

Copper(I) Halide π -Complexes with Allylacetone Azine. Synthesis and Crystal Structure of $2\text{CuX} \cdot$ $\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{N}-\text{N}=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ ($\text{X} = \text{Cl}^-, \text{Br}^-$)

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Abstract—The crystals of the $2\text{CuCl} \cdot \text{AAAZ}$ (**I**) and $2\text{CuBr} \cdot \text{AAAZ}$ (**II**) complexes were prepared by an electrochemical synthesis from $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ or CuBr_2 in ethanol–2-butanol mixture and from allylacetone azine (AAAZ) and structurally characterized (DARCh diffractometer, $\text{MoK}\alpha$ radiation, 1091 and 738 independent reflections with $F \geq 4\sigma(F)$, $R = 0.027$ and 0.034 for **I** and **II**, respectively). The crystals of the isostructural compounds are orthorhombic, space group $Pcab$, $Z = 8$. Unit cell parameters for **I**: $a = 19.199(7)$, $b = 11.780(5)$, $c = 13.493(4)$ Å, $V = 3052(3)$ Å³; for **II**: $a = 19.264(4)$, $b = 12.340(8)$, $c = 13.591(4)$ Å, $V = 3231(4)$ Å³. In both structures, the ligand is both π - and σ -coordinated to the copper atom, whose trigonal-pyramidal surroundings consists of the nitrogen and halogen atoms and C=C bond in the equatorial plane and apical halogen atom. One of the coordinated allyl groups is locally disordered, which is particularly pronounced for **II**.

In transition metal chemistry, azomethines are known as ligands forming coordination σ bonds [1]. Earlier, we prepared and structurally characterized the first copper(I) π -complexes with olefinic derivatives of azomethines (*N*-allyl-2-furylaldimine and *N*-allylbenzaldimine) and revealed the coordination capabilities of the C=C bond in the presence of the $>\text{C}=\text{N}-\text{R}$ group [2]. It was of interest to prepare copper(I) π -complexes with allyl-substituted ligands containing the $>\text{C}=\text{N}-$ groups of various natures, in particular, with allyl-substituted azine containing the $>\text{C}=\text{N}-\text{N}=\text{C}<$ group, and to study the behavior of the C=C bond toward Cu(I) in the presence of this group. For this purpose, the copper(I) chloride and bromide π -complexes with allylacetone azine $\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{N}-\text{N}=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (AAAZ) $2\text{CuCl} \cdot \text{AAAZ}$ (**I**) and $2\text{CuBr} \cdot \text{AAAZ}$ (**II**) were synthesized and structurally characterized.

EXPERIMENTAL

The AAAZ ligand was prepared by reacting equimolar quantities of allylacetone and hydrazine sulfate with a 20% aqueous solution of sodium hydroxide [3]. High-quality single crystals of **I** and **II** were synthesized from $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ or CuBr_2 and AAAZ by an ($U = 0.3$ V) electrochemical synthesis on copper electrodes in the ethanol–2-butanol mixture. In both cases, mixing of the solutions of starting components was accompanied by vigorous gas evolution and decoloration of the solution, probably, because of a partial reduction of Cu(II) to Cu(I) by the ligand. The moderately air-stable crystals of **I** were grown over 1.5 h as

colorless needles. The crystals of **II** of the same habitus were formed on the electrodes over two days.

The structures were determined using the arrays of diffraction data collected on a single-crystal DARCh diffractometer. The reflection intensities were corrected for the Lorentz and polarization effects. Absorption was corrected using the DIFABS program.

The crystal data and data collection parameters are listed in Table 1.

The structures were solved by the direct method; light atoms and H atoms were located from the difference Fourier syntheses. All the non-hydrogen atoms were refined by the full-matrix anisotropic method (hydrogen atoms isotropically) with the CSD program package [4].

Atomic coordinates and thermal parameters for structures **I** and **II** are listed in Table 2; bond lengths, bond angles, and torsion angles are given in Table 3.

