Crystal structure of *N*-(2-(aminoethyl)pyridyl)(salicylaldiminato)-copper(II) perchlorate dimer, $[Cu(C_{14}H_{13}N_2O)]_2(ClO_4)_2$

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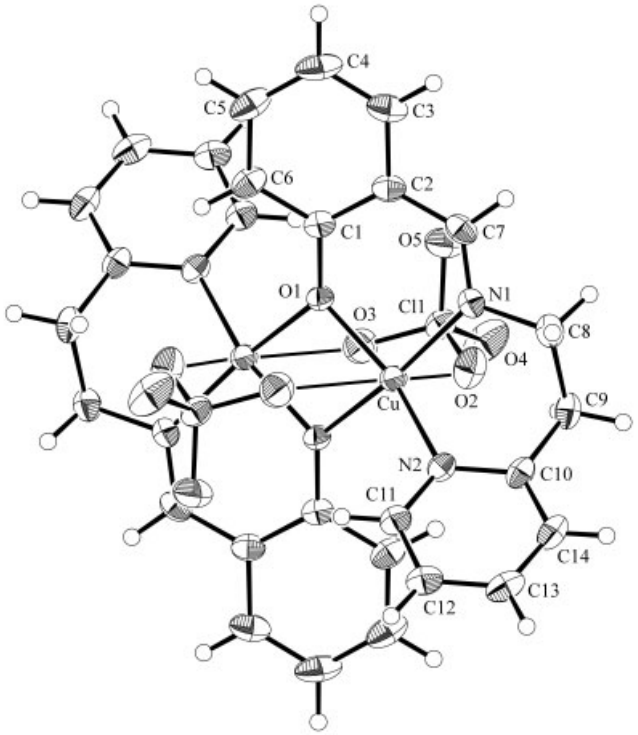

Abstract

$C_{14}H_{13}ClCuN_2O_5$, monoclinic, $P12_1/n1$ (No. 14), $a = 9.559(2)$ Å, $b = 11.024(2)$ Å, $c = 14.397(4)$ Å, $\beta = 104.75(2)°$, $V = 1467.1$ Å^3, $Z = 4$, $R_{gt}(F) = 0.034$, $wR_{ref}(F^2) = 0.089$, $T = 293$ K.

Source of material

The complex was prepared as in [1].

Discussion

The ligand in this compound was used as a 'capping' group in attempts to make thiocyanate-bridged Cu(II)-Fe(III) heterometallic complexes, by substitution of the available position on the Cu(II) tridentate Schiff base complex [1]. However, as one of the products, the copper complex dimerized, in a characteristic fashion, utilizing the phenoxo oxygen atom as bridging group. The O1 atoms bridge to two CuN_2O_2 chromophores, related by a centre of inversion, forming symmetric *d*(Cu—O1) and *d*(Cu—O1') of 1.938(2) Å and 1.968(2) Å, respectively; *d*(Cu—N1) = 1.955(2) Å and *d*(Cu—N2) = 1.984(2) Å. The O2 and O3 atoms of two perchlorate ions form weak Cu—O bonds in the axial positions so that *d*(Cu—O2) = 2.668(2) Å and *d*(Cu—O3) = 2.868(3) Å. The coordination geometry is therefore axially-distorted octahedral. The Cu–O1–Cu' angle is 102.40(8)° and the Cu···Cu' distance is 3.0444(9) Å. Fitting of the variable temperature magnetic susceptibility data yielded an exchange coupling constant, *J*, of –19 cm^{-1} ($g = 2.02$), which is low for such phenoxo-bridged Cu(II) systems [2].

Table 1. Data collection and handling.

Crystal:	green block, size 0.16 × 0.24 × 0.24 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	16.98 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC6R, $\omega/2\theta$
$2\theta_{max}$:	55.2°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3767, 3384
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2354
$N(param)_{refined}$:	209
Programs:	teXsan [3], SHELXS-86 [4], SHELXL-97 [5], DIFABS [6], PLATON [7], ORTEPII [8]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(3)	4*e*	0.1066	0.0404	0.6560	0.045
H(4)	4*e*	0.2557	–0.0278	0.5654	0.045
H(5)	4*e*	0.3288	0.1027	0.4633	0.045
H(6)	4*e*	0.2369	0.2970	0.4380	0.045
H(7)	4*e*	–0.0266	0.1917	0.7085	0.045
H(8a)	4*e*	–0.0225	0.3870	0.8262	0.057
H(8b)	4*e*	–0.1571	0.3093	0.7743	0.057
H(9a)	4*e*	–0.2607	0.4899	0.6919	0.057
H(9b)	4*e*	–0.2487	0.4919	0.8026	0.057
H(11)	4*e*	0.1097	0.7317	0.6611	0.045
H(12)	4*e*	0.1259	0.8738	0.7796	0.045
H(13)	4*e*	–0.0099	0.8471	0.8920	0.045
H(14)	4*e*	–0.1546	0.6774	0.8810	0.045

