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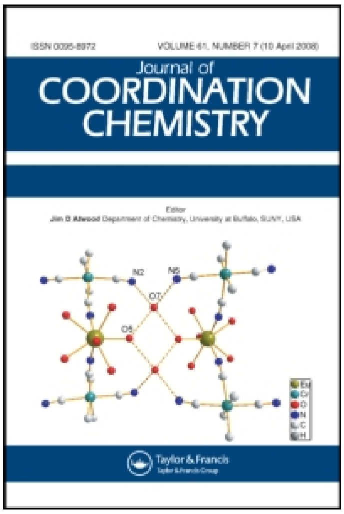

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Synthesis, Crystal and Molecular Structure of Mono- and Diaquadi(acetato-*O*)-*Bis*(2,4'-Bipyridyl) Copper(II)

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SYNTHESIS, CRYSTAL AND MOLECULAR STRUCTURE OF MONO- AND DIAQUADI(ACETATO-*O*)-*BIS*(2,4′-BIPYRIDYL) COPPER(II)

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The title compound has been synthesized and characterized by elemental analysis and conductivity studies. The crystal and molecular structure has been determined. There are two different types of molecules in the crystal: mono- and diaquadi(acetato-*O*)-*bis*(2,4′-bipyridyl) copper (II). Both copper atoms occupy special positions. The copper atoms show almost ideal square pyramidal (4 + 1) and square bipyramidal (4 + 2) coordination. Due to the Jahn–Teller effect, the axial Cu–O(water) bond distances are longer than respective equatorial Cu–O(acetate) bond distances. The bond valences of the copper were computed. An intramolecular strong hydrogen bond linking O(water) and O(acetate) atoms exists in the molecule. The differences of geometrical environment for copper in mono- and diaquadi(acetato-*O*)-*bis*(2,4′-bipyridyl) copper(II) are imposed by strong intermolecular hydrogen bonds creating a linear infinite chain structure along crystallographic *x* axis. Also weak intramolecular hydrogen bonds are present in the molecule.

Keywords: Hydrogen bond chain; Five coordinated copper(II); Six coordinated copper(II); Bond valence

INTRODUCTION

The self-assembly of metal compounds into one-, two- and three-dimensional supramolecular architectures is currently of considerable interest. The potential applications of crystal macroscopic physical properties are defined by the intermolecular electronic interactions present in the solid state [1–3]. Consequently, there is a need for the development and study of strong and highly directional intermolecular interactions, which are able to generate predetermined molecular arrangements. The high directionality of strong (O–H ⋯ O) and weak (C–H ⋯ O) hydrogen bonds makes them useful

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in crystal design for preparation of molecular materials with controlled physical properties [1,4–6]. The interactions of strong and weak hydrogen bonds play vital roles in molecular recognition in a wide variety of biological systems [7,8], as well as influencing crystal packing in crystals [1,9,10].

The second, very important, property of metal compounds is the geometry and bonding properties of the metal. It has been stated, that the bond length to bond valence correlation represents a measure of the strength of a bond that is independent of the atomic size [11]. The application of this correlation allows comparison of the relative importance of Cu–N and Cu–O bonds for different molecules and check of the valence-sum rule for copper atoms [12]. The valence-sum rule states that the sum of the valences of the bonds formed by an atom is equal to the valence (formal oxidation state) of the atom. Violation of the valence-sum rule can indicate mistakes in the interpretation of the structure by omission of the weak hydrogen bonds, or can show that bonds are strained as the result of the crystallographic constraints that prevent the bonds from attaining their ideal lengths [12,13]. In this work we attempt to show the influence of strong and weak hydrogen bonds on the molecular conformation and differentiation of bond lengths.

EXPERIMENTAL

Chemicals

2-4′-Bipyridyl (m.p. 61°C) and methanol (anhydroscan) were obtained from Aldrich and from Lab-scan., respectively. Other chemicals were p.a. from POCh-Gliwice.

Synthesis

A solution of 4.3 mmol of copper(II) acetate in 20 mL of water was added to a solution of 12.8 mmol of 2,4′-bipyridyl in 10 mL of water containing a few drops of 95% EtOH. The mixture was heated at 80°C for 15 min and allowed to cool. During several days, fine, crystalline compound was obtained. The product was dissolved in equivolume mixture of water and 95% EtOH, and the solution was kept at 277 K. After one month plate crystals had grown.

