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## Structure of the Mixed-Valence Salt Bis(*N,N'*-dibenzyl-4,4'-bipyridinium) Aquanonachlorotricuprate(2II, I)

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**Abstract.**  $[\text{C}_{24}\text{H}_{22}\text{N}_2]_2[\text{Cu}_3\text{Cl}_9(\text{H}_2\text{O})]$ ,  $M_r = 1204.64$ , monoclinic,  $C2/c$ ,  $a = 27.78$  (1),  $b = 24.408$  (5),  $c = 18.202$  (5) Å,  $\beta = 125.35$  (2)°,  $V = 10\,065$  (5) Å<sup>3</sup>,  $Z = 8$ ,  $D_x = 1.59$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 17.8$  cm<sup>-1</sup>,  $F(000) = 4879$ ,  $T = 295$  K,  $R = 0.0729$  for 2632 unique observed [ $F \geq 3\sigma(F)$ ] reflections and 278 parameters. The title compound is a mixed-valence salt with a Cu<sup>II</sup>:Cu<sup>I</sup> ratio of 2:1. The structure consists of trimers of loosely associated  $\text{CuCl}_4^{2-}$ ,  $\text{CuCl}_2^-$  and  $(\text{CuCl}_3\text{H}_2\text{O})^-$  anions hydrogen bonded into chains running along the *c* direction of the unit cell. These chains run through stacks of benzyl viologen cations lying in the *ab* plane.

**Introduction.** In recent years this laboratory has been investigating several mixed-valence Cu<sup>II</sup>/Cu<sup>I</sup> systems (Willett, 1987; Willett & Halvorson, 1988; Scott & Willett, 1990). One such compound studied in this laboratory is (paraquat)Cu<sub>2</sub>Cl<sub>4</sub>, a salt reported several years ago (Macfarlane & Williams, 1969; Prout & Murray-Rust, 1969). This compound consists of chains of  $\text{CuCl}_4^{2-}$  tetrahedra sharing edges, co-crystallized parallel to stacks of methyl viologen cations (paraquat). The past studies of this compound allude to a donor-acceptor relationship between the paraquat cations and the  $(\text{Cu}_2\text{Cl}_4)_n$  chains, and powder EPR shows a small Cu<sup>II</sup> signal. Powder conductivity data show semiconductive behavior. An analog of the paraquat salt, employing benzyl viologen in place of the methyl viologen, was synthesized in an effort to enhance these properties. It was postulated that the benzyl viologen dication, which has a more positive reduction potential than that of the methyl viologen, would increase the amount of charge transferred from anion to cation,

and thus the amount of Cu<sup>II</sup> character in the chain. The crystal and molecular structure of the product obtained will be presented in this paper.

**Experimental.** The crystals were prepared using the preparation method developed for (methyl viologen)-Cu<sub>2</sub>Cl<sub>4</sub> (Macfarlane & Williams, 1969). This method produced small brownish-orange needle-shaped crystals. A crystal with dimensions 0.25 × 0.20 × 0.35 mm was selected for data collection on a Syntex P<sub>2</sub> diffractometer, with a graphite monochromator, upgraded to Nicolet R3 specifications (Campana, Shepard & Litchman, 1981). Lattice constants were derived from 25 reflections in the range  $21 < 2\theta < 26^\circ$ . Data were collected with  $\omega$  scans (1.1°); two check reflections monitored every 96 reflections ( $\bar{2}00$  and  $\bar{4}22$ ) show no systematic excursions; 4287 total reflections out to  $2\theta = 45^\circ$ , 2632 unique with  $R(\text{merge}) = 0.024$ ;  $hkl$  ranges,  $0 \leq h \leq 13$ ,  $0 \leq k \leq 26$ ,  $-17 \leq l \leq 17$ . Empirical  $\psi$  scan absorption corrections applied (program XEMP of SHELXTL, Sheldrick, 1985) assuming an ellipsoidally shaped crystal (relative transmission in the range 0.789 to 0.906).

