# The Synthesis, Magnetic Properties, and Crystal Structure of Two Copper(II) Complexes Prepared from 2-Aminomethylpyridine

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# Abstract

The structures of Cu(amp)<sub>2</sub>(ClO<sub>4</sub>)<sub>2</sub> and [CuLCl<sub>2</sub>]<sub>2</sub> (where  $L = C_9 H_{12} N_2 O$ ) were determined by X-ray crystallographic techniques.  $Cu(amp)_2(ClO_4)_2$ crystallized in space group P1 with a = 7.630(2), b = 7.980(1), c = 7.972(5) Å,  $\alpha = 106.67(3), \beta = 108.75(3), \gamma = 95.90(2)^{\circ}$  and Z = 1. The structure was refined to R = 0.025 and  $R_{w} =$ 0.037 with 1146 reflections with  $I > 3\sigma(I)$ .  $[CuLCl_2]_2$  crystallized in space group P1 with a =7.093(1), b = 9.412(1), c = 9.541(2) Å,  $\alpha = 94.25(1)$ ,  $\beta = 103.69(2)$  and  $\gamma = 108.32(1)^{\circ}$ . The structure was refined to R = 0.040 and  $R_w = 0.051$  with 1265 reflections with  $I > 3\sigma(I)$ . CuLCl<sub>2</sub> forms a dimer through coordination of one of its chlorine atoms to the copper atom of an adjacent monomeric unit.  $Cu(amp)_2(ClO_4)_2$  forms a monomer with an octahedral coordination sphere. The perchlorate groups are weakly coordinated to the copper atom.  $Cu(amp)_2(ClO_4)_2$  exhibits Curie-Weiss behavior with g = 2.11 and  $\theta = 0.16$  K. [CuLCl<sub>2</sub>]<sub>2</sub> exhibits antiferromagnetic intra-dimer coupling with g = 2.09and  $2J = -3.50 \text{ cm}^{-1}$ .

# Introduction

We have been synthesizing and investigating the structural and magnetic properties of complexes resulting from the coordination of copper(II) with 2-aminomethylpyridine and its derivatives. In an earlier report we described a linear chain complex of copper-(II) chloride and 2-aminomethylpyridine [1]. Our previous reports of complexes that use 2-aminomethylpyridine as a building block also include the observation of binuclear [1, 2] species. In this report we describe some additional coordination chemistry of 2-aminomethylpyridine.

The coordination chemistry of 2-alkylpyridines with copper(II) has yielded a variety of interesting adducts. Hodgson and coworkers have reported ladder type linear chains with copper(II) bromides [3, 4], and similar complexes prepared from copper-(II) chlorides have been reported by our laboratory [1]. The simple coordination salts of copper(II) halides with aminoalkylpyridine show a propensity for clustering with all reported examples being either dimers or polymers. In order to investigate the electron and molecular structure of some monomeric complexes of 2-aminomethyl pyridine, we prepared these complexes using a non-coordinating anion such as perchlorate. We also attempted to prepare a copper(II) chloride complex with this ligand in a



nonaqueous environment by using triethylorthoformate as a dehydrating agent. However, a condensation reaction occurred between the aminomethylpyridine and one of the hydrolysis fragments of the triethylorthoformate (vide infra). The product of this condensation reaction (L) coordinates with Copper-(II) chloride to produce a dimeric complex  $[CuLCl_2]_2$ . The dimer exhibits antiferromagnetic coupling propagated through the chlorine bridge. We report here on the synthesis, the room temperature crystal structure, and the variable temperature magnetic susceptibility over the 300 K temperature region for the two complexes,  $Cu(amp)_2(ClO_4)_2$  and  $(CuLCl_2)_2$ , amp = 2-aminomethylpyridine and where L=  $C_{9}H_{12}N_{2}O.$ 

# Experimental

Syntheses

 $Cu(amp)_2(ClO_4)_2$ 

A solution of 200 mmol of 2-aminomethylpyridine in 100 ml of ethanol was reacted with a solution of 100 mmol of hydrated copper chloride also in ethanol. The reaction solution was heated for a few minutes, filtered and allowed to slowly evaporate yielding a blue crystal product suitable for X-ray and magnetic analysis.

# $[CuLCl_2]_2$

A solution consisting of 100 mmol of 2-aminomethylpyridine was dissolved in 100 ml of ethanol with 5 ml of triethylorothoformate. This solution was added while hot to a solution of 100 mmol of copper-(II) chloride in 100 ml ethanol also containing 5 ml of triethylorothoformate. The resulting mixture was heated for a few minutes and filtered. The filtered solution yielded small crystals of  $Cu(L)Cl_2$  which were used for X-ray and magnetic analysis.

# Magnetic Measurements

Polycrystalline samples of the complexes were measured on a model 905 Superconducting SQUID susceptometer purchased from SHE Corporation. The susceptometer is interface to an IBM 9000 computer system. Data were recorded over the 2--300 K temperature range. The general experimental technique used for data collection is described elsewhere.

#### **Crystal Structure Determination**

A single blue-green crystal of  $[CuLCl_2]_2$  and a single violet crystal of  $Cu(amp)_2(ClO_4)_2$  were mounted on an Enraf-Nonius CAD-4 diffractometer with graphite crystal monochromatized Mo K $\alpha$  radiation.

Lattice constants for  $Cu(amp)_2(ClO_4)_2$  were determined by a least-squares fit of 25 reflections with  $20 \le 2\theta \le 30^\circ$  resulting in a = 7.630(2), b =7.980(1), c = 7.972(5) Å,  $\alpha = 106.67(3)$ ,  $\beta = 108.75$ -(3) and  $\gamma = 95.90(2)^{\circ}$ . Unit cell dimensions and successful determination of the structure confirmed the space group as P1. Three dimensional intensity data were collected in the  $\omega:2\theta$  scan mode. A total of 1270 reflections were measured ( $0 \le 2\theta \le 50^\circ$ ) with 1146 considered observed  $(I > 3\sigma(I))$ . The data were corrected for absorbance as a function of psi (maximum absorbance, 18%). The structure was solved by placing Cu at the origin. All remaining atoms were located on successive Fourier maps. Subsequent full-matrix least-squares refinement on F of all atom positions and thermal parameters (except Cu positions) led to R = 0.025 and  $R_w =$ 0.037.

Lattice constants for  $[CuLCl_2]_2$  were determined by a least-squares fit of 25 reflections with  $18 \le 2\theta \le 37^\circ$  resulting in a = 7.093(1), b = 9.412(1), c = 9.541(2) Å,  $\alpha = 94.25(1)$ ,  $\beta = 103.69(2)$  and  $\gamma = 108.32(1)^\circ$ . Unit cell dimensions and successful determination of the structure confirmed the space group as  $P\overline{1}$ . A total of 1521 reflections were measured ( $0 \le 2\theta \le 44^\circ$ ) with 1265 considered observed ( $I > 3\sigma(I)$ ). The data were corrected for absorbance as a function of psi (maximum absorbance, 30%). The structure was solved using a Patterson function to locate the Cu atom. All other atoms were located on successive Fourier maps. Subsequent least-squares refinement of all atom positions and thermal parameters led to R = 0.040and  $R_w = 0.051$ .

## Results

The final fractional coordinates with estimated standard deviations (e.s.d.s) for each molecule are summarized for  $[CuLCl_2]_2$  and  $Cu(amp)_2(ClO_4)_2$  in Table I. Bond lengths and angles are shown in Tables II and III. Figure 1 shows a schematic drawing of one molecular unit of  $Cu(amp)_2(ClO_4)_2$  and Fig. 2 shows a schematic drawing of one dimeric unit of  $[CuLCl_2]_2$ . The molecule dimerizes by coordination



Fig. 1. ORTEP diagram of the formula unit of  $Cu(amp)_2$ -(ClO<sub>4</sub>)<sub>2</sub>.



Fig. 2. ORTEP diagram of the binuclear unit of [CuLCl<sub>2</sub>]<sub>2</sub>.