RESULTS AND DISCUSSION

Molecular compounds **I** and **II** are isostructural. Each of the two independent copper(I) atoms in the structures has the trigonal-pyramidal environment consisting of the nitrogen atom, halogen atom, and C=C bond in the equatorial plane and the apical halogen atom. The bridging function of the halogen atoms results in the formation of the [010]-directed helical polymeric fragments Cu_nX_n , with the sense of rotation changing according to the alternation of the Cu_2X_2 units ($\text{X} = \text{Cl}$ in structure **I** and Br in structure **II**). Each

Table 1. Crystal data and details of data collection for **I** and **II**

Parameter	I	II
<i>M</i>	390.3	479.2
<i>F</i> (000)	1584	1872
Space group	<i>Pcab</i>	<i>Pcab</i>
<i>a</i> , Å	19.199(7)	19.264(4)
<i>b</i> , Å	11.780(5)	12.340(8)
<i>c</i> , Å	13.493(4)	13.591(4)
<i>V</i> , Å ³	3052(3)	3231(4)
<i>Z</i>	8	8
ρ (calcd), g/cm ³	1.699(2)	1.970(2)
μ_{Mo} , cm ⁻¹	32.2	79.5
Radiation	MoK α	MoK α
Diffractometer	DARCh	DARCh
Scan mode	$\theta/2\theta$	$\theta/2\theta$
Number of reflections:		
measured	2055	1002
independent with $F \geq 4\sigma(F)$	1091	738
$2\theta_{\text{max}}$, deg.	47	50
Refined data	252	252
<i>R</i>	0.027	0.034
<i>R</i> _w	0.027	0.031
Weighing scheme	$[\sigma(F_o)^2 + 0.0004F_o^2]^{-1}$	$[\sigma(F_o)^2 + 0.0004F_o^2]^{-1}$
GOOF	1.07	1.15

unit is surrounded by the exceedingly flexible AAAZ molecule whose nearest nitrogen atom and the C=C bond are chelated to the copper atom. As a result, the AAAZ molecule, owing to the similar behavior of its second half, plays the role of a tetradentate ligand.

The structures of **I** and **II** are built from chains. Each chain is surrounded by six analogous chains (Fig. 1). Their outer organic parts are bonded via the van der Waals forces. Both inside and between the chains, hydrogen bonds of the C–H...X type are formed, additionally stabilizing the structure. The geometric parameters of the selected H bonds are given in Table 4. Noteworthy is the very strong C(7)–H(7.3)...Br(1) contact [H...Br 2.6(1) Å] that elongates the corresponding C–H bond to 1.18(9) Å.

Structure solution showed that the thermal motions of the C(9–12) atoms in **I** are to a large extent anisotropic and dominate in the direction perpendicular to the plane of the Cu(2)–m(11,12) and C(11)=C(12) bonds (Fig. 1). This is accompanied by the apparent shortening of the C=C double bond to 1.29(1) Å. In **II**, the shortening of the C(11)=C(12) bond to 1.20(2) Å is accompanied by changing the corresponding C=C–C angle (Table 3). The thermal motions of the C(9–12) atoms are also strongly anisotropic (Fig. 2). Despite the

fact that each of the C(9–12) atoms of complex **II** appeared in the difference Fourier map as two distinct maxima corresponding to two different positions, the geometry of the olefinic molecule failed to be improved. Because of this, Table 2 reports the average positions for two conformers. The coordinates of

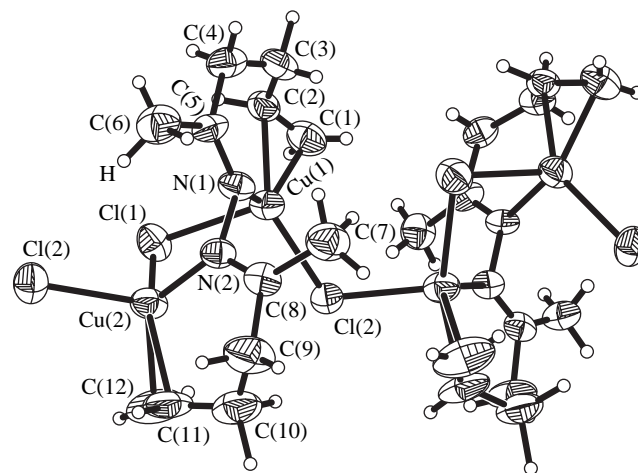
**Fig. 1.** Polymeric chain $(\text{Cu}_2\text{Cl}_2 \cdot \text{AAAZ})_n$ in structure **I**.