The structure solution was obtained *via* the direct methods routine SOLV in the SHELXTL (version 5.1) crystallographic program package and refinement also utilized that set of programs (Sheldrick, 1985). A difference synthesis based on the Cu and Cl positions yielded the C, N and O atom positions. H atoms, except for phenyl rings, were constrained to ideal positions (C—H and N—H = 0.96 Å) and assigned isotropic thermal parameters 1.2 times larger than the associated atoms. Phenyl ring H atoms were also constrained to ideal positions, but were assigned isotropic thermal parameters of

0.08 Å<sup>2</sup>. The final refinement included positional parameters on all non-H and non-phenyl ring atoms. The phenyl rings were constrained to be regular hexagons with C—C = 1.395 Å. The Cu, Cl and O atoms were refined on *F* with anisotropic thermal parameters, with all other atoms refined with isotropic thermal parameters.

The final refinement resulted in  $R = 0.0729$  [ $F > 3\sigma(F)$ ] and 0.1109 (all data), where  $wR = 0.0667$  and  $w = 1/[\sigma^2(F) + g(F)^2]$ , with  $g = 0.00067$ . The goodness of fit was 1.591,  $|\Delta/\sigma|_{\max} = 0.032$ . The largest peak on the final difference map was 0.5 e Å<sup>-3</sup> near the water O atom, while the most negative excursion was -0.5 e Å<sup>-3</sup>. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Atomic coordinates are listed in Table 1 and bond distances and angles for the anions and one of the benzyl viologen cations are given in Table 2. A view of the structure is shown in Fig. 1.\* A stereoview of the unit cell including only the anion position is shown in Fig. 2, and a unit-cell packing diagram showing cations only is in Fig. 3.

\* Lists of data collection parameters, anisotropic thermal parameters, H-atom parameters, structure factors and bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53875 (34 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Atomic coordinates ( $\times 10^4$ ) and isotropic thermal parameters ( $\text{\AA}^2 \times 10^3$ ) for (benzyl viologen)<sub>2</sub>Cu<sub>3</sub>Cl<sub>9</sub>(H<sub>2</sub>O)