IABLE I. Positional Parameters and their Es	stimated Standard	Deviations
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$\begin{tabular}{l l l l l l l l l l l l l l l l l l l $	Atom	x	у	Z	B (Å <sup>2</sup> ) <sup>a</sup>
$\begin{array}{cccc} \mbox{Cu} & 0.75106(8) & -0.5242(6) & 0.54936(6) & 3.45(1) \\ \mbox{Cl} 1 & 0.6780(2) & -0.3762(1) & 0.7491(2) & 5.33(3) \\ \mbox{Cl} 2 & 0.8567(2) & -0.7646(4) & 0.1402(4) & 5.99(9) \\ \mbox{Nl} & 0.8255(5) & -0.6589(4) & 0.6525(4) & 3.83(9) \\ \mbox{Nl} & 0.8255(5) & -0.6589(4) & 0.6525(4) & 3.83(9) \\ \mbox{Nl} & 0.8255(5) & -0.6589(4) & 0.6325(4) & 3.83(9) \\ \mbox{Cl} & 0.8912(8) & -0.7090(5) & 0.7361(6) & 4.7(1) \\ \mbox{Cl} & 0.8912(8) & -0.9521(6) & 0.7430(7) & 5.6(2) \\ \mbox{Cl} & 0.89703(8) & -0.9521(6) & 0.7430(7) & 5.6(2) \\ \mbox{Cl} & 0.8703(8) & -0.9523(5) & 0.5385(7) & 4.9(1) \\ \mbox{Cl} & 0.8703(8) & -0.9523(5) & 0.5385(7) & 4.9(1) \\ \mbox{Cl} & 0.7255(7) & -0.8052(3) & 0.3385(6) & 4.5(1) \\ \mbox{Cl} & 0.7255(7) & -0.8052(3) & 0.3385(6) & 4.5(1) \\ \mbox{Cl} & 0.7255(7) & -0.8052(3) & 0.3385(6) & 4.5(1) \\ \mbox{Cl} & 0.7255(7) & -0.8052(3) & 0.3385(6) & 4.5(1) \\ \mbox{Cl} & 0.7255(7) & -0.8052(3) & 0.3385(6) & 4.5(1) \\ \mbox{Cl} & 0.416(9) & -0.8127(7) & -0.1090(6) & 6.2(2) \\ \mbox{HI} & 0.920(6) & -0.618(3) & 0.652(5) & -0.0014(6) & 5.8(2) \\ \mbox{Cl} & 0.4979(9) & -0.7105(6) & 0.0344(6) & 5.8(2) \\ \mbox{Cl} & 0.4979(9) & -0.8127(7) & -0.1090(6) & 7.11* \\ \mbox{HI} & 0.920(6) & -1.034(6) & 0.531(5) & 6(1)* \\ \mbox{HI} & 0.920(6) & -1.040(6) & 0.738(6) & 7(1)* \\ \mbox{HI} & 0.597(6) & -0.687(4) & 0.351(5) & 6(1)* \\ \mbox{HI} & 0.597(6) & -0.687(4) & 0.317(5) & 5(1)* \\ \mbox{HI} & 0.395(6) & -0.655(5) & -0.002(5) & 5(1)* \\ \mbox{HI} & 0.395(6) & -0.687(4) & -0.112(7) & 8(2)* \\ \mbox{HI} & 0.3047(7) & -0.837(6) & -0.037(6) & 7(1)* \\ \mbox{HI} & 0.395(6) & -0.653(6) & -0.093(6) & 7(1)* \\ \mbox{HI} & 0.395(6) & -0.037(6) & 0.3538(6) & 4.7(1) \\ \mbox{Ol} & 0.307(6) & 0.3538(6) & -0.012(7) & 2.58(3) \\ \mbox{Ol} & 0.3038(6) & -0.0136(6) & 7329(6) & 5.7(1) \\ \mbox{Ol} & 0.3038(6) & -0.1058(6) & 0.3038(6) & 0.7328(6) & 5.7(1) \\ \mbox{Ol} & 0.3038(6) & -0.1058(15) & 0.338(6) & 4.7(1) \\ \mbox{Ol} & 0.3038(6) & -0.1058(15) & 0.338(6) & 4.7(1) \\ \mbox{Ol} & 0.3038(6) & -0.1058(16) & 0.3338(6) & 5.7(1) \\ \m$	For [Cu(C <sub>9</sub> H <sub>12</sub>	2N2O)Cl2]2			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Cu	0.75106(8)	-0.52482(6)	0.56936(6)	3.85(1)
$\begin{array}{cccccc} C12 & 0.8567(2) & -0.3762(1) & 0.7891(2) & 5.31(3) \\ 01 & 0.5790(5) & -0.7640(4) & 0.1402(4) & 5.909(9) \\ N1 & 0.8255(5) & -0.66989(4) & 0.65356(4) & 3.83(9) \\ N2 & 0.7036(5) & -0.65952(4) & 0.3839(4) & 4.1(1) \\ C1 & 0.8912(8) & -0.7090(5) & 0.7951(6) & 4.9(1) \\ C2 & 0.9145(9) & -0.8546(6) & 0.4439(6) & 5.6(1) \\ C3 & 0.8703(8) & -0.9521(5) & 0.5965(7) & 4.9(1) \\ C4 & 0.8098(7) & -0.9521(5) & 0.551(5) & 4.1(1) \\ C5 & 0.7289(6) & -0.817(5) & 0.551(5) & 4.1(1) \\ C6 & 0.7275(7) & -0.8052(5) & 0.3983(6) & 4.5(1) \\ C7 & 0.6340(7) & -0.6040(5) & 0.2538(6) & 4.9(1) \\ C8 & 0.4979(9) & -0.7105(6) & -0.0044(6) & 5.8(2) \\ C9 & 0.4169(9) & -0.8527(7) & -0.1080(6) & 6.2(2) \\ H1 & 0.920(6) & -0.618(5) & 0.862(5) & 5.1(5) \\ H1 & 0.920(6) & -0.618(5) & 0.862(5) & 5.1(7) \\ H3 & 0.905(7) & -1.040(6) & 0.7388(6) & 7(1)^* \\ H4 & 0.786(6) & -1.034(5) & 0.534(5) & 7(1)^* \\ H5 & 0.597(5) & -0.887(4) & 0.351(5) & 6(1)^* \\ H7 & 0.596(6) & -0.650(5) & 0.234(5) & 5(1)^* \\ H9 & 0.647(8) & -0.624(6) & -0.0137(5) & 8(2)^* \\ H11 & 0.345(6) & -0.683(6) & -0.099(6) & 7(1)^* \\ H12 & 0.350(7) & -0.843(6) & -0.099(6) & 7(1)^* \\ H7 & 0.596(6) & 0.7124(7) & 0.099(6) & 7(1)^* \\ H12 & 0.350(7) & -0.843(6) & -0.0137(5) & 8(2)^* \\ H11 & 0.345(5) & 0.594(5) & 0.0004(2) & 2.25(2) \\ O1 & 0.1805(5) & 0.5945(5) & 0.0024(6) & 4.1(1) \\ O2 & 0.3116(6) & 0.8985(5) & 0.156(15) & 3.6(1) \\ O4 & 0.4409(6) & 0.7124(7) & -0.0347(6) & 5.9(1) \\ O4 & 0.4409(6) & 0.7124(7) & -0.0347(6) & 5.9(1) \\ O4 & 0.4409(6) & 0.7124(7) & -0.0347(6) & 5.9(1) \\ O4 & 0.4409(6) & 0.7124(7) & -0.0347(6) & 5.2(1) \\ O5 & 0.7044(6) & 0.013(5) & 0.3536(6) & 4.4(1) \\ O6 & 0.5649(6) & 0.2269(7) & 1.02236(6) & 5.2(1) \\ O6 & 0.5649(6) & 0.2269(7) & 1.0233(6) & 5.2(1) \\ O6 & 0.5649(6) & 0.2269(7) & 1.0233(6) & 5.2(1) \\ O6 & 0.5649(6) & 0.2269(7) & 0.3037(6) & 2.39(1) \\ O1 & 0.1855(5) & -0.2393(6) & -0.101(5) & 2.7(1) \\ O1 & 0.183(7) & 0.0331(7) & 0.3537(7) & 2.3(1) \\ O2 & 0.0185(5) & 0.016(5) & 0.2393(6) & 5.2(1) \\ O3 & 0.0453(7) & 0.0333(7) & 0.3537(7) & 2.3(1) \\ O2 & 0.0183(7) & 0.033$	C11	0.6780(2)	-0.3392(1)	0.4495(1)	4.56(3)
01         0.5790(5)         -0.7469(4)         0.1402(4)         5.09(9)           N1         0.855(5)         -0.6599(4)         0.535(4)         3.83(9)           N2         0.7036(5)         -0.6592(4)         0.3839(4)         4.1(1)           C1         0.8912(8)         -0.7990(5)         0.7961(6)         4.9(1)           C2         0.9145(9)         -0.823(5)         0.595(7)         4.9(1)           C3         0.8703(8)         -0.9521(5)         0.595(7)         4.9(1)           C4         0.899(7)         -0.8252(5)         0.3983(6)         4.5(1)           C5         0.7789(6)         -0.0170(6)         -0.0044(6)         5.8(2)           C8         0.4979(9)         -0.7105(6)         -0.0044(6)         5.8(2)           C9         0.4169(9)         -0.8327(7)         -0.1080(6)         6.2(2)           H1         0.920(6)         -0.6317(5)         0.848(5)         7(1)*           H2         0.964(7)         -0.837(6)         0.9534(5)         7(1)*           H4         0.786(6)         -0.0837(6)         0.324(5)         4(1)*           H6         0.859(6)         -0.837(6)         0.324(5)         5(1)*           H1 <td>C12</td> <td>0.8567(2)</td> <td>-0.3762(1)</td> <td>0.7891(2)</td> <td>5.33(3)</td>	C12	0.8567(2)	-0.3762(1)	0.7891(2)	5.33(3)
N1         0.8256(5) $-0.6989(4)$ 0.6526(4)         3.33(9)           N2         0.736(5) $-0.6989(4)$ 0.339(4)         4.1(1)           C1         0.8912(8) $-0.7090(5)$ 0.7961(6)         4.9(1)           C2         0.9145(9) $-0.8324(6)$ 0.4730(7)         5.6(2)           C3         0.8703(8) $-0.9521(6)$ $0.7430(7)$ 5.6(2)           C4         0.8098(7) $-0.9521(5)$ $0.5551(5)$ 4.1(1)           C5         0.7896(6) $-0.8197(5)$ $0.5551(5)$ 4.1(1)           C6         0.7275(7) $-0.8052(5)$ $0.3983(6)$ 4.5(1)           C7         0.6340(7) $-0.6406(5)$ $0.2558(6)$ 4.5(1)           C8         0.4979(9) $-0.7105(6)$ $0.2553(6)$ 7(1)*           H1         0.920(6) $-0.618(5)$ $0.662(5)$ 7(1)*           H3         0.905(7) $-1.040(6)$ $0.738(6)$ 7(1)*           H4         0.786(6) $-0.837(6)$ $0.234(5)$ 5(1)*           H3         0.997(5) $-0.847(6)$ $-0.012(7)$ 8(2	01	0.5790(5)	-0.7469(4)	0.1402(4)	5.09(9)
N2         0.7036(5) $-0.6592(4)$ 0.3839(4)         4.1(1)           C1         0.8912(8) $-0.709(5)$ 0.7961(6)         4.9(1)           C2         0.9145(9) $-0.8364(6)$ 0.8429(6)         5.6(1)           C3         0.8703(8) $-0.9529(5)$ 0.5965(7)         4.9(1)           C5         0.7896(6) $-0.8152(5)$ 0.5983(6)         4.1(1)           C6         0.7275(7) $-0.6052(5)$ 0.5551(5)         4.1(1)           C6         0.7275(7) $-0.6406(5)$ 0.2558(6)         4.9(1)           C8         0.4979(9) $-0.7105(6)$ $-0.0180(6)$ 5.2(2)           C1         0.920(5) $-0.618(5)$ $0.682(5)$ 5(1)*           H1         0.920(5) $-0.837(6)$ $0.534(5)$ 7(1)*           H3         0.905(7) $-0.837(5)$ $0.534(5)$ 7(1)*           H4 $0.786(6)$ $-1.034(5)$ $0.534(5)$ 7(1)*           H4 $0.786(6)$ $-0.650(5)$ $0.234(5)$ 5(1)*           H2 $0.566(6)$ $-0.650(5)$ $0.234(5)$ 5(1)*	N1	0.8265(5)	-0.6989(4)	0.6526(4)	3.83(9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2	0.7036(5)	-0.6592(4)	0.3839(4)	4.1(1)
$\begin{array}{ccccc} C2 & 0.9145(9) & -0.8364(6) & 0.8429(6) & 5.6(1) \\ C3 & 0.8703(8) & -0.9521(6) & 0.7430(7) & 5.6(2) \\ C4 & 0.8098(7) & -0.9529(5) & 0.5965(7) & 4.9(1) \\ C5 & 0.7896(6) & -0.8197(5) & 0.5551(5) & 4.1(1) \\ C6 & 0.7275(7) & -0.8052(5) & 0.3983(6) & 4.5(1) \\ C7 & 0.6340(7) & -0.6406(5) & 0.2558(6) & 4.9(1) \\ C8 & 0.4979(9) & -0.7105(6) & -0.0044(6) & 5.8(2) \\ C9 & 0.4169(9) & -0.8527(7) & -0.1080(6) & 6.2(2) \\ H1 & 0.920(6) & -0.618(5) & 0.682(5) & 51(1)^* \\ H2 & 0.964(7) & -0.837(6) & 0.953(6) & 7(1)^* \\ H3 & 0.905(7) & -1.040(6) & 0.788(6) & 7(1)^* \\ H4 & 0.786(6) & -1.034(5) & 0.524(5) & 4(1)^* \\ H5 & 0.597(5) & -0.887(4) & 0.351(5) & 4(1)^* \\ H6 & 0.859(6) & -0.560(5) & 0.224(5) & 5(1)^* \\ H8 & 0.385(6) & -0.650(5) & 0.234(5) & 5(1)^* \\ H9 & 0.647(8) & -0.652(5) & -0.002(5) & 5(1)^* \\ H10 & 0.305(7) & -0.927(6) & -0.002(5) & 5(1)^* \\ H11 & 0.543(8) & -0.833(6) & -0.099(6) & 7(1)^* \\ \hline For Cu(amp)_2(CIO_{2})_2 \\ \hline Cu & 0.000 & 0.000 & 0.000 & 2.22 \\ C11 & 0.347(2) & 0.2750(2) & 0.9096(2) & 2.58(3) \\ C12 & 0.6554(2) & 0.2750(2) & 0.909(6) & 7(1)^* \\ \hline For CU(amp)_2(CIO_{2})_2 \\ \hline Cu & 0.000 & 0.000 & 0.000 & 2.22 \\ C11 & 0.347(8) & -0.833(6) & -0.099(6) & 7(1)^* \\ \hline For CU(amp)_2(CIO_{2})_2 \\ C12 & 0.6554(2) & 0.2750(2) & 0.9044(2) & 2.58(3) \\ C12 & 0.6554(2) & 0.2750(2) & 0.9044(2) & 2.58(3) \\ C12 & 0.6554(2) & 0.2750(2) & 0.0024(6) & 4.1(1) \\ C3 & 0.4509(7) & 0.6795(6) & 0.2593(6) & 5.3(1) \\ O4 & 0.4409(6) & 0.712(97) & -0.0347(6) & 5.3(1) \\ O4 & 0.4409(6) & 0.712(97) & 0.0347(6) & 5.3(1) \\ O4 & 0.4409(6) & 0.712(97) & 0.0347(6) & 5.3(1) \\ O4 & 0.4409(6) & 0.712(97) & 0.283(6) & 0.709(6) & 7.117 \\ C1 & -0.073(8) & 0.303(6) & 0.703(6) & 0.793(6) & 5.2(1) \\ N1 & -0.0268(5) & 0.1061(6) & 0.9935(6) & 4.4(1) \\ O3 & 0.4509(7) & 0.218(7) & 0.2387(6) & 2.3(1) \\ C1 & -0.073(8) & 0.0345(7) & 0.339(7) & 0.2387(6) & 2.3(1) \\ C1 & -0.073(8) & 0.0345(7) & 0.303(7) & -0.537(7) & 2.8(1) \\ C2 & -0.184(7) & -0.2489(7) & -0.337(7) & 2.8(1) \\ C1 & -0.1080(7) & -0.2489(7) & -0.390(7) & 7.7(1) \\ C1 & 0.1080(7) & -0.2489(7$	C1	0.8912(8)	-0.7090(5)	0.7961(6)	4.9(1)
$\begin{array}{ccccc} C3 & 0.8703(8) & -0.9621(6) & 0.7430(7) & 5.6(2) \\ C4 & 0.809(7) & -0.9529(5) & 0.5955(7) & 4.5(1) \\ C5 & 0.7896(6) & -0.8197(3) & 0.5551(5) & 4.1(1) \\ C7 & 0.6340(7) & -0.6406(5) & 0.2558(6) & 4.5(1) \\ C7 & 0.6340(7) & -0.6406(5) & 0.2558(6) & 4.5(1) \\ C8 & 0.4979(9) & -0.7103(6) & -0.0044(6) & 5.8(2) \\ C9 & 0.4169(9) & -0.8371(7) & -0.1080(6) & 6.2(2) \\ H1 & 0.920(6) & -0.618(5) & 0.862(5) & 5(1)^* \\ H3 & 0.905(7) & -1.040(6) & 0.788(6) & 7(1)^* \\ H4 & 0.786(6) & -1.034(5) & 0.524(5) & 4(1)^* \\ H5 & 0.597(5) & -0.887(4) & 0.351(5) & 4(1)^* \\ H6 & 0.859(6) & -0.654(5) & -0.023(5) & 5(1)^* \\ H8 & 0.385(6) & -0.654(5) & -0.023(5) & 5(1)^* \\ H9 & 0.647(8) & -0.654(6) & -0.012(7) & 8(2)^* \\ H10 & 0.305(7) & -0.927(6) & -0.085(6) & 8(2)^* \\ H11 & 0.543(8) & -0.893(6) & -0.190(6) & 7(1)^* \\ H12 & 0.350(7) & -0.927(6) & -0.099(6) & 7(1)^* \\ H11 & 0.3471(2) & 0.7244(2) & 0.969(8(2) & 2.36(3) \\ C11 & 0.3471(2) & 0.7244(2) & 0.996(8(2) & 2.36(3) \\ C11 & 0.3471(2) & 0.7244(2) & 0.909(6) & 7(1)^* \\ H11 & 0.545(5) & 0.0393(6) & -0.190(6) & 7(1)^* \\ C4 & 0.409(6) & 0.7129(7) & -0.347(6) & 5.9(1) \\ C3 & 0.4509(7) & 0.6795(6) & 0.2593(6) & 5.3(1) \\ C4 & 0.409(6) & 0.7129(7) & -0.347(6) & 5.9(1) \\ C3 & 0.7043(6) & 0.1031(5) & 0.3347(6) & 5.9(1) \\ C3 & 0.7043(6) & 0.1031(5) & 0.3347(6) & 5.9(1) \\ C3 & 0.7043(6) & 0.1031(5) & 0.2493(5) & 1.53(6) \\ C3 & 0.7043(6) & 0.0057(7) & 0.2493(6) & 5.3(1) \\ C4 & 0.1002(7) & 0.278(7) & 0.339(7) & 0.2393(6) & 5.3(1) \\ C5 & 0.1057(7) & 0.238(6) & -0.105(16) & -2.37(7) \\ C1 & -0.1738(8) & 0.0547(8) & 0.2931(8) & 3.3(1) \\ C2 & -0.1834(7) & 0.1288(7) & 0.3990(7) & 2.3(1) \\ C4 & 0.1002(7) & 0.338(7) & -0.3287(7) & 3.1(1) \\ C5 & 0.1057(7) & -0.348(7) & 0.3077(7) & 2.8(1) \\ C4 & 0.1002(7) & -0.333(7) & -0.337(7) & 2.3(1) \\ C5 & 0.1057(7) & -0.348(7) & -0.3990(7) & 2.3(1) \\ C4 & 0.1002(7) & -0.348(7) & -0.3990(7) & 2.3(1) \\ C5 & 0.1057(7) & -0.348(7) & -0.3990(7) & 2.3(1) \\ C4 & 0.1002(7) & -0.398(7) & -0.3991(7) & 2.7(1) \\ C11 & -0.1090(7) & -0.289(7) & -0.3091(7) & 2.7(1) \\ C12 & -0.261$	C2	0.9145(9)	-0.8364(6)	0.8429(6)	5.6(1)