Table 2. Atomic coordinates * and thermal parameters** for structures **I** and **II**

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> , Å ²	Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> , Å ²
Cu(1)	0.58278(3)	0.06394(6)	0.71500(5)	3.55(2)	H(1.2)	0.506(2)	-0.094(3)	0.687(3)	2.0(9)
	0.58125(8)	0.0542(1)	0.7121(1)	4.41(5)		0.504(4)	-0.099(7)	0.686(7)	5(3)
Cu(2)	0.69211(3)	0.28241(6)	0.75397(5)	3.81(2)	H(2.1)	0.460(2)	0.130(3)	0.710(3)	4(1)
	0.69315(7)	0.2670(1)	0.7507(1)	4.69(5)		0.462(4)	0.126(7)	0.708(7)	6(3)
Cl(1)	0.60008(7)	0.2615(1)	0.6472(1)	4.11(4)	H(3.1)	0.410(2)	0.004(5)	0.847(3)	6(1)
Br(1)	0.59926(7)	0.2469(1)	0.63379(9)	4.95(4)		0.414(5)	0.014(7)	0.837(7)	5(3)
Cl(2)	0.67950(7)	-0.0304(1)	0.6683(1)	4.18(4)	H(3.2)	0.483(2)	-0.023(3)	0.851(3)	1.9(9)
Br(2)	0.68147(7)	-0.0470(1)	0.6656(1)	4.89(4)		0.488(4)	-0.038(7)	0.861(6)	3(2)
N(1)	0.5985(2)	0.1286(3)	0.8570(3)	2.9(1)	H(4.1)	0.460(2)	0.184(3)	0.890(2)	1(1)
	0.5992(5)	0.1202(7)	0.8507(6)	3.7(3)		0.456(5)	0.187(7)	0.888(6)	5(3)
N(2)	0.6683(2)	0.1692(3)	0.8653(3)	3.1(1)	H(4.2)	0.464(2)	0.119(4)	0.974(3)	5(1)
	0.6685(4)	0.1571(7)	0.8588(6)	3.4(3)		0.463(4)	0.118(7)	0.964(6)	4(3)
C(1)	0.4972(3)	-0.0257(5)	0.6660(4)	4.8(2)	H(6.1)	0.533(2)	0.281(3)	1.015(3)	3(1)
	0.4945(7)	-0.035(1)	0.668(1)	6.7(5)		0.533(4)	0.286(7)	1.009(6)	5(3)
C(2)	0.4763(2)	0.0545(4)	0.7302(4)	3.7(2)	H(6.2)	0.599(3)	0.311(5)	0.972(4)	8(2)
	0.4733(5)	0.045(1)	0.7285(9)	4.7(4)		0.609(5)	0.299(9)	0.964(8)	11(4)
C(3)	0.4626(3)	0.0349(5)	0.8391(4)	4.0(2)	H(6.3)	0.601(3)	0.217(5)	1.045(4)	9(2)