	x	y	z	U*
Cu(1)	2400 (1)	3322 (1)	2354 (1)	48 (1)
Cu(2)	1912 (1)	4948 (1)	-1582 (1)	55 (1)
Cu(3)	3293 (1)	5151 (1)	1841 (2)	86 (2)
Cl(1)	1794 (2)	2601 (1)	1903 (2)	58 (3)
Cl(2)	2704 (2)	4035 (1)	1921 (2)	58 (3)
Cl(3)	1849 (2)	3854 (2)	2628 (2)	58 (3)
Cl(4)	3252 (2)	2855 (2)	3048 (2)	61 (3)
Cl(5)	1629 (2)	4243 (2)	-2529 (3)	64 (3)
Cl(6)	1031 (2)	5160 (2)	-1882 (2)	53 (3)
Cl(7)	2461 (2)	5115 (2)	-95 (2)	67 (3)
Cl(8)	4038 (2)	4795 (2)	1962 (2)	54 (3)
Cl(9)	2890 (2)	5683 (2)	2259 (2)	65 (3)
O	2569 (4)	5098 (3)	-1746 (6)	55 (7)
N(1)	966 (5)	4300 (4)	-318 (7)	53 (3)
N(2)	1867 (5)	1329 (4)	211 (6)	40 (3)
N(3)	1785 (5)	3592 (4)	5224 (7)	43 (3)
N(4)	1065 (5)	787 (4)	5030 (7)	50 (3)
C(1)	400 (7)	4355 (6)	-991 (10)	77 (5)
C(2)	38 (7)	4640 (5)	-864 (9)	60 (5)
C(3)	196 (6)	4863 (5)	-76 (8)	36 (4)
C(4)	792 (7)	4776 (6)	628 (10)	69 (5)
C(5)	1167 (7)	4489 (6)	504 (9)	68 (5)
C(6)	1063 (4)	3057 (4)	-431 (5)	58 (4)
C(7)	858	2540	-813	71 (5)
C(8)	734	2425	-1657	85 (6)
C(9)	816	2827	-2119	86 (6)
C(10)	1021	3345	-1737	73 (5)
C(11)	1145	3460	-893	47 (4)
C(12)	1372 (7)	3995 (6)	-456 (10)	79 (5)
C(13)	2162 (6)	1670 (5)	898 (8)	49 (4)
C(14)	2417 (6)	2123 (5)	821 (8)	47 (4)
C(15)	2374 (6)	2252 (4)	56 (8)	38 (4)
C(16)	2094 (7)	1858 (6)	-609 (10)	69 (5)
C(17)	1828 (6)	1415 (6)	-548 (9)	57 (4)
C(18)	424 (4)	1105 (3)	-969 (5)	45 (4)
C(19)	-107	1357	-1251	64 (5)
C(20)	-166	1619	-625	64 (5)
C(21)	307	1627	283	63 (5)
C(22)	839	1374	565	54 (4)
C(23)	897	1113	-61	42 (4)
C(24)	1509 (6)	893 (5)	241 (8)	50 (4)
C(25)	1779	3551 (5)	4490 (8)	50 (4)
C(26)	2063 (6)	3126 (5)	4397 (8)	49 (4)
C(27)	2364 (6)	2727 (4)	5062 (7)	31 (4)
C(28)	2336 (6)	2801 (5)	5785 (8)	43 (4)
C(29)	2061 (6)	3229 (5)	5872 (8)	45 (4)
C(30)	693 (4)	3457 (4)	5380 (4)	56 (4)
C(31)	132	3236	4997	58 (4)
C(32)	-325	3362	4108	68 (5)
C(33)	-222	3707	3603	56 (4)
C(34)	339	3928	3986	46 (4)
C(35)	797	3802	4874	42 (4)
C(36)	1424 (6)	4015 (5)	5292 (9)	54 (4)
C(37)	1144 (6)	676 (5)	5809 (9)	51 (4)
C(38)	726 (6)	362 (5)	5798 (8)	47 (4)
C(39)	223 (5)	163 (4)	4997 (7)	27 (3)
C(40)	193 (6)	296 (5)	4236 (8)	52 (4)
C(41)	610 (6)	594 (5)	4264 (8)	53 (4)
C(42)	1316 (4)	1500 (3)	3619 (6)	59 (5)
C(43)	1094	1909	2966	76 (5)
C(44)	812	2365	3020	77 (5)
C(45)	753	2410	3727	70 (5)
C(46)	974	2001	4381	58 (4)
C(47)	1256	1545	4326	47 (4)
C(48)	1538 (6)	1129 (6)	5070 (9)	68 (5)

\* The equivalent isotropic  $U$  is defined as one-third of the trace of the orthogonalized  $U_{ij}$  tensor.

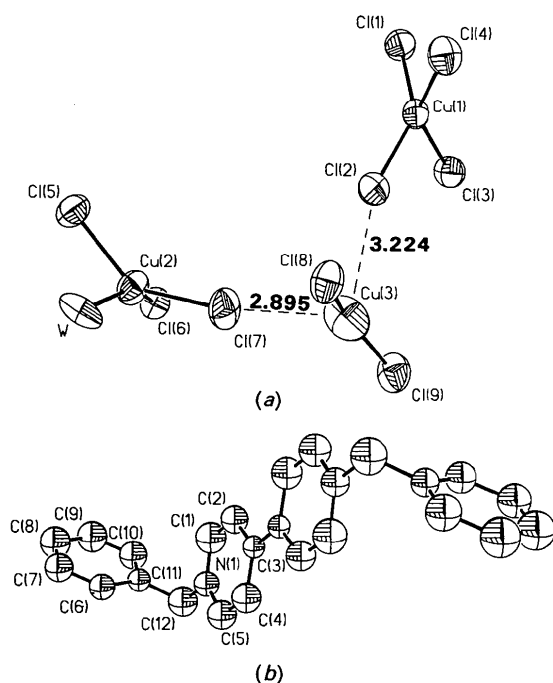


Fig. 1. (a) A view of the anion portion of the structure showing thermal ellipsoids and intratrimer bonds (Å). (b) A view of one of the benzyl viologen cations showing thermal ellipsoids.