$\begin{array}{ccccc} C4 & 0.8098(7) & -0.9529(5) & 0.5956(7) & 4.9(1) \\ C5 & 0.7395(6) & -0.8197(5) & 0.5551(5) & 4.1(1) \\ C6 & 0.7275(7) & -0.8052(5) & 0.3983(6) & 4.5(1) \\ C7 & 0.6340(7) & -0.6406(5) & 0.2558(6) & 4.9(1) \\ C8 & 0.4979(9) & -0.7105(6) & -0.0044(6) & 5.8(2) \\ C9 & 0.4169(9) & -0.837(7) & -0.1080(6) & 6.2(2) \\ H1 & 0.920(6) & -0.618(5) & 0.862(5) & 5(1)* \\ H2 & 0.964(7) & -1.040(6) & 0.788(6) & 7(1)* \\ H4 & 0.736(6) & -1.034(5) & 0.524(5) & 4(1)* \\ H5 & 0.597(5) & -0.887(4) & 0.351(5) & 4(1)* \\ H6 & 0.859(6) & -0.813(5) & 0.351(5) & 4(1)* \\ H6 & 0.859(6) & -0.650(5) & -0.002(5) & 5(1)* \\ H9 & 0.647(8) & -0.624(6) & -0.012(7) & 8(2)* \\ H10 & 0.350(7) & -0.833(6) & -0.025(5) & 5(1)* \\ H10 & 0.350(7) & -0.833(6) & -0.025(5) & 5(1)* \\ H11 & 0.543(8) & -0.893(6) & -0.098(6) & 7(1)* \\ For Cu(amp)_2(CO_4)_2 \\ Cu & 0.000 & 0.000 & 0.000 & 2.2 \\ C11 & 0.3471(2) & 0.7244(2) & 0.9944(2) & 2.52(3) \\ O1 & 0.1805(5) & 0.243(5) & 0.154(5) & 3.6(1) \\ O2 & 0.3116(6) & 0.8985(5) & 0.155(5) & 3.6(1) \\ O2 & 0.3116(6) & 0.8985(5) & 0.155(5) & 3.6(1) \\ O2 & 0.3116(6) & 0.8985(5) & 0.155(5) & 3.6(1) \\ O3 & 0.4509(7) & 0.6795(6) & 0.7192(6) & 5.3(1) \\ O4 & 0.4409(6) & 0.7129(7) & -0.347(6) & 5.3(1) \\ O3 & 0.4509(7) & 0.6795(6) & 0.7593(6) & 5.3(1) \\ O3 & 0.4509(7) & 0.3038(6) & 0.7502(6) & 5.3(1) \\ O4 & 0.4409(6) & 0.7129(7) & -0.347(6) & 5.3(1) \\ O4 & 0.4409(6) & 0.7129(7) & -0.347(6) & 5.3(1) \\ O4 & 0.5184(6) & 0.3038(6) & 0.7502(6) & 5.3(1) \\ O7 & 0.8356(5) & 0.4075(6) & 0.9983(6) & 4.4(1) \\ O8 & 0.5184(6) & 0.3038(6) & 0.7502(6) & 5.3(1) \\ O1 & -0.1738(8) & 0.0547(8) & 0.2373(6) & 5.3(1) \\ O1 & -0.1738(8) & 0.0547(8) & 0.2373(7) & 3.3(1) \\ C5 & 0.105(77) & 0.2481(7) & 0.3681(6) & 2.4(1) \\ C6 & 0.2655(77) & 0.303(7) & -0.3873(7) & 3.3(1) \\ C5 & 0.105(77) & -0.345(7) & 0.3077(7) & 2.8(1) \\ C5 & 0.105(77) & -0.345(7) & 0.3077(7) & 2.8(1) \\ C5 & 0.105(77) & -0.345(7) & 0.3077(7) & 2.8(1) \\ C5 & 0.105(77) & -0.345(7) & 0.3077(7) & 2.8(1) \\ C5 & 0.105(77) & -0.345(7) & 0.3077(7) & 2.8(1) \\ C5 & 0.105(77) & -0.345(7) & 0.3077(7) & $	C3	0.8703(8)	-0.9621(6)	0.7430(7)	5.6(2)
$\begin{array}{ccccc} C5 & 0.7896(6) & -0.8197(5) & 0.5551(5) & 4.1(1) \\ C6 & 0.7275(7) & -0.8052(5) & 0.3983(6) & 4.5(1) \\ C7 & 0.6340(7) & -0.6406(5) & 0.2558(6) & 4.5(1) \\ C8 & 0.4979(9) & -0.7105(6) & -0.0044(6) & 5.8(2) \\ C9 & 0.4169(9) & -0.8527(7) & -0.1080(6) & 6.2(2) \\ H1 & 0.920(6) & -0.618(5) & 0.862(5) & 5(1)* \\ H3 & 0.905(7) & -1.040(6) & 0.788(6) & 7(1)* \\ H4 & 0.786(6) & -1.034(5) & 0.524(5) & 4(1)* \\ H5 & 0.597(5) & -0.887(4) & 0.351(5) & 6(1)* \\ H6 & 0.859(6) & -0.813(5) & 0.361(5) & 6(1)* \\ H8 & 0.385(6) & -0.650(5) & 0.234(5) & 5(1)* \\ H8 & 0.385(6) & -0.665(5) & -0.002(5) & 5(1)* \\ H1 & 0.395(6) & -0.687(6) & -0.012(7) & 8(2)* \\ H11 & 0.596(6) & -0.693(6) & -0.012(7) & 8(2)* \\ H11 & 0.345(8) & -0.927(6) & -0.085(6) & 8(2)* \\ H11 & 0.345(8) & -0.927(6) & -0.099(6) & 7(1)* \\ \hline For Cu(amp)_2(ClO_d)_2 \\ C1 & 0.000 & 0.000 & 0.000 & 2.2 \\ C1 & 0.000 & 0.000 & 0.000 & 2.2 \\ C1 & 0.350(7) & -0.843(6) & -0.190(6) & 7(1)* \\ \hline For Cu(amp)_2(ClO_d)_2 \\ C2 & 0.516(5) & 0.5945(5) & 0.0024(6) & 4.1(1) \\ 0.3 & 0.4509(7) & 0.6795(6) & 0.2593(6) & 5.3(1) \\ 0.4 & 0.400(6) & 0.7129(7) & -0.0347(6) & 5.9(1) \\ 0.5 & 0.7043(6) & 0.1031(5) & 0.3943(6) & 0.7502(6) & 5.9(1) \\ 0.5 & 0.7043(6) & 0.1031(5) & 0.3945(6) & 4.7(1) \\ 0.6 & 0.5649(6) & 0.2694(7) & 1.0283(6) & 5.3(1) \\ 0.6 & 0.5649(6) & 0.2694(7) & 1.0283(6) & 5.3(1) \\ 0.71 & 0.1365(5) & 0.0475(6) & 0.2993(6) & 4.4(1) \\ 0.6 & 0.5649(6) & 0.2260(5) & 0.1002(5) & 2.5(1) \\ N3 & 0.0385(6) & -0.1061(6) & -0.2387(6) & 2.3(1) \\ 0.7 & 0.835(5) & 0.0473(8) & 0.2931(6) & 4.4(1) \\ 0.8 & 0.5318(6) & -0.1061(6) & -0.2387(6) & 2.3(1) \\ 0.1 & -0.1738(8) & 0.0547(8) & 0.29317(7) & 2.3(1) \\ 0.5 & 0.1057(7) & 0.2483(7) & 0.4552(7) & 3.3(1) \\ 0.5 & 0.1057(7) & 0.2483(7) & 0.3077(7) & 2.8(1) \\ 0.5 & 0.1057(7) & 0.2485(7) & -0.3037(7) & 2.37(1) \\ 0.4 & 0.1002(7) & -0.3303(7) & -0.5371(7) & 2.8(1) \\ 0.5 & 0.1057(7) & 0.2485(7) & -0.3091(7) & 2.7(1) \\ 0.11 & -0.1094(7) & -0.3303(7) & -0.3591(7) & 2.7(1) \\ 0.12 & -0.2618(7) & -0.2898(7) & -0.3091(7) & 2.7(1) \\ 0.12 & -0.2618(7) & -0.2898(7) & $	C4	0.8098(7)	-0.9529(5)	0.5965(7)	4.9(1)
C6 $0.7275(7)$ $-0.8052(5)$ $0.3983(6)$ $4.5(1)$ C7 $0.6340(7)$ $-0.6406(5)$ $0.2558(6)$ $4.9(1)$ C8 $0.4979(9)$ $-0.8527(7)$ $-0.1080(6)$ $5.3(2)$ H1 $0.920(6)$ $-0.618(5)$ $0.862(5)$ $5(1)^*$ H2 $0.954(7)$ $-0.837(6)$ $0.933(6)$ $7(1)^*$ H3 $0.995(7)$ $-1.040(6)$ $0.788(6)$ $7(1)^*$ H4 $0.736(6)$ $-1.054(5)$ $0.524(5)$ $4(1)^*$ H5 $0.597(5)$ $-0.887(4)$ $0.351(5)$ $6(1)^*$ H6 $0.859(6)$ $-0.656(5)$ $-0.002(5)$ $5(1)^*$ H7 $0.596(6)$ $-0.656(5)$ $-0.002(5)$ $5(1)^*$ H8 $0.3857(7)$ $-0.833(6)$ $-0.012(7)$ $8(2)^*$ H10 $0.305(7)$ $-0.927(6)$ $-0.002(5)$ $5(2)^*$ H11 $0.343(8)$ $-0.834(6)$ $-0.199(6)$ $7(1)^*$ For Cu(amp)_2(CDo_2)_2         Cu	C5	0.7896(6)	-0.8197(5)	0.5551(5)	4.1(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	0.7275(7)	-0.8052(5)	0.3983(6)	4.5(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7	0.6340(7)	-0.6406(5)	0.2558(6)	4.9(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8	0.4979(9)	-0.7105(6)	-0.0044(6)	5.8(2)
H1       0.920(6) $-0.618(5)$ 0.82(5)       5(1)*         H2       0.964(7) $-0.837(6)$ 0.953(6)       7(1)*         H3       0.905(7) $-1.040(6)$ 0.788(6)       7(1)*         H4       0.786(6) $-1.034(5)$ 0.524(5)       4(1)*         H5       0.557(5) $-0.887(4)$ 0.351(5)       6(1)*         H7       0.596(6) $-0.624(6)$ $-0.002(5)$ 5(1)*         H8       0.385(6) $-0.624(6)$ $-0.012(7)$ 8(2)*         H10       0.305(7) $-0.624(6)$ $-0.012(7)$ 8(2)*         H11       0.543(8) $-0.893(6)$ $-0.999(6)$ 7(1)*         H12       0.350(7) $-0.843(6)$ $-0.190(6)$ 7(1)*         For Cu(amp) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub> Cu       0.000       0.000       0.200       2.58(3)         C11       0.3471(2) $0.7244(2)$ 0.0968(2)       2.58(3)         C12       0.6653(2) $0.759(5)$ $0.0224(6)$ 4.1(1)         O22       0.3116(6) $0.8985(5)$ $0.1024(6)$ 4.1(1)         O2       0.3116(6) $0.2594(7)$ $1.0283(6)$	C9	0.4169(9)	-0.8527(7)	-0.1080(6)	6.2(2)
H2 $0.964(7)$ $-0.837(6)$ $0.936(6)$ $7(1)^{\bullet}$ H3 $0.905(7)$ $-1.040(6)$ $0.788(6)$ $7(1)^{\bullet}$ H4 $0.786(6)$ $-1.034(5)$ $0.524(5)$ $4(1)^{\bullet}$ H5 $0.597(5)$ $-0.837(4)$ $0.351(5)$ $6(1)^{\bullet}$ H6 $0.839(6)$ $-0.655(5)$ $0.234(5)$ $5(1)^{\bullet}$ H8 $0.385(6)$ $-0.652(6)$ $-0.022(5)$ $5(1)^{\bullet}$ H9 $0.647(8)$ $-0.624(6)$ $-0.012(7)$ $8(2)^{\bullet}$ H11 $0.335(7)$ $-0.833(6)$ $-0.099(6)$ $7(1)^{\bullet}$ For Cu(amp) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub> Cu $0.000$ $0.000$ $2.2$ Cu $0.000$ $0.000$ $0.000$ 2.2         Cl1 $0.3471(2)$ $0.7244(2)$ $0.9968(2)$ 2.58(3)         O1 $0.1805(5)$ $0.5945(5)$ $0.0024(6)$ 4.1(1)         O2 $0.3116(6)$ $0.8985(5)$ $0.1561(5)$ 3.6(1)         O3 $0.4409(6)$ $0.7129(7)$ $-0.337(6)$ 5.9(1)         O4 $0.4409(6)$ <	H1	0.920(6)	-0.618(5)	0.862(5)	5(1)*
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н2	0.964(7)	-0.837(6)	0.953(6)	7(1)*
H4       0.786(6)       -1.034(5)       0.524(5)       4(1)*         H5       0.597(5)       -0.887(4)       0.351(5)       4(1)*         H6       0.859(6)       -0.560(5)       0.234(5)       5(1)*         H7       0.596(6)       -0.655(5)       -0.002(5)       5(1)*         H9       0.647(8)       -0.624(6)       -0.012(7)       8(2)*         H10       0.305(7)       -0.927(6)       -0.085(6)       8(2)*         H11       0.543(8)       -0.893(6)       -0.099(6)       7(1)*         H12       0.350(7)       -0.843(6)       -0.190(6)       7(1)*         H12       0.350(7)       -0.843(6)       -0.190(6)       7(1)*         For Cu(amp) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub> -       -       -       -       -         Cu       0.000       0.000       0.000       2.52(3)       -         O1       0.1805(5)       0.5945(5)       0.156(15)       3.6(1)       0.3         O2       0.3116(6)       0.8985(5)       0.156(15)       3.6(1)       0.3       -         O3       0.4509(7)       0.6795(6)       0.2593(6)       5.3(1)       0       -         O3       0.4409(6)       0.7122	H3	0.905(7)	-1.040(6)	0.788(6)	7(1)*
H5 $0.597(5)$ $-0.887(4)$ $0.351(5)$ $4(1)^*$ H6 $0.859(6)$ $-0.813(5)$ $0.351(5)$ $6(1)^*$ H7 $0.596(6)$ $-0.656(5)$ $0.02(5)$ $5(1)^*$ H8 $0.385(6)$ $-0.624(6)$ $-0.012(7)$ $8(2)^*$ H10 $0.305(7)$ $-0.927(6)$ $-0.085(6)$ $8(2)^*$ H11 $0.543(8)$ $-0.937(6)$ $-0.099(6)$ $7(1)^*$ For Cu(amp)_2(ClO4)_2 $Cu$ $0.000$ $0.000$ $2.2$ $2.58(3)$ Cl $0.33471(2)$ $0.7244(2)$ $0.9968(2)$ $2.58(3)$ Cl1 $0.3471(2)$ $0.7244(2)$ $0.9968(2)$ $2.58(3)$ Cl2 $0.3116(6)$ $0.8985(5)$ $0.1024(6)$ $4.1(1)$ O2 $0.3116(6)$ $0.8985(5)$ $0.1561(5)$ $3.6(1)$ O2 $0.3116(6)$ $0.8985(5)$ $0.1561(5)$ $3.6(1)$ O3 $0.4509(7)$ $0.6795(6)$ $0.2593(6)$ $5.3(1)$ O4 $0.4409(6)$ $0.7129(7)$ $-0.0347(6)$ $5.9(1)$ O5	H4	0.786(6)	-1.034(5)	0.524(5)	4(1)*
H6 $0.859(6)$ $-0.813(5)$ $0.361(5)$ $6(1)^*$ H7 $0.596(6)$ $-0.560(5)$ $0.234(5)$ $5(1)^*$ H8 $0.385(6)$ $-0.6624(6)$ $-0.012(7)$ $8(2)^*$ H10 $0.305(7)$ $-0.927(6)$ $-0.085(6)$ $8(2)^*$ H11 $0.543(8)$ $-0.893(6)$ $-0.099(6)$ $7(1)^*$ H12 $0.350(7)$ $-0.843(6)$ $-0.190(6)$ $7(1)^*$ For Cu(amp) <sub>2</sub> (CO <sub>4</sub> ) <sub>2</sub> $CU$ $0.000$ $0.000$ $2.2$ Cu $0.000$ $0.000$ $0.000$ $2.2$ Cl1 $0.3471(2)$ $0.7244(2)$ $0.9968(2)$ $2.58(3)$ O1 $0.1805(5)$ $0.5945(5)$ $0.0024(6)$ $4.1(1)$ O2 $0.3116(6)$ $0.8983(5)$ $0.1561(5)$ $3.6(1)$ O3 $0.4509(7)$ $0.6795(6)$ $0.2593(6)$ $5.3(1)$ O4 $0.4409(6)$ $0.7129(7)$ $-0.0347(6)$ $5.9(1)$ O5 $0.7043(6)$ $0.1031(5)$ $0.8346(6)$ $4.7(1)$ O6 $0.5649(6)$	Н5	0.597(5)	-0.887(4)	0.351(5)	4(1)*
$\begin{array}{ccccccc} H7 & 0.596(6) & -0.560(5) & 0.234(5) & 5(1)^{\bullet} \\ H8 & 0.385(6) & -0.665(5) & -0.002(5) & 5(1)^{\bullet} \\ H9 & 0.647(8) & -0.624(6) & -0.012(7) & 8(2)^{\bullet} \\ H10 & 0.305(7) & -0.927(6) & -0.085(6) & 8(2)^{\bullet} \\ H11 & 0.543(8) & -0.893(6) & -0.099(6) & 7(1)^{\bullet} \\ H12 & 0.350(7) & -0.843(6) & -0.190(6) & 7(1)^{\bullet} \\ \hline \\ For Cu(amp)_2(ClO_4)_2 \\ \hline \\ Cu & 0.000 & 0.000 & 0.000 & 0.000 & 2.2 \\ Cl1 & 0.3471(2) & 0.7244(2) & 0.0968(2) & 2.58(3) \\ Cl2 & 0.6563(2) & 0.2750(2) & 0.9044(2) & 2.52(3) \\ Ol & 0.1805(5) & 0.5945(5) & 0.0024(6) & 4.1(1) \\ O2 & 0.3116(6) & 0.8985(5) & 0.0524(6) & 5.3(1) \\ O3 & 0.4509(7) & 0.6795(6) & 0.2593(6) & 5.3(1) \\ O4 & 0.4409(6) & 0.7129(7) & -0.0347(6) & 5.9(1) \\ O5 & 0.7043(6) & 0.0131(5) & 0.8364(6) & 4.7(1) \\ O6 & 0.5649(6) & 0.2694(7) & 1.0283(6) & 5.2(1) \\ O7 & 0.8365(5) & 0.4073(6) & 0.9983(6) & 4.4(1) \\ O8 & 0.5318(6) & 0.3038(6) & 0.7502(6) & 5.0(1) \\ N1 & -0.0268(5) & 0.1061(5) & 0.2493(5) & 1.93(9) \\ N2 & 0.1970(6) & 0.2260(5) & 0.1002(5) & 2.5(1) \\ N3 & 0.0385(6) & -0.1061(6) & -0.2387(6) & 2.9(1) \\ N4 & -0.1855(5) & -0.2398(6) & -0.1001(5) & 2.7(1) \\ Cl & -0.1738(8) & 0.0547(8) & 0.2931(8) & 3.3(1) \\ C2 & -0.1854(7) & 0.1288(7) & 0.3550(7) & 2.8(1) \\ C3 & -0.0433(7) & 0.2778(7) & 0.5990(7) & 2.9(1) \\ C4 & 0.1002(7) & 0.3319(7) & 0.5550(7) & 2.8(1) \\ C5 & 0.1057(7) & 0.2413(7) & 0.3681(6) & 2.4(1) \\ C6 & 0.2655(7) & 0.3045(7) & -0.2873(7) & 3.1(1) \\ C6 & 0.2655(7) & 0.303(7) & -0.2873(7) & 3.1(1) \\ C6 & 0.1057(7) & 0.2413(7) & 0.3681(6) & 2.4(1) \\ C6 & 0.2655(7) & 0.303(7) & -0.2873(7) & 3.1(1) \\ C7 & 0.1838(7) & -0.2781(8) & -0.5868(7) & 3.7(1) \\ C1 & -0.199(7) & -0.2485(6) & -0.1701(6) & 2.7(1) \\ C1 & -0.199(7) & -0.2485(6) & -0.371(7) & 2.8(1) \\ C7 & 0.1838(7) & -0.288(7) & -0.3091(7) & 2.7(1) \\ C12 & -0.2618(7) & -0.2888(7) & -0.3091(7) & 2.7(1) \\ C12 & -0.2618(7) & -0.2888(7) & -0.3091(7) & 2.7(1) \\ C12 & -0.2618(7) & -0.2888(7) & -0.3091(7) & 2.7(1) \\ C12 & -0.2618(7) & -0.2888(7) & -0.3091(7) & 2.7(1) \\ C12 & -0.2618(7) & -0.2888(7) & -0.3091(7) & 2.7(1) \\ C12 & -$	H6	0.859(6)	-0.813(5)	0.361(5)	6(1)*