Chemical Analysis and Conductivity Measurement

The C, H and N contents were determined by standard microanalytical technique (Carbo-Erba analyzer). Copper analysis was carried out complexometrically in mineralized sample.

Analytical data for $C_{24}H_{24}CuN_4O_5 \cdot C_{24}H_{26}CuN_4O_6$ (%): Found: Cu, 12.15; N, 10.43; C, 55.48; H, 4.87. Calculated: Cu, 12.20; N, 10.75; C, 55.33; H, 4.84.

Conductivity measurement was performed on a conductivitymeter of the OK-102/1 type equipped with an OK 902 electrode at 25 ± 0.05°C. Molar conductivity of the complex was measured using a $1.0 \cdot 10^{-3}$ M solution in methanol and has a value of $\Delta_M = 17.9\,\Omega^{-1}\,cm^2\,mol^{-1}$. These prove that in methanol the title compound is a nonelectrolyte [14].

X-ray Crystal Structure Analysis of the Title Compound

A plate crystal of title compound of approximate dimensions $0.36 \times 0.28 \times 0.17$ mm was mounted on a KM-4-CCD automatic diffractometer equipped with CCD detector, and used for data collection. X-ray intensity data were collected with graphite monochromated MoK_α radiation ($\lambda = 0.71073$ Å) at room temperature with ω scan mode. A 30 s exposure time was used. Half of an Ewald sphere was collected. The unit cell parameters were determined from least-squares refinement of the setting angles of the 3767 strongest reflections. Details concerning crystal data and refinement are given in Table I.

Examination of two reference frames monitored after each 50 frames measured showed 0.11% loss of the intensity. During the data reduction decay correction coefficient was taken into account. Lorentz-polarization correction was applied to the intensity data. Numerical absorption correction was used. The maximum and minimum transmission factors were 0.849 and 0.716. The structure of the title compound was solved by direct methods and subsequently completed by the difference Fourier recycling. All the non-hydrogen atoms were refined anisotropically using full-matrix, least-squares technique on F^2. All the hydrogen atoms were found from difference Fourier synthesis after four cycles of anisotropic refinement, and refined as "riding" on the adjacent carbon atoms with individual isotropic temperature factors equal 1.2 times the value of equivalent temperature factor of the parent carbon atom. The solution and refinements were performed with SHELXS97 [15] and SHELXL97 [16]. The graphical manipulations were performed using the XP routine of the

TABLE I Crystal data and structure refinement for title compound

Empirical formula	$C_{24}H_{24}CuN_4O_5 \cdot C_{24}H_{26}CuN_4O_6$
Formula weight	1042.04
Temperature	293(2) K
Wavelength	$\lambda(MoK_\alpha) = 0.71073$ Å
Crystal system, space group	monoclinic, $C2/c$
Unit cell dimensions	$a = 25.1733(9)$ $b = 5.9301(3)$ $c = 30.9790(12)$ Å $\beta = 95.906(7)^\circ$
Volume	4600.0(3) Å^3
Z, Calculated density	4, 1.505 mg/m^3
Absorption coefficient	0.996 mm^{-1}
$F(000)$	2160
Crystal size	$0.36 \times 0.28 \times 0.17$ mm
θ range for data collection	3.38–25.05
Index ranges	$-29 \le h \le 29$, $-0 \le k \le 7$, $0 \le l \le 36$
Reflections collected/unique	4063/4063
Refinement method	full-matrix least-squares on F^2
Max. and min. transmission	0.849 and 0.716
Data/restraints/parameters	4063/0/332
Goodness-of-fit on F^2	1.052
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0388$, $wR2 = 0.0921$
R indices (all data)	$R1 = 0.0524$, $wR2 = 0.0999$
Largest diff. peak and hole	0.562 and -0.464 e. Å^{-3}

TABLE II Selected structural data for title compound. Distances in Å, angles in deg