**Discussion.** The design strategy succeeded, in one sense, in that the Cu<sup>II</sup>:Cu<sup>I</sup> ratio in the inorganic chain was increased to 2:1. However, this increase came at the expense of the simple chain of edge-shared tetrahedra present in (paraquat)Cu<sub>2</sub>Cl<sub>4</sub>. The assignment of the oxidation number to the metal ions is made on the basis of the coordination geome-

Table 2. Selected bond lengths (Å) and angles (°) for (benzyl viologen)<sub>2</sub>Cu<sub>3</sub>Cl<sub>9</sub>(H<sub>2</sub>O)

Cu(1)—Cl(1)	2.238 (4)	N(1)—C(1)	1.326 (16)
Cu(1)—Cl(2)	2.267 (5)	N(1)—C(5)	1.339 (20)
Cu(1)—Cl(3)	2.274 (6)	N(1)—C(12)	1.492 (26)
Cu(1)—Cl(4)	2.243 (5)	C(1)—C(2)	1.349 (29)
Cu(2)—Cl(5)	2.232 (4)	C(2)—C(3)	1.348 (21)
Cu(2)—Cl(6)	2.237 (6)	C(3)—C(4)	1.405 (17)
Cu(2)—Cl(7)	2.246 (4)	C(3)—C(3A)	1.436 (34)
Cu(2)—W	2.045 (13)	C(4)—C(5)	1.378 (30)
Cu(3)—Cl(8)	2.135 (6)	C(12)—C(11)	1.467 (16)
Cu(3)—Cl(9)	2.122 (6)		
Cl(1)—Cu(1)—Cl(2)	146.1 (2)	Cl(8)—Cu(3)—Cl(9)	153.3 (2)
Cl(1)—Cu(1)—Cl(3)	94.0 (2)	C(1)—N(1)—C(5)	120.3 (17)
Cl(2)—Cu(1)—Cl(3)	94.1 (2)	C(1)—N(1)—C(12)	120.1 (13)
Cl(1)—Cu(1)—Cl(4)	97.6 (2)	C(5)—N(1)—C(12)	119.5 (12)
Cl(2)—Cu(1)—Cl(4)	95.9 (2)	C(13)—N(2)—C(17)	121.1 (13)
Cl(3)—Cu(1)—Cl(4)	142.3 (2)	N(1)—C(1)—C(2)	119.7 (15)
Cl(5)—Cu(2)—Cl(6)	98.2 (2)	C(1)—C(2)—C(3)	125.1 (12)
Cl(5)—Cu(2)—Cl(7)	139.5 (2)	C(2)—C(3)—C(3A)	125.3 (13)
Cl(6)—Cu(2)—Cl(7)	97.9 (2)	C(2)—C(3)—C(4)	113.3 (16)
Cl(5)—Cu(2)—O	88.4 (3)	C(4)—C(3)—C(3A)	121.3 (15)
Cl(6)—Cu(2)—O	149.9 (3)	C(3)—C(4)—C(5)	122.1 (15)
Cl(7)—Cu(2)—O	95.8 (3)	C(10)—C(11)—C(12)	122.1 (9)
N(1)—C(5)—C(4)	119.4 (13)	N(1)—C(12)—C(11)	114.0 (14)
C(6)—C(11)—C(12)	117.9 (9)		