H8 $0.385(6)$ $-0.665(5)$ $-0.002(5)$ $5(1)^*$ H9 $0.647(8)$ $-0.624(6)$ $-0.012(7)$ $8(2)^*$ H10 $0.305(7)$ $-0.927(6)$ $-0.035(6)$ $8(2)^*$ H11 $0.543(8)$ $-0.893(6)$ $-0.099(6)$ $7(1)^*$ For Cu(amp) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub> Cu $0.000$ $0.000$ $0.000$ $2.2$ Cu $0.000$ $0.000$ $0.000$ $2.58(3)$ Cl2 $0.6563(2)$ $0.7244(2)$ $0.0968(2)$ $2.53(3)$ Ol1 $0.1805(5)$ $0.754(5)$ $0.1024(6)$ $4.1(1)$ O2 $0.3116(6)$ $0.8985(5)$ $0.1561(5)$ $3.6(1)$ O3 $0.4509(7)$ $0.6795(6)$ $0.2593(6)$ $5.3(1)$ O4 $0.4409(6)$ $0.7129(7)$ $-0.0347(6)$ $5.2(1)$ O5 $0.7043(6)$ $0.1031(5)$ $0.8364(6)$ $4.7(1)$ O6 $0.5494(6)$ $0.2694(7)$ $1.0283(6)$ $5.2(1)$ O7 $0.8365(5)$ $0.1061(5)$ $0.2493(5)$ $1.93(9)$ N1	Н7	0.596(6)	-0.560(5)	0.234(5)	5(1)*
H9 $0.647(8)$ $-0.624(6)$ $-0.012(7)$ $8(2)^*$ H10 $0.305(7)$ $-0.927(6)$ $-0.089(6)$ $7(1)^*$ H11 $0.543(8)$ $-0.893(6)$ $-0.099(6)$ $7(1)^*$ H12 $0.350(7)$ $-0.843(6)$ $-0.190(6)$ $7(1)^*$ For Cu(amp) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub> $Cloadelta(2)$ $2.58(3)$ $2.2$ Cu $0.000$ $0.000$ $0.000$ $2.2$ Cl1 $0.3471(2)$ $0.7244(2)$ $0.0968(2)$ $2.58(3)$ Cl2 $0.6563(2)$ $0.2750(2)$ $0.9044(2)$ $2.52(3)$ O1 $0.1805(5)$ $0.5945(5)$ $0.0024(6)$ $4.1(1)$ O2 $0.3116(6)$ $0.8985(5)$ $0.1561(5)$ $3.6(1)$ O3 $0.4509(7)$ $0.6795(6)$ $0.2593(6)$ $5.3(1)$ O4 $0.4409(6)$ $0.712(7)$ $-0.0347(6)$ $5.9(1)$ O5 $0.7043(6)$ $0.1031(5)$ $0.8364(6)$ $4.7(1)$ O6 $0.5649(6)$ $0.2594(7)$ $1.0283(6)$ $5.0(1)$ N1 $-0.0268(5)$ <t< td=""><td>H8</td><td>0.385(6)</td><td>-0.665(5)</td><td>-0.002(5)</td><td>5(1)*</td></t<>	H8	0.385(6)	-0.665(5)	-0.002(5)	5(1)*
H100.305(7) $-0.927(6)$ $-0.085(6)$ $8(2)^{\bullet}$ H110.543(8) $-0.893(6)$ $-0.099(6)$ $7(1)^{\bullet}$ For Cu(amp)_2(ClO <sub>4</sub> )22 $-0.843(6)$ $-0.190(6)$ $7(1)^{\bullet}$ For Cu(amp)_2(ClO <sub>4</sub> )2Cu0.0000.0000.0002.2Cu10.3471(2)0.7244(2)0.0968(2)2.58(3)Cu20.6563(2)0.2593(5)0.0024(6)4.1(1)O20.3116(6)0.8985(5)0.1561(5)3.6(1)O30.4509(7)0.6795(6)0.2593(6)5.3(1)O40.409(6)0.7129(7) $-0.0347(6)$ 5.9(1)O50.7043(6)0.1013(5)0.8364(6)4.7(1)O60.2694(7)1.0283(6)5.2(1)O70.8365(5)0.1061(5)0.2493(5)1.93(9)N20.1071(6)0.2694(7)1.0283(6)4.4(1)O60.338(6)0.1061(5)0.2493(5)1.93(9)N20.1071(6)0.2260(5)0.1002(5)2.5(1)N4 $-0.1738(8)$ 0.0547(8)0.2387(6)2.9(1)C40.1037(7)0.348(7)0.3287(7)3.2(1)C3 $-0.1834(7)$ 0.2778(7)0.399(7)2.9(1)C4 $-0.1836(7)$ $-0.278(7)$ $0.3077(7)$ 2.8(1)C1 $-0.1836(7)$ $-0.278(8)$ $-0.2873(7$	H9	0.647(8)	-0.624(6)	-0.012(7)	8(2) <b>*</b>
H11 $0.543(8)$ $-0.893(6)$ $-0.099(6)$ $7(1)^*$ H12 $0.350(7)$ $-0.843(6)$ $-0.190(6)$ $7(1)^*$ For Cu(amp)2(CIO <sub>4</sub> )2Cu $0.000$ $0.000$ $0.000$ $2.2$ Cu $0.0471(2)$ $0.7244(2)$ $0.9968(2)$ $2.58(3)$ Cl2 $0.6563(2)$ $0.7250(2)$ $0.9044(2)$ $2.52(3)$ O1 $0.1805(5)$ $0.5945(5)$ $0.0024(6)$ $4.1(1)$ O2 $0.3116(6)$ $0.8985(5)$ $0.1661(5)$ $3.6(1)$ O3 $0.4509(7)$ $0.6795(6)$ $0.2593(6)$ $5.3(1)$ O4 $0.4409(6)$ $0.7129(7)$ $-0.0347(6)$ $5.9(1)$ O5 $0.7043(6)$ $0.1031(5)$ $0.8364(6)$ $4.7(1)$ O6 $0.5649(6)$ $0.2694(7)$ $1.0283(6)$ $5.2(1)$ O7 $0.8365(5)$ $0.1061(5)$ $0.2493(5)$ $1.93(9)$ N2 $0.1970(6)$ $0.2260(5)$ $0.1002(5)$ $2.5(1)$ N3 $0.0385(6)$ $-0.1061(6)$ $-0.2387(6)$ $2.9(1)$ N4 $-0.1855(5)$ $-0.2398(6)$ $-0.1001(5)$ $2.7(1)$ C2 $-0.1834(7)$ $0.1288(7)$ $0.4552(7)$ $3.2(1)$ C3 $-0.0433(7)$ $0.2778(7)$ $0.5950(7)$ $2.8(1)$ C4 $0.1002(7)$ $0.3319(7)$ $0.3077(7)$ $2.8(1)$ C5 $0.1057(7)$ $0.2413(7)$ $0.3077(7)$ $2.8(1)$ C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.2781(8)$ $-0.2873(7$	H10	0.305(7)	-0.927(6)	-0.085(6)	8(2)*
H12 $0.350(7)$ $-0.843(6)$ $-0.190(6)$ $7(1)^*$ For Cu(amp) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub> Cu $0.000$ $0.000$ $0.000$ $2.2$ C11 $0.3471(2)$ $0.7244(2)$ $0.0968(2)$ $2.58(3)$ C12 $0.6563(2)$ $0.2750(2)$ $0.9044(2)$ $2.52(3)$ O1 $0.1805(5)$ $0.5945(5)$ $0.0024(6)$ $4.1(1)$ O2 $0.3116(6)$ $0.8985(5)$ $0.1561(5)$ $3.6(1)$ O3 $0.4509(7)$ $0.6795(6)$ $0.2593(6)$ $5.3(1)$ O4 $0.4409(6)$ $0.7129(7)$ $-0.0347(6)$ $5.9(1)$ O5 $0.7043(6)$ $0.1031(5)$ $0.8364(6)$ $4.7(1)$ O6 $0.5649(6)$ $0.2694(7)$ $1.0283(6)$ $5.2(1)$ O7 $0.8365(5)$ $0.4075(6)$ $0.9983(6)$ $4.4(1)$ O8 $0.5184(6)$ $0.3038(6)$ $0.7502(6)$ $5.0(1)$ N1 $-0.0268(5)$ $0.1061(5)$ $0.2493(5)$ $1.93(9)$ N2 $0.1970(6)$ $0.2260(5)$ $0.1002(5)$ $2.5(1)$	H11	0.543(8)	-0.893(6)	-0.099(6)	7(1)*
For $Cu(amp)_2(ClO_4)_2$ Cu         0.000         0.000         0.000         2.2           Cl1         0.3471(2)         0.7244(2)         0.0968(2)         2.58(3)           Cl2         0.6563(2)         0.2750(2)         0.9044(2)         2.52(3)           Ol1         0.1805(5)         0.5945(5)         0.0024(6)         4.1(1)           O2         0.3116(6)         0.8985(5)         0.1561(5)         3.6(1)           O3         0.4509(7)         0.6795(6)         0.2593(6)         5.3(1)           O4         0.4409(6)         0.7129(7)         -0.0347(6)         5.9(1)           O5         0.7043(6)         0.1031(5)         0.8364(6)         4.7(1)           O6         0.5649(6)         0.2694(7)         1.0283(6)         5.2(1)           O7         0.8365(5)         0.4075(6)         0.9983(6)         4.4(1)           O8         0.5318(6)         0.3038(6)         0.7502(6)         5.0(1)           N1         -0.0268(5)         0.1061(5)         0.2493(5)         1.93(9)           N2         0.1970(6)         0.2260(5)         0.1002(5)         2.5(1)           N3         0.0385(6)         -0.1061(6)         -0.2387(6	H12	0.350(7)	-0.843(6)	-0.190(6)	7(1)*
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	For Cu(amp)2	(ClO <sub>4</sub> ) <sub>2</sub>			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Cu	0.000	0.000	0.000	2.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11	0.3471(2)	0.7244(2)	0.0968(2)	2.58(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12	0.6563(2)	0.2750(2)	0.9044(2)	2.52(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	01	0.1805(5)	0.5945(5)	0.0024(6)	4.1(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2	0.3116(6)	0.8985(5)	0.1561(5)	3.6(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O3	0.4509(7)	0.6795(6)	0.2593(6)	5.3(1)
O5 $0.7043(6)$ $0.1031(5)$ $0.8364(6)$ $4.7(1)$ O6 $0.5649(6)$ $0.2694(7)$ $1.0283(6)$ $5.2(1)$ O7 $0.8365(5)$ $0.4075(6)$ $0.9983(6)$ $4.4(1)$ O8 $0.5318(6)$ $0.3038(6)$ $0.7502(6)$ $5.0(1)$ N1 $-0.0268(5)$ $0.1061(5)$ $0.2493(5)$ $1.93(9)$ N2 $0.1970(6)$ $0.2260(5)$ $0.1002(5)$ $2.5(1)$ N3 $0.0385(6)$ $-0.1061(6)$ $-0.2387(6)$ $2.9(1)$ N4 $-0.1855(5)$ $-0.2398(6)$ $-0.1001(5)$ $2.7(1)$ C1 $-0.1738(8)$ $0.0547(8)$ $0.2931(8)$ $3.3(1)$ C2 $-0.1854(7)$ $0.1288(7)$ $0.4552(7)$ $3.2(1)$ C3 $-0.0433(7)$ $0.2778(7)$ $0.5990(7)$ $2.9(1)$ C4 $0.1002(7)$ $0.3319(7)$ $0.3681(6)$ $2.4(1)$ C5 $0.1057(7)$ $0.2413(7)$ $0.3681(6)$ $2.4(1)$ C6 $0.2655(7)$ $0.3045(7)$ $-0.2873(7)$ $3.1(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$	04	0.4409(6)	0.7129(7)	-0.0347(6)	5.9(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O5	0.7043(6)	0.1031(5)	0.8364(6)	4.7(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O6	0.5649(6)	0.2694(7)	1.0283(6)	5.2(1)
08 $0.5318(6)$ $0.3038(6)$ $0.7502(6)$ $5.0(1)$ N1 $-0.0268(5)$ $0.1061(5)$ $0.2493(5)$ $1.93(9)$ N2 $0.1970(6)$ $0.2260(5)$ $0.1002(5)$ $2.5(1)$ N3 $0.0385(6)$ $-0.1061(6)$ $-0.2387(6)$ $2.9(1)$ N4 $-0.1855(5)$ $-0.2398(6)$ $-0.1001(5)$ $2.7(1)$ C1 $-0.1738(8)$ $0.0547(8)$ $0.2931(8)$ $3.3(1)$ C2 $-0.1854(7)$ $0.1288(7)$ $0.4552(7)$ $3.2(1)$ C3 $-0.0433(7)$ $0.2778(7)$ $0.5990(7)$ $2.9(1)$ C4 $0.1002(7)$ $0.319(7)$ $0.5550(7)$ $2.8(1)$ C5 $0.1057(7)$ $0.2413(7)$ $0.3681(6)$ $2.4(1)$ C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	07	0.8365(5)	0.4075(6)	0.9983(6)	4.4(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	08	0.5318(6)	0.3038(6)	0.7502(6)	5.0(1)
N2 $0.1970(6)$ $0.2260(5)$ $0.1002(5)$ $2.5(1)$ N3 $0.0385(6)$ $-0.1061(6)$ $-0.2387(6)$ $2.9(1)$ N4 $-0.1855(5)$ $-0.2398(6)$ $-0.1001(5)$ $2.7(1)$ C1 $-0.1738(8)$ $0.0547(8)$ $0.2931(8)$ $3.3(1)$ C2 $-0.1854(7)$ $0.1288(7)$ $0.4552(7)$ $3.2(1)$ C3 $-0.0433(7)$ $0.2778(7)$ $0.5990(7)$ $2.9(1)$ C4 $0.1002(7)$ $0.3319(7)$ $0.5550(7)$ $2.8(1)$ C5 $0.1057(7)$ $0.2413(7)$ $0.3681(6)$ $2.4(1)$ C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	N1	-0.0268(5)	0.1061(5)	0.2493(5)	1.93(9)
N3 $0.0385(6)$ $-0.1061(6)$ $-0.2387(6)$ $2.9(1)$ N4 $-0.1855(5)$ $-0.2398(6)$ $-0.1001(5)$ $2.7(1)$ C1 $-0.1738(8)$ $0.0547(8)$ $0.2931(8)$ $3.3(1)$ C2 $-0.1854(7)$ $0.1288(7)$ $0.4552(7)$ $3.2(1)$ C3 $-0.0433(7)$ $0.2778(7)$ $0.5990(7)$ $2.9(1)$ C4 $0.1002(7)$ $0.3319(7)$ $0.5550(7)$ $2.8(1)$ C5 $0.1057(7)$ $0.2413(7)$ $0.3681(6)$ $2.4(1)$ C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	N2	0.1970(6)	0.2260(5)	0.1002(5)	2.5(1)
N4 $-0.1855(5)$ $-0.2398(6)$ $-0.1001(5)$ $2.7(1)$ C1 $-0.1738(8)$ $0.0547(8)$ $0.2931(8)$ $3.3(1)$ C2 $-0.1854(7)$ $0.1288(7)$ $0.4552(7)$ $3.2(1)$ C3 $-0.0433(7)$ $0.2778(7)$ $0.5990(7)$ $2.9(1)$ C4 $0.1002(7)$ $0.3319(7)$ $0.5550(7)$ $2.8(1)$ C5 $0.1057(7)$ $0.2413(7)$ $0.3681(6)$ $2.4(1)$ C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	N3	0.0385(6)	-0.1061(6)	-0.2387(6)	2.9(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N4	-0.1855(5)	-0.2398(6)	-0.1001(5)	2.7(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1	-0.1738(8)	0.0547(8)	0.2931(8)	3.3(1)
C3 $-0.0433(7)$ $0.2778(7)$ $0.5990(7)$ $2.9(1)$ C4 $0.1002(7)$ $0.3319(7)$ $0.5550(7)$ $2.8(1)$ C5 $0.1057(7)$ $0.2413(7)$ $0.3681(6)$ $2.4(1)$ C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	C2	-0.1854(7)	0.1288(7)	0.4552(7)	3.2(1)
C4 $0.1002(7)$ $0.3319(7)$ $0.5550(7)$ $2.8(1)$ C5 $0.1057(7)$ $0.2413(7)$ $0.3681(6)$ $2.4(1)$ C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	C3	-0.0433(7)	0.2778(7)	0.5990(7)	2.9(1)
C5 $0.1057(7)$ $0.2413(7)$ $0.3681(6)$ $2.4(1)$ C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	C4	0.1002(7)	0.3319(7)	0.5550(7)	2.8(1)
C6 $0.2655(7)$ $0.3045(7)$ $0.3077(7)$ $2.8(1)$ C7 $0.1838(7)$ $-0.0547(8)$ $-0.2873(7)$ $3.1(1)$ C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	C5	0.1057(7)	0.2413(7)	0.3681(6)	2.4(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	0.2655(7)	0.3045(7)	0.3077(7)	2.8(1)
C8 $0.1906(7)$ $-0.1459(7)$ $-0.4684(6)$ $3.6(1)$ C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	C7	0.1838(7)	-0.0547(8)	-0.2873(7)	3.1(1)
C9 $0.0423(9)$ $-0.2781(8)$ $-0.5868(7)$ $3.7(1)$ C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	C8	0.1906(7)	-0.1459(7)	-0.4684(6)	3.6(1)
C10 $-0.1094(7)$ $-0.3303(7)$ $-0.5371(7)$ $2.8(1)$ C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	C9	0.0423(9)	-0.2781(8)	-0.5868(7)	3.7(1)
C11 $-0.1080(7)$ $-0.2485(6)$ $-0.3710(6)$ $2.0(1)$ C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ $2.7(1)$	C10	-0.1094(7)	-0.3303(7)	-0.5371(7)	2.8(1)
C12 $-0.2618(7)$ $-0.2898(7)$ $-0.3091(7)$ 2.7(1)	C11	-0.1080(7)	-0.2485(6)	-0.3/10(6)	2.0(1)
	C12	-0.2618(7)	-0.2898(7)	-0.3091(7)	2./(1)