I		*II*	
Cu(1)–O(1)	1.9532(19)	Cu(51)–O(51)	1.9763(18)
Cu(1)–N(1)	2.029(2)	Cu(51)–N(51)	2.032(2)
Cu(1)–O(3)	2.236(3)	Cu(51)–O(53)	2.427(2)
N(1)–C(1)	1.334(4)	N(51)–C(51)	1.335(3)
N(1)–C(5)	1.323(4)	N(51)–C(55)	1.340(4)
C(1)–C(2)	1.377(4)	C(51)–C(52)	1.380(4)
C(2)–C(3)	1.389(4)	C(52)–C(53)	1.393(4)
C(3)–C(4)	1.381(4)	C(53)–C(54)	1.389(4)
C(3)–C(6)	1.488(4)	C(53)–C(56)	1.476(4)
C(4)–C(5)	1.376(4)	C(54)–C(55)	1.385(4)
C(6)–N(2)	1.340(4)	C(56)–N(52)	1.342(4)
C(6)–C(10)	1.381(4)	C(56)–C(60)	1.388(4)
N(2)–C(7)	1.338(4)	N(52)–C(57)	1.348(4)
C(7)–C(8)	1.369(5)	C(57)–C(58)	1.380(5)
C(8)–C(9)	1.363(5)	C(58)–C(59)	1.354(6)
C(9)–C(10)	1.378(4)	C(59)–C(60)	1.385(4)
O(1)–C(11)	1.261(4)	O(51)–C(61)	1.280(3)
C(11)–O(12)	1.233(4)	C(61)–O(52)	1.223(3)
C(11)–C(12)	1.510(4)	C(61)–C(62)	1.507(4)
O(1)#1–Cu(1)–O(1)	177.57(13)	O(51)#2–Cu(51)–O(51)	180.0
O(1)#1–Cu(1)–N(1)	90.70(8)	O(51)#2–Cu(51)–N(51)	92.16(8)
O(1)–Cu(1)–N(1)	89.49(8)	O(51)–Cu(51)–N(51)	87.84(8)
N(1)–Cu(1)–N(1)#1	170.89(14)	N(51)–Cu(51)–N(51)#2	180.0
O(1)–Cu(1)–O(3)	88.78(6)	O(51)–Cu(51)–O(53)	93.03(7)
		O(51)–Cu(51)–O(53)#2	86.97(7)
N(1)–Cu(1)–O(3)	94.55(7)	N(51)–Cu(51)–O(53)	94.13(8)
		N(51)–Cu(51)–O(53)#2	85.87(8)
		N(51)#2–Cu(51)–O(53)#2	94.13(8)
		O(53)#2–Cu(51)–O(53)	180.0
C(5)–N(1)–C(1)	117.1(3)	C(55)–N(51)–C(51)	117.6(2)
C(5)–N(1)–Cu(1)	118.9(2)	C(55)–N(51)–Cu(51)	120.74(18)
C(1)–N(1)–Cu(1)	124.1(2)	C(51)–N(51)–Cu(51)	121.62(18)
N(1)–C(1)–C(2)	123.2(3)	N(51)–C(51)–C(52)	123.0(3)
C(1)–C(2)–C(3)	120.0(3)	C(51)–C(52)–C(53)	119.8(3)
C(4)–C(3)–C(2)	116.1(3)	C(54)–C(53)–C(52)	117.0(3)
C(4)–C(3)–C(6)	122.5(3)	C(54)–C(53)–C(56)	121.8(3)
C(2)–C(3)–C(6)	121.4(3)	C(52)–C(53)–C(56)	121.1(3)
C(5)–C(4)–C(3)	120.5(3)	C(55)–C(54)–C(53)	119.7(3)
N(1)–C(5)–C(4)	123.2(3)	N(51)–C(55)–C(54)	122.8(3)
N(2)–C(6)–C(10)	121.8(3)	N(52)–C(56)–C(60)	123.1(3)
N(2)–C(6)–C(3)	116.6(3)	N(52)–C(56)–C(53)	115.7(3)
C(10)–C(6)–C(3)	121.6(3)	C(60)–C(56)–C(53)	121.2(3)
C(7)–N(2)–C(6)	117.5(3)	C(57)–N(52)–C(56)	116.6(3)
N(2)–C(7)–C(8)	124.2(4)	N(52)–C(57)–C(58)	123.5(4)
C(9)–C(8)–C(7)	117.6(3)	C(59)–C(58)–C(57)	118.9(3)
C(8)–C(9)–C(10)	119.9(4)	C(58)–C(59)–C(60)	119.6(4)
C(9)–C(10)–C(6)	119.0(3)	C(59)–C(60)–C(56)	118.3(4)
C(11)–O(1)–Cu(1)	122.25(19)	C(61)–O(51)–Cu(51)	128.92(18)
O(2)–C(11)–O(1)	125.3(3)	O(52)–C(61)–O(51)	124.6(3)
O(2)–C(11)–C(12)	118.5(3)	O(52)–C(61)–C(62)	119.5(3)
O(1)–C(11)–C(12)	116.1(3)	O(51)–C(61)–C(62)	115.9(2)