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	4*e*	–0.02157(4)	0.49651(3)	0.60114(2)	0.0374(2)	0.0300(2)	0.0309(2)	0.0032(2)	0.0103(1)	0.0006(1)
Cl(1)	4*e*	–0.34248(8)	0.37857(6)	0.42885(5)	0.0290(4)	0.0440(4)	0.0433(3)	0.0049(3)	0.0058(3)	–0.0039(3)
O(1)	4*e*	0.0436(2)	0.3952(2)	0.5104(1)	0.031(1)	0.0288(9)	0.0338(9)	0.0052(7)	0.0086(8)	0.0022(7)
O(2)	4*e*	–0.2972(2)	0.4420(2)	0.5188(2)	0.046(1)	0.080(2)	0.045(1)	–0.010(1)	0.012(1)	–0.016(1)
O(3)	4*e*	–0.2776(3)	0.4363(2)	0.3603(2)	0.064(2)	0.057(1)	0.045(1)	0.012(1)	0.018(1)	0.009(1)
O(4)	4*e*	–0.4957(2)	0.3838(3)	0.3945(2)	0.025(1)	0.102(2)	0.095(2)	0.008(1)	0.001(1)	–0.032(2)
O(5)	4*e*	–0.2947(3)	0.2559(2)	0.4412(2)	0.075(2)	0.039(1)	0.114(2)	0.010(1)	0.041(2)	0.011(1)
N(1)	4*e*	–0.0345(2)	0.3603(2)	0.6855(2)	0.031(1)	0.037(1)	0.033(1)	–0.002(1)	0.0064(9)	0.0041(9)
N(2)	4*e*	–0.0264(2)	0.6210(2)	0.6998(2)	0.031(1)	0.038(1)	0.033(1)	0.003(1)	0.0067(9)	–0.0032(9)
C(1)	4*e*	0.1069(3)	0.2859(2)	0.5301(2)	0.026(1)	0.033(1)	0.034(1)	0.001(1)	–0.003(1)	–0.005(1)
C(2)	4*e*	0.0760(3)	0.2113(2)	0.6013(2)	0.037(2)	0.034(1)	0.039(1)	0.004(1)	–0.000(1)	0.000(1)
C(3)	4*e*	0.1318(4)	0.0923(3)	0.6120(2)	0.066(2)	0.034(2)	0.052(2)	0.007(2)	0.002(2)	0.006(1)
C(4)	4*e*	0.2221(4)	0.0517(3)	0.5590(3)	0.074(3)	0.040(2)	0.061(2)	0.027(2)	–0.001(2)	–0.003(2)
C(5)	4*e*	0.2626(4)	0.1290(3)	0.4963(2)	0.053(2)	0.062(2)	0.043(2)	0.027(2)	0.002(2)	–0.010(2)
C(6)	4*e*	0.2075(3)	0.2457(3)	0.4807(2)	0.036(2)	0.050(2)	0.038(1)	0.013(1)	0.001(1)	–0.004(1)
C(7)	4*e*	0.0000(3)	0.2515(3)	0.6707(2)	0.036(2)	0.036(1)	0.038(1)	–0.002(1)	0.001(1)	0.010(1)
C(8)	4*e*	–0.0992(3)	0.3794(3)	0.7677(2)	0.039(2)	0.049(2)	0.038(1)	0.000(1)	0.011(1)	0.007(1)
C(9)	4*e*	–0.1931(3)	0.4919(3)	0.7548(2)	0.030(2)	0.060(2)	0.038(1)	–0.001(2)	0.012(1)	0.002(1)
C(10)	4*e*	–0.1062(3)	0.6050(3)	0.7644(2)	0.025(1)	0.049(2)	0.032(1)	0.010(1)	0.004(1)	–0.000(1)
C(11)	4*e*	0.0566(3)	0.7205(3)	0.7063(2)	0.033(2)	0.041(2)	0.041(2)	0.003(1)	0.005(1)	–0.003(1)
C(12)	4*e*	0.0665(3)	0.8064(3)	0.7767(2)	0.039(2)	0.041(2)	0.049(2)	0.005(1)	0.001(1)	–0.006(1)
C(13)	4*e*	–0.0141(4)	0.7904(3)	0.8435(2)	0.050(2)	0.052(2)	0.041(2)	0.016(2)	0.003(1)	–0.011(1)
C(14)	4*e*	–0.1001(3)	0.6894(3)	0.8367(2)	0.039(2)	0.060(2)	0.038(2)	0.015(2)	0.012(1)	–0.003(1)

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