Atom	x	у	<i>z</i>	$B(\mathbb{A}^2)^{\mathbf{a}}$
H1	-0.254(9)	0.007(9)	0.203(9)	7*
H2	-0.28(1)	0.086(9)	0.480(9)	7*
Н3	-0.050(9)	0.322(9)	0.713(9)	7*
H4	0.183(9)	0.404(9)	0.615(9)	7*
Н5	0.3807	0.2709	0.3621	7*
Н6	0.3022	0.4395	0.3448	7*
H7	0.2960	0.2051	0.0587	7*
H8	0.1365	0.3123	0.0465	7*
Н9	0.2674	0.0642	-0.2049	7*
H10	0.2943	-0.1273	-0.5016	7*
H11	0.0450	-0.3510	-0.7025	7*
H12	-0.2019	-0.4225	-0.6226	7*
H13	-0.3117	-0.4126	-0.3683	7*
H14	-0.3579	0.2249	-0.3505	7*
H15	-0.1279	-0.3254	-0.0627	7*
H16	-0.2894	-0.2236	-0.0556	7*

<sup>a</sup> Starred atoms were refined isotropically; anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as:  $(4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab\cos(\gamma)B(1,2) + ac\cos(\beta)B(1,3) + bc\cos(\alpha)B(2,3)]$ .