Symmetry transformations used to generate equivalent atoms: #1 $-x, y, -z+\frac{1}{2}$; #2 $-x, -y+1, -z$.

SHELXTL [17] and ORTEP [18]. Atomic scattering factors were those incorporated in the computer programs. Interatomic bond distances and angles are listed in Table II. Atomic coordinates and equivalent isotropic displacement parameters are listed in Table III.

TABLE III Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for title compound. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	$U_{(eq)}$
Cu(1)	0	570(1)	2500	29(1)
N(1)	732(1)	842(4)	2284(1)	32(1)
C(1)	871(1)	2487(6)	2025(1)	45(1)
C(2)	1375(1)	2679(6)	1892(1)	46(1)
C(3)	1766(1)	1112(5)	2030(1)	32(1)
C(4)	1612(1)	−608(6)	2290(1)	51(1)
C(5)	1100(1)	−679(6)	2409(1)	47(1)
C(6)	2318(1)	1298(6)	1901(1)	37(1)
N(2)	2440(1)	3219(5)	1706(1)	50(1)
C(7)	2934(1)	3416(7)	1587(1)	56(1)
C(8)	3323(1)	1808(7)	1660(1)	53(1)
C(9)	3194(1)	−132(7)	1861(1)	56(1)
C(10)	2687(1)	−413(6)	1983(1)	51(1)
O(1)	338(1)	500(3)	3096(1)	36(1)
C(11)	498(1)	2264(5)	3297(1)	33(1)
C(12)	746(1)	1942(6)	3757(1)	51(1)
O(2)	472(1)	4189(4)	3145(1)	57(1)
O(3)	0	−3201(5)	2500	49(1)
Cu(51)	0	5000	0	28(1)
N(51)	−758(1)	4920(4)	170(1)	27(1)
C(51)	−1065(1)	3092(5)	104(1)	33(1)
C(52)	−1576(1)	2961(5)	227(1)	32(1)
C(53)	−1793(1)	4803(5)	426(1)	29(1)
C(54)	−1476(1)	6716(5)	487(1)	35(1)
C(55)	−965(1)	6708(5)	358(1)	34(1)
C(56)	−2330(1)	4691(5)	576(1)	34(1)
N(52)	−2468(1)	2692(5)	734(1)	48(1)
C(57)	−2950(1)	2576(8)	886(1)	61(1)
C(58)	−3306(2)	4351(8)	868(1)	61(1)
C(59)	−3166(1)	6332(7)	694(1)	59(1)
C(60)	−2667(1)	6550(6)	548(1)	45(1)
O(51)	204(1)	6719(3)	538(1)	31(1)
C(61)	448(1)	6033(5)	897(1)	30(1)
C(62)	428(1)	7589(5)	1280(1)	41(1)
O(52)	681(1)	4229(4)	946(1)	61(1)
O(53)	247(1)	1413(4)	341(1)	54(1)

RESULTS AND DISCUSSION

A perspective view of the structure together with the atom numbering scheme is shown in Fig. 1, hydrogen atoms being omitted for clarity. The structure is plotted with 50% probability of displacement ellipsoids.

There are two different types of molecules in the crystal structure: monoaquadi(acetato-*O*)-*bis*(bipyridyl) copper(II) (**I** hereafter) and diaquadi(acetato-*O*)-*bis*(bipyridyl) copper (II) (**II** hereafter). The asymmetric unit includes a half of each molecule. The Cu(1) and O(3) atoms of molecule (**I**) lies on a twofold axis (special positions *e* of C2/c space group at 0, y, ¼ [19]). The Cu(51) atom of molecule (**II**) occupies a special position *b* at 0, ½, 0 [19] with site symmetry $\bar{1}$.