tries and on Cu—Cl bond distances. The Cu<sup>II</sup> species have pseudo-*D*<sub>2d</sub> symmetry with Cu—Cl bond distances of approximately 2.25 Å (Halvorson, Patterson & Willett, 1990), while the Cu<sup>I</sup> site has a slightly bent two-coordinate geometry with much shorter Cu—Cl lengths of 2.13 Å (Jardine, 1975). As can be observed from Fig. 1(a), the anionic chain portion of the structure is strikingly different from that of (methyl viologen)Cu<sub>2</sub>Cl<sub>4</sub>. Its chain structure is built up from CuCl<sub>4</sub><sup>2-</sup> tetrahedra sharing edges, while the chain in the title compound is a weakly bonded corkscrew consisting of trimeric units of CuCl<sub>4</sub><sup>2-</sup>, (CuCl<sub>3</sub>H<sub>2</sub>O)<sup>-</sup> and CuCl<sub>2</sub><sup>-</sup> anions, as shown in Fig. 1(a). The intratrimer bonding network is made up off long Cl—Cu(3) contacts, where Cu(3) is Cu<sup>I</sup>; Cl(2)—Cu(3) = 3.224 Å from the CuCl<sub>4</sub><sup>2-</sup> anion, and Cl(7)—Cu(3) = 2.895 Å from the (CuCl<sub>3</sub>H<sub>2</sub>O)<sup>-</sup> anion. There are two trimeric units in the repeat unit, the second generated using a *c* glide operation (Fig. 2). The *c* glide equivalent of the (CuCl<sub>3</sub>H<sub>2</sub>O)<sup>-</sup> anion has an O—Cl(3) contact of 3.032 Å, and an O—Cl(9) contact of 3.097 Å.

The crystal packing in the benzyl viologen salt also contrasts with that of the paraquat salt. In the paraquat compound the one-dimensional chains run parallel to stacks of methyl viologen cations, whereas in the benzyl viologen salt the chains run through holes in layers of the cations. These layers lie parallel to the *ab* plane. This can be observed in Fig. 3 where the channels are marked with crosses; the chains must twist in order to make it through the cation layers. In the paraquat structure the channels are much more linear, and the greater one-dimensional character of the (Cu<sub>2</sub>Cl<sub>4</sub>)<sub>n</sub> chains in this salt is probably derived from this. The non-planarity of the cations in the benzyl viologen case does not allow them to stack in such a linear fashion.

The structure of the title compound is also very different from other mixed-valence structures being studied in this laboratory. The compound (3-aminopyridinium)<sub>4</sub>Cu<sub>4</sub>Br<sub>10</sub> (Willett & Halvorson, 1988) is composed of tetrameric units made up of two Cu<sup>I</sup> species (disordered between tetrahedral CuBr<sub>4</sub><sup>2-</sup> and trigonal planar CuBr<sub>3</sub><sup>2-</sup> geometries), and two five-coordinate Cu<sup>II</sup> species of CuBr<sub>3</sub>N<sub>2</sub>, where N is the amino nitrogen of the cation. There are direct Br bridges between the Cu<sup>II</sup> and Cu<sup>I</sup> centers in this compound, with the bridging Cu—Br distance being only slightly longer than the non-bridging distances. Thus, the bridging network is much stronger than in the title compound, which possesses only semicoordinate Cu<sup>I</sup>—Cl distances in the Cu<sup>II</sup>—Cl—Cu<sup>I</sup> bridges, and very weak hydrogen-bonding interactions. The compound (Et<sub>4</sub>N)Cu<sub>2</sub>Cl<sub>4</sub> (Willett, 1987) possesses infinite chains of alternating CuCl<sub>4</sub><sup>2-</sup> and CuCl<sub>3</sub><sup>2-</sup> tetrahedra sharing edges, with a strong bibrigged interaction between Cu<sup>II</sup> and Cu<sup>I</sup>

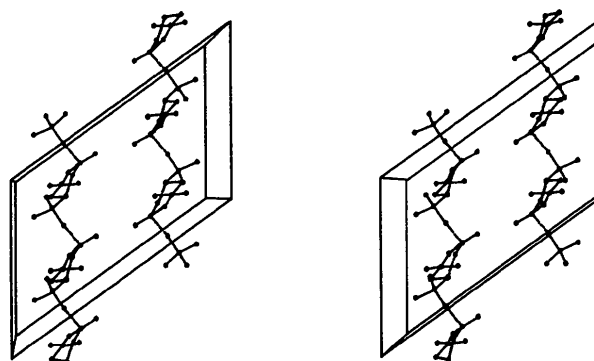


Fig. 2. A stereoview of the unit cell as viewed down the *b* axis. The cation portion has been omitted for clarity, and only one layer of chains is shown.