TABLE II. Bond Distances<sup>a</sup> (Å)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
For [Cu(C	C9H12N2O)Cl2	]2						
Cu	Cl1	2.283(1)	N2	C7	1.252(6)	C6	н5	0.98(4)
Cu	Cl1	2.862(1)	C1	C2	1.354(7)	C6	Н6	1.09(4)
Cu	C12	2.253(1)	C1	H1	0.96(5)	C7	Н7	0.90(5)
Cu	N1	2.036(3)	C2	C3	1.366(7)	C8	C9	1.466(8)
Cu	N2	1.991(3)	C2	H2	1.02(5)	C8	Н8	1.02(4)
01	C7	1.326(5)	C3	C4	1.379(7)	C8	Н9	1.14(6)
01	C8	1.473(6)	C3	Н3	0.95(5)	C9	H10	0.96(6)
N1	C1	1.358(6)	C4	C5	1.382(6)	C9	H11	1.06(5)
N1	C5	1.329(5)	C4	H4	0.94(4)	C9	H12	0.84(6)
N2	C6	1.449(5)	C5	C6	1.485(6)			
For Cu(an	np)2(ClO4)2							
Cu	02	2.632(8)	C12	O5	1.454(9)	C1	C2	1.294(14)
Cu	O5	2.564(9)	C12	06	1.388(7)	C2	C3	1.435(15)
Cu	N1	2.010(7)	C12	07	1,468(8)	C3	C4	1.321(13)
Cu	N2	1.999(7)	C12	08	1.386(7)	C4	C5	1.474(12)
Cu	N3	1.977(8)	N1	C1	1.337(12)	C5	C6	1.537(11)
Cu	N4	2.035(8)	N1	C5	1.288(13)	C7	C8	1,439(13)
Cl1	01	1.387(7)	N2	C6	1.478(11)	C8	C9	1.33(2)
C11	02	1.418(8)	N3	C7	1.350(11)	C9	C10	1.401(14)
Cl1	O3	1.449(8)	N3	C11	1.395(12)	C10	C11	1.293(13)
C11	O4	1.435(8)	N4	C12	1.491(11)	C11	C12	1.454(12)