The copper atoms adopt almost ideal square pyramidal $(4+1)$ and square bipyramidal $(4+2)$ coordination for (**I**) and (**II**) respectively. The four basal bonds are formed by nitrogen atoms of 2,4′-bipyridyl, its symmetry equivalent generated via a $-x$, $y-z+\frac{1}{2}$ symmetry transformation for (**I**) and $-x$, $-y+1$, $-z$ for (**II**), oxygen

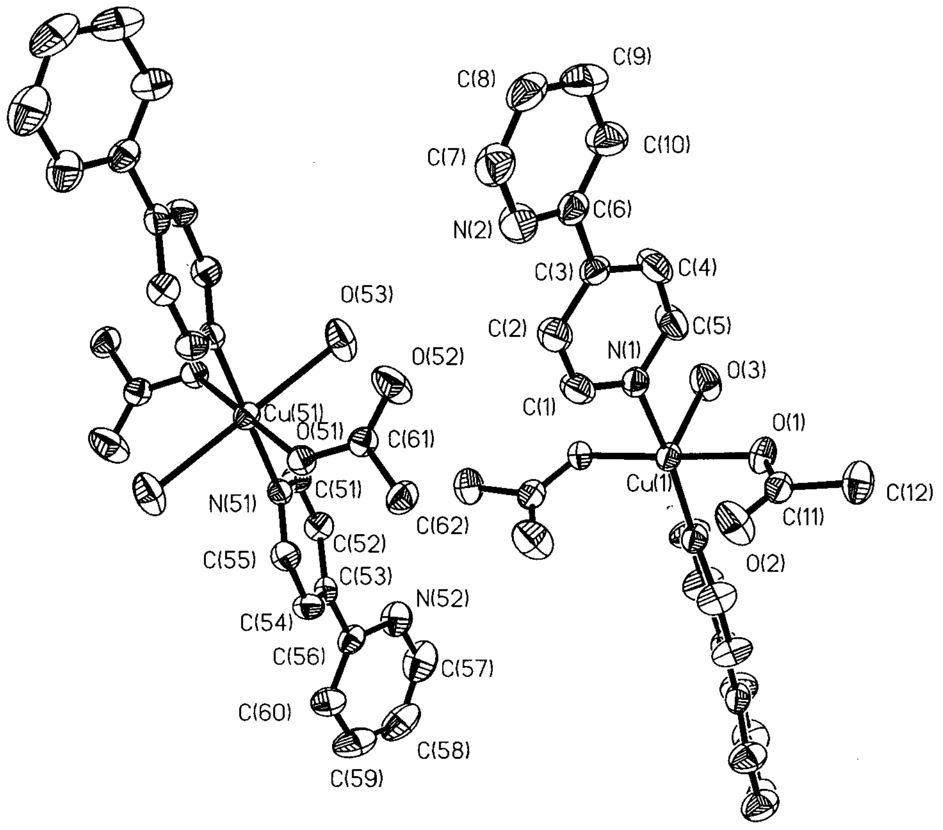

FIGURE 1 The molecular conformation title compound with atom numbering plotted with 50% probability of displacement ellipsoids. Hydrogen atoms are omitted for clarity.

TABLE IV Dihedral angles (deg) of copper polyhedra

Plane 1	*Plane 2*	*Angle*
Cu(1), N(1), N(1)#1, O(1), O(1)#1	Cu(1), N(1), N(1)#1, O(3)	90.00(1)
Cu(1), N(1), N(1)#1, O(1), O(1)#1	Cu(1), O(1), O(1)#1, O(3)	90.00(1)
Cu(1), N(1), N(1)#1, O(3)	Cu(1), O(1), O(1)#1, O(3)	89.39(8)
Cu(51), N(51), N(51)#2, O(51), O(51)#2	Cu(51), N(51), N(51)#1, O(53), O(53)#2	87.12(6)
Cu(51), N(51), N(51)#2, O(51), O(51)#2	Cu(51), O(51), O(51)#1, O(53), O(53)#2	85.97(8)
Cu(51), N(51), N(51)#2, O(53), O(53)#2	Cu(51), O(51), O(51)#1, O(53), O(53)#2	88.05(8)

