(5)—C(31)	118.7 (5)
N(1)—Cu(1)—N(2)	169.7 (2)	N(4)—Cu(2)—O(7)	85.5 (2)
N(1)—Cu(1)—N(3)	100.0 (2)	N(4)—Cu(2)—N(5)	170.3 (2)
N(2)—Cu(1)—N(3)	82.3 (2)	O(7)—Cu(2)—N(5)	102.8 (2)
O(1)—Cu(1)—O(3')	91.0 (2)	O(6)—Cu(2)—N(6)	169.0 (2)
N(3)—Cu(1)—O(3')	95.2 (2)	N(5)—Cu(2)—N(6)	82.2 (2)
C(2)—C(1)—O(2)	119.5 (6)	C(18)—C(17)—O(6)	119.5 (6)
C(1)—C(2)—C(3)	111.6 (5)	C(17)—C(18)—C(19)	111.7 (5)
C(3)—C(2)—N(1)	114.5 (5)	C(19)—C(18)—N(4)	111.0 (5)
C(3)—C(4)—O(3)	117.6 (6)	C(19)—C(20)—O(7)	117.2 (6)
O(3)—C(4)—O(4)	124.3 (6)	O(7)—C(20)—O(8)	125.2 (6)
C(5)—C(6)—C(7)	118.4 (7)	C(21)—C(22)—C(23)	119.0 (6)
C(7)—C(8)—C(9)	125.4 (6)	C(23)—C(24)—C(25)	125.1 (6)
C(9)—C(8)—C(15)	119.1 (6)	C(25)—C(24)—C(31)	118.4 (6)
C(9)—C(10)—C(11)	120.0 (7)	C(25)—C(26)—C(27)	121.4 (7)
C(10)—C(11)—C(16)	119.2 (6)	C(26)—C(27)—C(32)	118.1 (6)
C(11)—C(12)—C(13)	119.6 (7)	C(27)—C(28)—C(29)	119.3 (7)
C(13)—C(14)—N(3)	122.3 (6)	C(29)—C(30)—N(6)	123.3 (6)
C(8)—C(15)—N(2)	123.4 (6)	C(24)—C(31)—N(5)	123.4 (6)
C(11)—C(16)—C(15)	120.5 (6)	C(27)—C(32)—C(31)	120.5 (6)
C(15)—C(16)—N(3)	116.4 (6)	C(31)—C(32)—N(6)	116.6 (6)
C(14)—N(3)—C(16)	118.3 (6)	C(30)—N(6)—C(32)	117.4 (6)

Symmetry code: (i)  $-x, y - \frac{1}{2}, 1 - z$ .

Non-water H atoms were refined using a riding model and a fixed isotropic  $U$ . Water H atoms were found in a  $\Delta F$  synthesis and refined with constrained distances and isotropic  $U$ .

The structure was solved by direct methods and refined by full-matrix least squares. *SHELXTL/PC* (Sheldrick, 1991) was used for all calculations and drawings.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, least-squares-planes data and short intermolecular contacts have been deposited with the IUCr (Reference: HU1069). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## Complexation with Ligands Containing a Dipyridylmethane Unit. Structures of a Free Ligand and Two Copper(II) Complexes

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## Abstract

The crystal structures of the metal-free ligand 6,6'-(1-methoxypropylidene)bis(2-pyridinecarboxylic acid) monohydrate,  $C_{16}H_{16}N_2O_5 \cdot H_2O$  (1), the complex aqua-{6,6'-[1-(2-pyridylmethoxy)propylidene]bis(2-pyridinecarboxylato-*N,O*)}copper(II),  $[Cu(C_{21}H_{17}N_3O_5)(H_2O)]$  (2), and the dimeric complex bis[ $\mu$ -6,6'-{(methoxy)[3-(3-pyridylmethoxy)phenyl]methylene}bis(2-pyridinecarboxylato-*N,N',O,O''*:*N''*)]dicopper(II) monohydrate,  $[Cu_2(C_{26}H_{19}N_3O_6)_2] \cdot H_2O$  (3), have been studied by X-ray diffraction. In the crystal of (1) the dipyridylmethane moiety adopts an *anti* conformation, with the two aromatic rings almost perpendicular to each other. This molecular conformation, as well as the crystal packing, are stabilized by hydrogen bonds involving the water molecule. The  $Cu^{II}$  ion in (2) has square-pyramidal coordination, with the apex position occupied by the water O atom. The aromatic rings are slightly bent from the plane formed by the two *cis*-positioned N atoms and the two carboxylic O atoms of the ligand molecule. The apical water O atoms link successive molecules into infinite chains *via* hydrogen bonds. The chains, held together by weak electrostatic interactions besides the van der Waals forces, are arranged so as to form a layer structure. (3) also contains a five-coordinate  $Cu^{II}$  ion with a square-pyramidal coordination polyhedron. The axial position is occupied by