	0.4611(6)	0.032(1)	0.8364(9)	5.4(5)		0.601(5)	0.229(8)	1.017(8)	9(3)
C(4)	0.4799(3)	0.1312(5)	0.9063(4)	4.0(2)	H(7.1)	0.728(2)	-0.037(4)	0.998(3)	6(1)
	0.4789(6)	0.126(1)	0.8999(8)	4.7(4)		0.734(6)	-0.019(7)	1.000(8)	9(3)
C(5)	0.5532(2)	0.1697(4)	0.9158(3)	2.9(1)	H(7.2)	0.653(2)	0.022(4)	1.013(3)	5(1)
	0.5547(6)	0.1608(9)	0.9092(7)	3.4(4)		0.662(6)	0.021(8)	1.025(8)	10(4)
C(6)	0.5704(3)	0.2547(5)	0.9942(4)	4.5(2)	H(7.3)	0.661(3)	-0.040(5)	0.945(4)	8(2)
	0.5704(5)	0.239(1)	0.9856(9)	5.4(4)		0.652(5)	-0.072(8)	0.932(7)	5(3)
C(7)	0.6886(3)	0.0082(5)	0.9731(4)	4.6(2)	H(9.1)	0.805(2)	0.104(3)	0.952(3)	2.1(9)
	0.6856(6)	-0.001(1)	0.9649(9)	5.3(4)		0.810(5)	0.066(9)	0.930(8)	11(4)
C(8)	0.7098(2)	0.1077(4)	0.9169(3)	3.1(1)	H(9.2)	0.792(3)	0.215(5)	0.931(4)	12(2)
	0.7090(6)	0.0974(9)	0.9112(8)	3.6(4)		0.795(5)	0.162(8)	0.960(8)	11(4)
C(9)	0.7847(3)	0.1406(6)	0.9173(4)	5.6(2)	H(10.1)	0.876(2)	0.147(4)	0.843(4)	6(1)
	0.7843(6)	0.123(1)	0.9093(9)	6.9(5)		0.878(5)	0.138(8)	0.838(8)	9(3)
C(10)	0.8172(3)	0.1586(6)	0.8180(5)	5.9(2)	H(10.2)	0.805(3)	0.093(6)	0.763(5)	12(2)
	0.8176(7)	0.167(2)	0.832(1)	12.7(8)		0.805(5)	0.110(8)	0.765(8)	10(3)
C(11)	0.8005(2)	0.2645(6)	0.7647(5)	5.6(2)	H(11.1)	0.814(4)	0.314(7)	0.818(6)	16(3)
	0.7998(6)	0.236(1)	0.761(1)	8.5(6)		0.812(6)	0.304(9)	0.821(9)	14(4)
C(12)	0.7852(3)	0.2808(7)	0.6723(5)	7.6(3)	H(12.1)	0.788(3)	0.342(7)	0.632(6)	17(3)
	0.7892(7)	0.266(1)	0.679(1)	9.1(6)		0.794(6)	0.338(8)	0.665(8)	13(4)
H(1.1)	0.496(2)	-0.003(4)	0.598(3)	6(1)	H(12.2)	0.770(3)	0.225(6)	0.651(5)	13(2)
	0.495(4)	0.001(7)	0.607(6)	5(3)		0.779(6)	0.215(8)	0.638(8)	13(4)