Symmetry transformations used to generate equivalent atoms:#1 $-x, y, -z+1/2$;#2 $-x, -y+1, -z$.

atom of carboxylate group (coordinated in monodentate mode) and its symmetry equivalent. The coordination of the metal is completed by axial water molecules. Due to the Jahn–Teller effect the axial Cu–O(water) bond distances are longer by 0.283(3) Å for (**I**) and 0.451(2) Å for (**II**) than respective equatorial Cu–O(acetate) bond distances. All least squares planes of copper polyhedra, except one in molecule (**I**), are ideally planar, which is caused by symmetry elements. For the least squares plane calculated through Cu(1)–O(1)–N(1) and the N(1) symmetry equivalent the maximum deviation occurs for the N(1) atom (0.1133(17) Å) and the copper atom deviates by -0.04793 Å. All dihedral angles between these planes are close to 90.0° (for details, see Table IV).

The bond valences were computed as $\nu_{ij} = \exp[(R_{ij} - d_{ij})/0.37]$ [20–22], where R_{ij} is the bond-valence parameter (in the formal sense R_{ij} is the single-bond length between i and j atoms)[12]. The $R_{\mathrm{Cu-O}}$ and $R_{\mathrm{Cu-N}}$ were taken as 1.679[23], and 1.713[12], respectively. The compound bond valences of the copper in molecule (**I**) are $\nu_{\mathrm{Cu(1)-O(1)}} = 0.477$, $\nu_{\mathrm{Cu(1)-O(3)}} = 0.222$, $\nu_{\mathrm{Cu(1)-N(1)}} = 0.426$ v.u. (valence units), thus the computed valence of the Cu(1) atom is 2.03 v.u. For molecule (**II**) copper bond valences are $\nu_{\mathrm{Cu(51)-O(51)}} = 0.448$, $\nu_{\mathrm{Cu(51)-O(53)}} = 0.132$, $\nu_{\mathrm{Cu(51)-N(51)}} = 0.422$ v.u., which yields a valence of the Cu(51) atom equal to 2.00 v.u. Weakening of the Cu–O(water) bond in molecule (**II**) can be explained by the greater coordination number of Cu(51) than Cu(1).

The overall arrangement of acetate groups is close to that reported for the related mono- and diaquadi(acetato-*O*)-*bis*(substitutepyridyl) copper(II) complexes [24,25]. The least squares planes calculated through all atoms of acetate group and through copper and oxygen atoms make an angle 6.62(12) and 20.25(11)° for molecule (**I**) and (**II**), respectively. The increasing angle in molecule (**II**) is caused by the strong intramolecular hydrogen bond linking O(53) and O(52) atoms (D···A distance 2.662(3) Å, D–H···A angle 151.9(3)°, where *D* – donor and *A* – acceptor, hereafter).