<sup>a</sup> Numbers in parentheses are estimated standard deviations in the least significant digits.

of C11 to the Cu atom of an adjacent monomeric unit (Cu  $\rightarrow$  Cl1, 2.862(1) Å). The coordination sphere about the metal atom is distorted square pyramid (4 + 1) resulting from the formation of two single chlorine atom bridges between metal atoms forming a dimer related by an inversion center. The Cu-Cu distance is 3.683(1) Å. The distortion of the coordination plane is primarily due to constraints imposed by the bidentate ligand resulting in the formation of a five membered ring at the copper atom. Although

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	For [Cu(C9	H <sub>12</sub> N <sub>2</sub> 0)Cl <sub>2</sub> ] <sub>2</sub>										
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CII	Си	CII	89.30(3)	CI	C2	H2	120.0(3)	01	C7	N2	123.4(4)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CII	Cu	CI2	92.43(4)	C	C2	H2	121.0(3)	01	C1	H7	112.0(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CI1	Cu	IN	172.45(9)	3	C3	C4	118.4(5)	N2	C1	H7	124.0(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CII	Cu	N2	92.8(1)	C2	C	H3	112.0(3)	01	<b>C8</b>	60	106.7(4)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CII	Cu	CI2	99.36(4)	C4	C	H3	129.0(3)	01	ŝ	H8	110.0(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CII	Cu	NI	93.73(9)	C3	C4	S	119.6(4)	01	C8	6H	98.0(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CI1	Cu	N2	88.6(1)	C3	C4	H4	121.0(3)	60	C8	H8	111.0(2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CI2	Cu	NI	93.9(1)	CS	C4	H4	119.0(3)	60	C8	6H	117.0(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	CI2	Cu	N2	170.6(1)	NI	S	C4	121.9(4)	H8	C8	6H	113.0(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	NI	ũ	N2	80.4(1)	NI	S	C6	117.1(4)	C8	60	H10	112.0(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C7	01	C8	117.9(4)	C4	S	C6	121.0(4)	C8	ව	H11	105.0(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C1	IN	S	117.6(4)	N2	C6	cs	110.3(3)	C8	ల	H12	112.0(4)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	N2	C7	115.4(4)	N2	ce Ce	H5	110.0(2)	H10	ల	H11	109.0(4)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	NI	CI	C2	123.0(4)	N2	C6	H6	111.0(2)	H10	ల	H12	97.0(5)
C2       C1       H1       122.0(3)       C5       H6       102.0(2)         Por Cu(amp) <sub>2</sub> (ClO <sub>4</sub> )       C3       119.5(5)       H5       C6       H6       114.0(3)         Por Cu(amp) <sub>2</sub> (ClO <sub>4</sub> )       C1       C3       117.0(4)       O1       C11       O2         O2       C4       N1       92.2(3)       O1       C11       O2       114.0(3)         O2       C4       N1       92.2(3)       O1       C11       O2       111.8(5)       C1       C2       C3         O2       C4       N1       92.2(3)       O1       C11       O3       106.0(6)       C3       C4       C4         O2       C4       N1       92.2(3)       O3       C11       O3       106.0(6)       C3       C4       C3       C4       C3       C4	NI	C1	HI	115.0(3)	cs	C6	HS	108.0(2)	H11	ల	H12	121.0(5)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C2	CI	HI	122.0(3)	cs	C6	H6	102.0(2)				
For Cu(amp) <sub>2</sub> (Clo <sub>4</sub> )         For Cu(amp) <sub>2</sub> (Clo <sub>4</sub> )           02         Cu         05         177.0(4)         01         Cl1         02         Cl         02         Cl         02         Cl         03         177.0(4)         01         Cl1         02         111.8(5)         Cl         Cl         02         Cl         03         105.7(5)         Cl         Cl         Cl         Cl         03         105.7(5)         Cl	CI	C	C	119.5(5)	HS	C6	H6	114.0(3)				
For Cu(amp) <sub>2</sub> (ClO <sub>4</sub> )         For Cu(amp) <sub>2</sub> (ClO <sub>4</sub> )           02         Cu         03         177.0(4)         01         Cl1         02         Cl         03         177.0(4)         01         Cl1         03         105.7(5)         Cl         Cl </td <td></td>												
02       Cu       03       177.0(4)       01       Cu       03       177.0(4)       01       Cu       03       105.7(5)       C2       C3       C3       C1       03       105.7(5)       C2       C3       C3       C1       C3       C4       C4       C3       C4       C4       C3       C4       C4       C3       C4       C4       C3	For Cu(am)	p)2(ClO4)2										
02         Cu         NI         92.2(3)         01         Cl         N1         92.2(3)         01         Cl         N2         77.7(3)         01         Cl         N1         92.2(3)         01         Cl         N3         85.1(3)         01         Cl         03         105.7(5)         C2         C3         C4         C5         C4         C5         C4         C5         C4         C5         C4 <thc4< th=""> <thc4< th=""> <thc4< th=""></thc4<></thc4<></thc4<>	02	Cu	05	177.0(4)	01	CII	02	111.8(5)	CI	C2	C	121.9(8)
02       Cu       N2       77.7(3)       01       Cl       04       106.0(6)       C3       C4       C5         02       Cu       N3       85.1(3)       02       Cl       03       109.9(5)       N1       C5       C4       C5         02       Cu       N4       98.4(3)       02       Cl       03       109.9(6)       N1       C5       C4	02	Cu	IN	92.2(3)	01	CII	03	105.7(5)	C2	C3	C4	119.4(9)
02       Cu       N3       85.1(3)       02       Cl       03       109.9(5)       N1       C5       C4         02       Cu       N4       98.4(3)       02       Cl       03       109.9(6)       N1       C5       C6         03       Cu       N1       90.2(3)       03       Cl1       04       113.5(6)       C4       C5       C6         05       Cu       N3       92.5(3)       03       Cl1       04       113.5(6)       C4       C5       C6         05       Cu       N3       92.5(3)       03       Cl1       04       113.5(6)       C4       C5       C6         05       Cu       N3       92.5(3)       05       C12       06       109.7(6)       N3       C7       C8       C6         05       Cu       N3       92.5(3)       05       C12       06       107.6(6)       C7       C6       C5       C6       C	02	Cu	N2	77.7(3)	01	CII	04	106.0(6)	C	C4	CS	120.1(8)
02         Cu         N4         98.4(3)         02         Cl         N1         90.2(3)         02         Cl         N1         90.2(3)         03         Cl         N1         C         C         N1         C         C         N1         C         C         N1         C         C         C         N1         C         C         C         N1         C <thc< th=""> <thc< th=""> <thc< th=""></thc<></thc<></thc<>	02	Cu	N3	85.1(3)	02	CII	03	109.9(5)	NI	CS	C4	120.0(8)
05         Cu         N1         90.2(3)         0.3         Cl1         04         113.5(6)         C4         C5         C6           05         Cu         N2         100.8(3)         05         Cl2         06         109.7(6)         N2         C6         C5         C6         C5         C6         C7         C8         C6         C6         C6         C7         C8         C10         C10         C10	02	Cu	N4	98.4(3)	02	CII	<b>0</b> 4	109.9(6)	NI	S	C6	118.0(9)
05         Cu         N2         100.8(3)         05         Cl2         06         109.7(6)         N2         C6         C5           05         Cu         N3         92.5(3)         05         Cl2         06         109.7(6)         N2         C6         C5           05         Cu         N4         83.0(3)         05         Cl2         07         106.0(5)         N3         C7         C8           05         Cu         N1         Cu         N2         81.6(3)         05         Cl2         08         107.6(6)         C7         C8         C9         C1         N3         C7         C8         C1         N3         C1         N1         N3         C1         N3         C1         N3         C1         N1         N3         C1         N1         <	05	Cn	IN	90.2(3)	03	CII	<b>0</b>	113.5(6)	C4	S	C6	121.9(8)
05         Cu         N3         92.5(3)         05         Cl2         07         106.0(5)         N3         C7         C8           05         Cu         N4         83.0(3)         05         Cl2         08         107.6(6)         C7         C8         C9           N1         Cu         N2         81.6(3)         06         Cl2         08         107.6(6)         C7         C8         C9           N1         Cu         N3         177.2(5)         06         Cl2         08         108.3(6)         C9         C10           N1         Cu         N4         99.8(3)         07         Cl2         08         113.7(5)         N3         C11         C10           N1         Cu         N3         97.4(3)         C1         N1         C5         119.5(8)         N3         C11         C10           N2         Cu         N4         175.9(4)         C7         N3         C11         C12           N3         Cu         N3         C11         113.7(5)         N3         C11         C12           N3         Cu         N4         175.9(4)         C7         N3         C11         C12	05	Cu	N2	100.8(3)	05	CI2	90	109.7(6)	N2	C6	S	107.1(7)
05         Cu         N4         83.0(3)         05         Cl2         08         107.6(6)         C7         C8         C9           NI         Cu         N2         81.6(3)         06         Cl2         07         111.4(6)         C8         C9         C10           NI         Cu         N3         177.2(5)         06         Cl2         07         111.4(6)         C8         C9         C10           NI         Cu         N3         177.2(5)         06         Cl2         08         108.3(6)         C9         C10         C11           N1         Cu         N3         97.4(3)         07         Cl2         08         113.7(5)         N3         C11         C10           N2         Cu         N3         97.4(3)         C1         N1         C5         119.5(8)         N3         C11         C12           N3         Cu         N4         175.9(4)         C7         N3         C11         C12           N3         Cu         N4         175.9(4)         C7         N3         C11         C12           N3         Cu         N4         N1         C1         C12         C3	05	Cu	N3	92.5(3)	05	CI2	07	106.0(5)	N3	C7	C8	121.0(1)
NI         Cu         N2         81.6(3)         06         Cl2         07         111.4(6)         C8         C9         C10           NI         Cu         N3         177.2(5)         06         Cl2         08         108.3(6)         C9         C10         C11           NI         Cu         N3         177.2(5)         06         Cl2         08         108.3(6)         C9         C10         C11           NI         Cu         N4         99.8(3)         07         Cl2         08         113.7(5)         N3         C11         C10           N2         Cu         N3         97.4(3)         C1         N1         C5         119.5(8)         N3         C11         C12           N2         Cu         N4         175.9(4)         C7         N3         C11         118.0(9)         C10         C11         C12           N3         Cu         N4         N1         C1         C12         C13         C12         C13         C12         C12         C12         C12         C12         C12         C13         C12         C13         C13         C11         C12         C13         C12         C13         C12<	05	Cu	N4	83.0(3)	05	CI2	08	107.6(6)	C1	C8	60	116.3(8)
NI         Cu         N3         177.2(5)         06         Cl2         08         108.3(6)         C9         C10         C11           NI         Cu         N4         99.8(3)         07         Cl2         08         113.7(5)         N3         C11         C10         C11           N2         Cu         N3         97.4(3)         C1         N1         C5         119.5(8)         N3         C11         C12         C12           N2         Cu         N4         175.9(4)         C7         N3         C11         C12         C12         N3         C11         C12         C12         C12         C12         C13         C12         C12         C12         C13         C12         C13         C12         C12         C12         C13         C12         C12 </td <td>NI</td> <td>ũ</td> <td>N2</td> <td>81.6(3)</td> <td>90</td> <td>CI2</td> <td>07</td> <td>111.4(6)</td> <td>C8</td> <td>60</td> <td>C10</td> <td>122.4(9)</td>	NI	ũ	N2	81.6(3)	90	CI2	07	111.4(6)	C8	60	C10	122.4(9)
NI         Cu         N4         99.8(3)         07         Cl2         08         113.7(5)         N3         Cl1         Cl0           N2         Cu         N3         97.4(3)         C1         N1         C5         119.5(8)         N3         C11         C12         C12           N2         Cu         N4         175.9(4)         C7         N3         C11         C12         C12 <td>NI</td> <td>ũ</td> <td>N3</td> <td>177.2(5)</td> <td>90</td> <td>CI2</td> <td>08</td> <td>108.3(6)</td> <td>ల</td> <td>C10</td> <td>C11</td> <td>119.5(9)</td>	NI	ũ	N3	177.2(5)	90	CI2	08	108.3(6)	ల	C10	C11	119.5(9)
N2 Cu N3 97.4(3) C1 N1 C5 119.5(8) N3 C11 C12 N2 Cu N4 175.9(4) C7 N3 C11 118.0(9) C10 C11 C12 N3 Cu N4 81.0(3) N1 C1 C7 173.0(9) NA C13 C11	NI	Cu	N4	99.8(3)	07	CI2	08	113.7(5)	N3	C11	C10	122.4(9)
N2 Cu N4 175.9(4) C7 N3 C11 118.0(9) C10 C11 C12 N3 Cu N4 81.0(3) N1 C1 C3 123.0(9) N4 C13 C11	N2	Cn	N3	97.4(3)	CI	NI	CS	119.5(8)	N3	C11	C12	114.2(8)
N <sup>2</sup> C <sub>1</sub> , N <sup>4</sup> 81 0(3) N1 C1 C2 123 0(0) N4 C13 C11	N2	Cu	<b>N4</b>	175.9(4)	C7	N3	C11	118.0(9)	C10	C11	C12	123.4(8)
	N3	ũ	N4	81.0(3)	NI	C1	C2	123.0(9)	N4	C12	C11	109.2(7)
		In parvitutives ut		mann avriativita u	ו נווע ועמוני ועמאו אווון ו	calle ulgues.						