* Atomic coordinates and thermal parameters in the upper row correspond to **I** and in the lower row, to **II**.

** $B_{eq} = 1/3 \sum_i \sum_j B_{ij} a_i^* a_j^* \hat{a}_i \hat{a}_j$ for non-hydrogen atoms.

Table 3. Bond lengths, * bond angles, and torsion angles in structures **I** and **II**

Bond**	<i>d</i> , Å		Angle**	ω , deg.	
	I	II		I	II
Cu(1)–X(1)	2.522(5)	2.629(8)	X(1)Cu(1)X(2)	104.2(2)	105.1(2)
Cu(1)–X(2)	2.254(7)	2.384(6)	X(1)Cu(1)N(1)	88.7(2)	89.5(3)
Cu(1)–N(1)	2.083(6)	2.08(1)	X(1)Cu(1) <i>m</i> (1,2)	111.0(3)	111.3(4)
Cu(1)–C(1)	2.062(9)	2.09(1)	X(2)Cu(1)N(1)	108.5(3)	108.1(3)
Cu(1)–C(2)	2.057(8)	2.09(1)	X(2)Cu(1) <i>m</i> (1,2)	126.9(3)	125.5(3)
Cu(1)– <i>m</i> (1,2)	1.947(8)	1.98(1)	N(1)Cu(1) <i>m</i> (1,2)	110.7(3)	111.4(5)
			C(1)Cu(1)C(2)	38.1(2)	37.7(5)
Cu(2)–X(1)	2.293(6)	2.420(5)	X(1)Cu(2)X(2)	106.8(2)	108.4(2)
Cu(2)–X(2)	2.454(5)	2.572(8)	X(1)Cu(2)N(2)	102.5(3)	103.2(3)
Cu(2)–N(2)	2.060(6)	2.06(1)	X(1)Cu(2) <i>m</i> (11,12)	126.2(3)	125.5(5)
Cu(2)–C(11)	2.096(8)	2.09(1)	X(2)Cu(2)N(2)	104.4(3)	104.6(3)
Cu(2)–C(12)	2.100(9)	2.09(1)	X(2)Cu(2) <i>m</i> (11,12)	104.4(3)	105.3(5)
Cu(2)– <i>m</i> (11,12)	1.997(8)	2.01(1)	N(2)Cu(2) <i>m</i> (11,12)	110.7(3)	108.1(5)
			C(11)Cu(2)C(12)	35.9(3)	33.2(6)
C(1)–C(2)	1.344(9)	1.35(2)			
C(2)–C(3)	1.511(8)	1.49(2)	C(1)C(2)C(3)	124.8(6)	125(1)
C(3)–C(4)	1.490(9)	1.48(2)	C(2)C(3)C(4)	115.9(6)	117(1)
C(4)–C(5)	1.48(1)	1.53(2)	C(3)C(4)C(5)	119.8(6)	119(1)
C(5)–N(1)	1.273(8)	1.27(1)	C(4)C(5)N(1)	118.5(6)	119(1)
C(5)–C(6)	1.493(9)	1.45(2)	C(4)C(5)C(6)	118.4(6)	117(1)
			N(1)C(5)C(6)	123.1(6)	125(1)
C(7)–C(8)	1.454(9)	1.49(2)	N(2)C(8)C(7)	124.4(6)	124(1)
			N(2)C(8)C(9)	117.1(6)	117(1)
N(1)–N(2)	1.427(9)	1.42(1)	C(5)N(1)N(2)	117.7(6)	117(1)
N(2)–C(8)	1.283(8)	1.29(1)	N(1)N(2)C(8)	115.9(6)	116(1)
C(8)–C(9)	1.49(1)	1.49(2)	C(7)C(8)C(9)	118.5(6)	119(1)
C(9)–C(10)	1.49(1)	1.34(2)	C(8)C(9)C(10)	115.9(6)	125(1)
C(10)–C(11)	1.48(1)	1.33(3)	C(9)C(10)C(11)	117.8(6)	134(2)
C(11)–C(12)	1.29(1)	1.20(2)	C(10)C(11)C(12)	130.1(7)	157(2)

Torsion angles

Angle**	ϕ , deg.		Angle	ϕ , deg.	
	I	II		I	II
Cu(1)X(1)Cu(2)X(2)	–134.4	–132.6	C(2)C(3)C(4)C(5)	–63.8	–65.5
Cu(1)X(2)Cu(2)X(1)	–2.5	–3.7	C(3)C(4)C(5)N(1)	–8.6	–10.8
Cu(1)N(1)C(5)C(4)	26.4	23.9	C(3)C(4)C(5)C(6)	–171.3	–169.2
Cu(1)N(1)C(5)C(6)	153.7	156.1	C(4)C(5)N(1)N(2)	178.1	177.8
Cu(1)C(1)C(2)C(3)	96.9	95.9	C(6)C(5)N(1)N(2)	2.0	2.2
Cu(1)N(1)N(2)C(8)	106.3	105.5	C(5)N(1)N(2)C(8)	–97.0	–96.4
Cu(1)N(1)N(2)Cu(2)	–53.4	–56.2	N(1)N(2)C(8)C(7)	6.0	3.0
Cu(2)N(2)C(8)C(7)	–161.6	–160.9	N(1)N(2)C(8)C(9)	173.1	170.8
Cu(2)N(2)C(8)C(9)	17.5	12.9	C(7)C(8)C(9)C(10)	–128.4	–144.2
Cu(2)N(2)N(1)C(5)	103.3	101.9	N(2)C(8)C(9)C(10)	50.7	–29.9
Cu(2)C(12)C(11)C(10)	100.9	114.2	C(8)C(9)C(10)C(11)	–75.7	–31.9
C(1)C(2)C(3)C(4)	–146.0	–144.6	C(9)C(10)C(11)C(12)	–136.4	–117.4

* C–H bond lengths range from 0.75(4) to 1.19(5) Å for **I** and from 0.8(1) to 1.2(1) Å for **II**.** X = Cl in structure **I** and Br in structure **II**; *m*(1,2) and *m*(11,12) are midpoints of the C(1)=C(2) and C(11)=C(12) bonds, respectively.