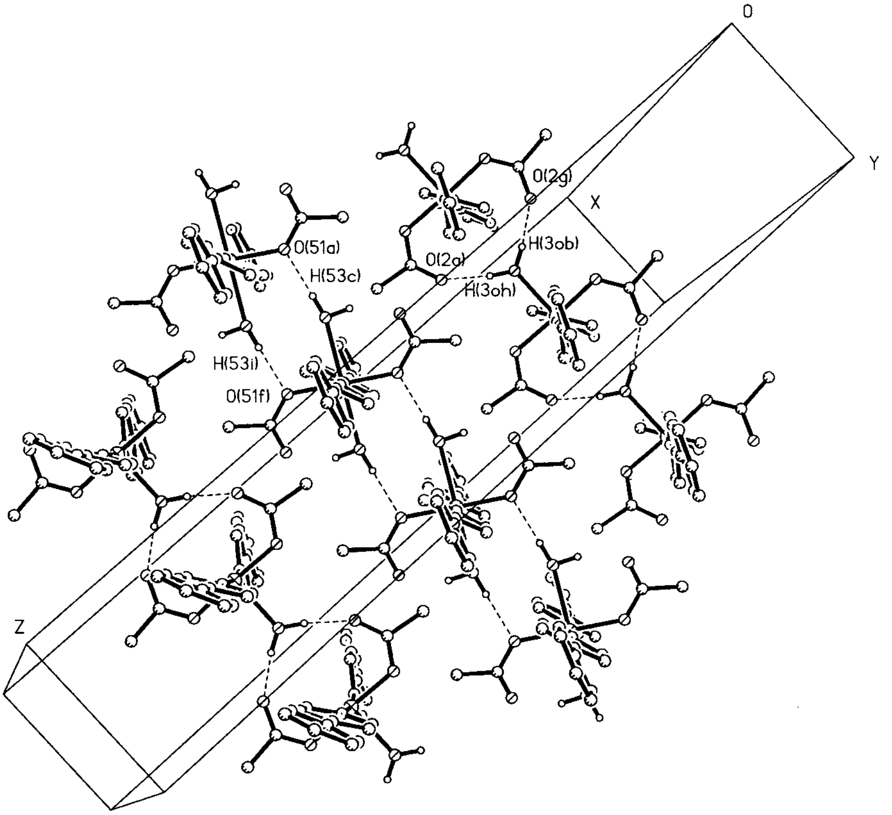

FIGURE 2 Fragment of crystal packing of title compound showing hydrogen bond infinite chains. Carbon bonded hydrogen atoms, not involved into intermolecular hydrogen bonds, are omitted for clarity.

The differences in the geometry of the copper environment in molecules (**I**) and (**II**) are imposed by intermolecular strong hydrogen bonds creating a linear infinite chain structure along the x axis (Fig. 2). In molecule (**I**) O(2) acting as an acceptor and its symmetry equivalent create chelating hydrogen bonds to O(3#) atom (generated by $-x$, $y-1$, $-z+\frac{1}{2}$ symmetry transformation) with a D$\cdots$A distance of 2.703(3) Å and a D$-$H$\cdots$A angle of 172.5(3)°. Molecules of (**II**) are assembled to a hydrogen bond chain via $-$O(53)$-$H(53O)O(51#) hydrogen bond (atom O(51#) generated by x, $y-1$, z symmetry transformation) with a D$\cdots$A distance of 2.855(3) Å, and a D$-$H$\cdots$A angle of 168.5(3)°. This hydrogen bond also explains the deviation of hydrogen atoms of water molecule O(51) from the copper polyhedra symmetry plane.

All pyridyl rings are planar within experimental error. The dihedral angle between two pyridyl rings in 2,4′-bipyridyl is 9.79(19) and 37.43(9) Å for (**I**) and (**II**), respectively. The smaller dihedral angle in molecule (**I**) is imposed by a weak intramolecular hydrogen bond linking C(2) and N(2) atoms (D$\cdots$A distance of 2.819(4) Å and D$-$H$\cdots$A angle of 100.5(4)°). The dihedral angle between the pyridyl ring indicated by N(1) and its symmetry equivalent is 67.92(9)°, and for the pyridyl ring indicated by N(51) and its symmetry equivalent is 0.00(14)°. The pyridyl ring attached to copper makes a dihedral angle with the least squares plane calculated through copper, nitrogen, acetate oxygen atom and their symmetry equivalents of 56.19(9) and 38.58(11)° for (**I**) and (**II**) respectively. The smaller dihedral angle in molecule (**II**) is imposed by a weak intramolecular hydrogen bond linking C(55) and O(51) atoms (D$\cdots$A distance of 2.937(3) Å and a D$-$H$\cdots$A angle of 106.7(3)°).

A rather short distance between O(53) and O(53$) (generated by $-x$, $-y$, $-z$ symmetry transformation) equal to 2.875(4) Å exists in the molecule. The described structure clearly illustrates the great influence of strong and weak hydrogen bonds on the conformation of molecules and differentiation of bond lengths.

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Supporting Information Available: Tables of crystal data and structure refinement, anisotropic displacement coefficients, atomic coordinates and equivalent isotropic displacement parameters for non-hydrogen atoms, H-atom coordinates and isotropic displacement parameters, bond lengths and interbond angles have been deposited with the Cambridge Crystallographic Data Centre under No. CCDC157451.

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