Cu(II) Complexes Prepared from 2-Aminomethylpyridine

TABLE III. Bond Angles<sup>a</sup> (°)

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the ligand has three possible coordination sites, only two (N1 and N2) are actually coordinated to the copper atoms.

 $Cu(amp)_2(ClO_4)_2$  has a pseudo inversion center at the copper position. However, the copper atom sits slightly above (0.505 Å) the coordination plane (N1, N2, N3 and N4).

The coordination sphere about the copper atom is a distorted octahedron with two perchlorate groups weakly coordinated axially to the copper atom through O2 and O5, 2.632(8) and 2.564(9) respectively. Additional distortion results from the formation of two five membered rings upon coordination of the copper atom to N1 and N2, and N3 and N4. There appear to be no significant intermolecular interactions.

The magnetic susceptibility data for the complexes are plotted in Figs. 3 and 4. The data for the



Fig. 3. The inverse magnetic susceptibility of  $Cu(amp)_2$ -(ClO<sub>4</sub>)<sub>2</sub> plotted as a function of temperature. The line drawn through the points is the best fit of the data to the Curie– Weiss law as described in the text.



Fig. 4. The magnetic susceptibility of  $(CuLCl_2)_2$  plotted as a function of temperature. The curve drawn through the points is the best fit of the data to the dimer equation as described in the text.

monomeric complex  $Cu(amp)_2(ClO_4)_2$  is shown in Fig. 3 as the inverse magnetic susceptibility plotted as a function of temperature. The data show a straight line dependence that is consistent with the simple Curie—Weiss law.

$$\chi = \frac{Ng^2 \mu_{\rm B}^2 S(S+1)}{3k(T-\theta)}$$

where all the parameters have their usual meaning and S = 1/2 for copper(II). The magnetic data were fitted to this equation with the parameters listed in Table IV.

TABLE IV. Magnetic Parameters for the Complexes Cu-(amp)<sub>2</sub>(ClO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O and (CuLCl<sub>2</sub>)<sub>2</sub> as Described in Text

	Cu(amp)(ClO <sub>4</sub> ) <sub>2</sub> ·2H <sub>2</sub> O	[CuLCl] <sub>2</sub>
g	2.11	2.09
ө 2J	0.16 K	$-3.50 \text{ cm}^{-1}$

Magnetic susceptibility data for the dimeric complex  $[CuLCl_2]_2$  are plotted in Fig. 4 as a function of temperature over the 2-300 K temperature range. The data exhibit a maximum in the magnetic susceptibility at about 3 K. This behavior is consistent with an antiferromagnetic interaction between the two copper(II) ions.

The equation that describes the behavior of the magnetic susceptibility of the spin-coupled copper(II) dimer may be written as follows:

$$\chi = \frac{2Ng^2\mu_{\rm B}^2}{kT} \frac{e^x}{1+3e^2}$$

where X = 2J/kT and 2J is the splitting between the singlet and the triplet with a negative J having a ground singlet. The magnetic data for the binuclear complex were fit to this equation but with a correction for a temperature independent paramagnetism of  $120 \times 10^{-6}$  emu/(mol Cu) for the two copper(II) ions and a small amount of paramagnetic (monomeric) impurity. The best fitted values are listed in Table IV.

# Discussion

The preparation of the dimeric complex  $[CuLCl_2]_2$ was somewhat surprising because the sequence of reactions was not expected. The solvent triethylorthoformate  $[HC(OCH_2CH_3)_3]$  is an excellent drying agent that may be used in reactions in which water must be removed. In the presence of water, the triethylorthoformate follows eqn. (1).



The ethylformate ester will then react with 2-aminomethylpyridine following eqn. (2).



The ligand L has a *trans* configuration about the immine bond and coordinates as a bidentate ligand to the copper(II) ion through the two nitrogen atoms. The  $CuLCl_2$  units then dimerize through the bridging chlorines.

The study of magneto-structural relationships in exchanged coupled systems continues to be an area of active research by many laboratories [5-10], much of this research concerns copper(II) magnetic interaction. Many theories have been proposed to describe and predict the magnetic behavior of exchange coupled systems [11-20].

The bridging center geometry between 4, 5 and 6 coordinate doubly bridged metal ions is often divided into two categories. These categories are illustrated by parallel plane bridging (I) in which the bridging ligands are equatorially bound to both metal ions and perpendicular plane (II) bridging in which the bridging ligands are axially bound to one metal ion and equatorial bound to the other. The binuclear complex [CuLCl<sub>2</sub>]<sub>2</sub> has bridging of the perpendicular plane type (II). Initial successes predicting magnetic properties from structural parameters were realized from an empirical correlation of the magnetostructural parameters of hydroxide bridged complexes of type I by Hatfield and Hodgson [21] and verified by several other laboratories. Many chlorine bridged binuclear and polymeric complexes have been synthesized [22-28] but attempts to correlate the magneto-structural properties have met with only limited success. The situation for chlorine bridge complexes is much more complicated due to the low lying d-orbitals that are involved in the magnetic exchange overlap pathways.

# Supplementary Material

Molar magnetic susceptibility data corrected for diamagnetism with Pascal constants are available from the authors on request.

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