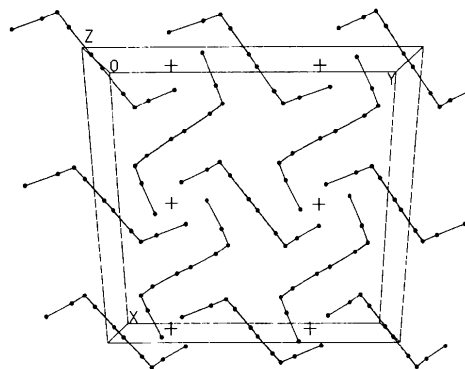


Fig. 3. A packing diagram of the unit cell as viewed down the chain axis (*c* axis). This is only one cationic layer ( $\frac{1}{2}$  along *c*). The anionic portion has been omitted for clarity, and only the atoms C(8), C(11), C(12), N(1), C(3) and their symmetry equivalents [Fig. 1(b)] are shown. The chains run through the channels marked with crosses.

sites. Another mixed-valence salt studied is the (hydrazinium)<sub>2</sub>Cu<sub>3</sub>Cl<sub>6</sub> salt, which has both bonded Cu<sup>I</sup>—Cl—Cu<sup>II</sup> bridges and bonded/semicoordinate Cu<sup>I</sup>—Cl...Cu<sup>II</sup> bridges (Scott & Willett, 1990). All of these compounds display the class II behavior of Robin & Day (1967) with broad intervalence absorption bands in the visible region of the spectrum (Scott, 1990). This transition probably arises *via* the strong Cu<sup>I</sup>—Cl—Cu<sup>II</sup> bridges present in these salts.

The Cu<sup>I</sup>...Cl—Cu<sup>II</sup> interactions in the title compound involve the two long Cu<sup>I</sup>...Cl contacts of 2.895 and 3.224 Å, shown as dashed lines in Fig. 1(a). The presence of such weak linkages makes the crystallographic assignment of the salt as a class I or class II mixed-valence system ambiguous. Clearly, the non-linearity of the CuCl<sub>2</sub><sup>-</sup> anion shows that some small perturbation is induced at the Cu<sup>I</sup> site. Nevertheless, the interaction must be much less than that in (Et<sub>4</sub>N)Cu<sub>2</sub>Cl<sub>4</sub> (Willett, 1987) and related systems (Scott, 1990). Spectroscopic investigation will not be much assistance, since the visible region of the spectrum is dominated by the broad tail of a BV electronic transition.

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## Structure of Dichlorobis(2-chloroimidazole)copper(II)

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**Abstract.** [CuCl<sub>2</sub>(C<sub>3</sub>H<sub>3</sub>ClN<sub>2</sub>)<sub>2</sub>], *M<sub>r</sub>* = 339.5, monoclinic, *C*2/*c*, *a* = 7.988 (1), *b* = 12.276 (2), *c* = 11.633 (2) Å, β = 90.4 (2)°, *V* = 1140.7 (3) Å<sup>3</sup>, *Z* = 4, *D<sub>x</sub>* = 1.98 g cm<sup>-3</sup>, λ(Mo *K*α) = 0.7107 Å, μ = 27.01 cm<sup>-1</sup>, *F*(000) = 668, room temperature, *R* = 0.030 for 1257 reflections with *F* > 7σ(*F*). The structure consists of discrete four-coordinate molecular units. The 2-chloroimidazole ligands are bonded through the N(3) atoms. The coordination about the Cu atom is intermediate between tetrahedral and square planar.

**Introduction.** Coordination about the Cu atom in complexes of the type CuL<sub>2</sub>X<sub>2</sub>, containing pyridines and azoles, is found to depend also upon effects of non-bonding groups on the ligands. For example, in complexes with *X* = Cl, the metal is five-coordinate for *L* = 2-methylpyridine (Marsh, Hatfield & Hodgson, 1982) and six-coordinate for *L* = pyridine (Morosin, 1975), four-coordinate for *L* = *N*-methylimidazole (van Ooijen, Reedijk & Spek, 1979) and five-coordinate for *L* = imidazole (Lundberg, 1972). This paper reports the structure of the 2-