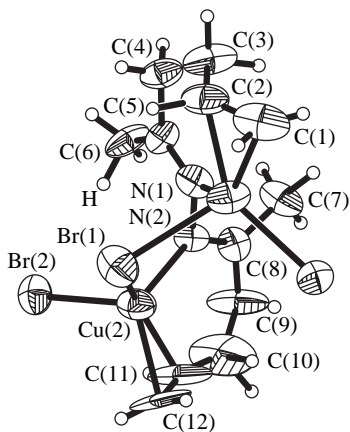
Table 4. Geometric parameters of hydrogen bonds in structures **I** and **II**

Bond C–H...X*	Distance, Å		CHX angle, deg.
	H...X	C–H	
C(4)–H(4.2)...X(1)	3.00(4)	0.97(4)	142(3)
	3.09(8)	0.92(8)	141(7)
C(6)–H(6.1)...X(1)	3.15(4)	0.84(4)	146(3)
	3.09(9)	0.97(9)	135(6)
C(6)–H(6.2)...X(2)	3.08(5)	0.91(5)	161(4)
	3.0(1)	1.1(1)	157(8)
C(7)–H(7.1)...X(2)	2.91(5)	0.98(5)	136(3)
	2.9(1)	1.1(1)	153(8)
C(7)–H(7.3)...X(1)	2.89(5)	0.87(5)	165(5)
	2.6(1)	1.18(9)	169(7)

* The values in the upper row correspond to **I** and in the lower row, to **II**; X = Cl (**I**), Br (**II**).

hydrogen atoms at the C atoms of the disordered allyl group in structure **II** are borrowed from structure **I** (for which they were found from difference Fourier syntheses) and refined isotropically.

The coordination polyhedra of the copper atoms are close to a tetrahedron: copper is markedly offset from the planes of equatorial ligands [0.40 and 0.56 Å in **I** and 0.44 and 0.61 Å in **II** for Cu(1) and Cu(2), respectively]. The orientation of the C=C bond is to a large extent determined by the steric factors: the angle τ between the plane of equatorial ligands and C=C bond is 13° and 14° in **I** and 12° and 4° in **II** for Cu(1) and Cu(2), respectively. The τ value (4°) for the Cu(2) atom in structure **II** is small because of the occurrence of the two conformations of the C(10)C(11)C(12) group, whose average position is found experimentally. The local disorder of the coordinated allyl group is probably

**Fig. 2.** Fragment of structure **II**.

stabilized by the hydrogen bonds of the (=C)–H...Br(2) type.

Despite the strong Cu(1)–(C=C) interaction [Cu(1)–*m*(1,2) distance is 1.947(8) Å in **I** and 1.98(1) Å in **II**], the coordinated olefinic bond C(1)=C(2) is only slightly elongated [to 1.344(9) Å in **I** and 1.35(2) Å in **II**], evidencing considerable predominance of the (M ← L)_σ component over the (M → L)_π component [5]. For the Cu(2) atom, the metal–olefin interaction is less efficient: the Cu(2)–*m*(11,12) distance is 1.997(8) Å in **I** and 2.01(1) Å in **II**.

Owing to the efficient Cu–N interaction in the copper(I) chloride π -complexes with *N*-allyl-2-furylaldimine and *N*-allylbenzaldimine, the metal atoms in these complexes are separately coordinated in the π and σ modes [Cu–N 1.932(4) and 1.941(5) Å, respectively] [2]. In **I** and **II**, the nitrogen atoms form weaker Cu–N contacts [2.083(6) and 2.060(6) Å in **I** and 2.08(1) and 2.06(1) Å in **II** for Cu(1) and Cu(2), respectively], allowing combined π - and σ -coordination of the copper atom.

Calculations with using the HYPERCHEM program and a modified version of the iterative SCF MO LCAO method in the INDO approximation [6] show that the charges on Cu(1) and Cu(2) in structure **I** are $-0.11\bar{e}$ and $-0.12\bar{e}$, respectively. The charge on each nitrogen atom ($-0.05\bar{e}$) is virtually equal to the charge on the nitrogen atom in the CuCl complexes with *N*-allyl-2-furylaldimine and *N*-allylbenzaldimine ($-0.04\bar{e}$) [2]. A considerable negative charge on the copper(I) atoms indicates that the nitrogen atoms in the AAZ molecule also possess donor properties, though weaker than in aldimines, thus favoring the combined π - and σ -coordination of copper by ligand.

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