Crystal structure of diaqua-di(2-methoxyacetato)copper(II), $C_6H_{14}CuO_8$

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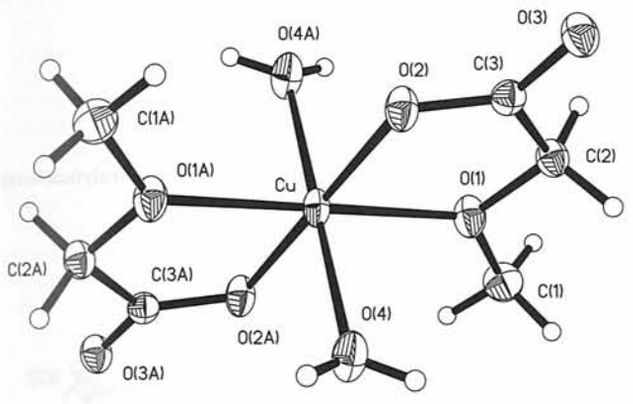
Received March 17, 2003, accepted in revised form and available on-line July 30, 2003; CCDC-No. 1267/1064



Abstract

$C_6H_{14}CuO_8$, monoclinic, $P12_1/n1$ (No. 14), $a = 6.955(1)$ Å, $b = 10.123(2)$ Å, $c = 7.226(1)$ Å, $\beta = 96.57(1)°$, $V = 505.4$ Å^3, $Z = 2$, $R_{gt}(F) = 0.026$, $wR_{ref}(F^2) = 0.069$, $T = 292$ K.

Source of material

Reagents and solvents used were of commercially available quality. A solution of 2-methoxyacetic acid (maaH, 2 mmol, 180 mg) in methanol (10 mL) was added to a stirred solution of $CuCl_2 \cdot 2H_2O$ (1 mmol, 171 mg) in water (10 mL). The resulting solution was filtered and washed with water and methanol after staying still in air for about 4 days. Large purple rod-like crystals of $Cu(maa)_2(H_2O)_2$ were obtained almost quantitatively (yield 96%). Elemental analysis: found – C, 26.12%; H, 5.12%; calc. for $C_6H_{14}O_8Cu$ – C, 25.95%; H, 5.08%.

Experimental details

The two H atoms attached to the coordination water molecules were located from difference Fourier maps and refined isotropically, mainly because these hydrogen atoms were able to rotate around the O4–Cu1 axis.

Discussion

The new Cu(II) complex with 2-methoxyacetate is a rarely-seen isologue of the Co(II) complex [1].

The complex is also a discrete electronically neutral one. One copper(II) atom, two acetate ligand anions and two coordination water molecules constitute each simplest structure unit. The Cu atom is six-coordinated by six oxygen atoms, two of which come from the two coordinated water molecules and the rest four from the two acetate ligands, forming a slightly distorted octahedron. Each methoxyacetate anion in the complex is bidentate with one ether oxygen atom and one oxygen from the carboxylate. All the carboxylates are unidentate groups. All oxygen atoms from the carboxylates and the water molecules contribute to the formation of the hydrogen bonds. Every structural unit is joined by strong H-bonds to four neighboring structure units. The strong hydrogen bonds join the monomer units along z-axis to form a 1D chain. In each 1D chain, the large planes in which the metal atoms are located are parallel each other at a short distance of 3.454(1) Å. Two different chains are alternatively arranged at the angle of 65.51(2)° for the title Cu(II) complex (comparable to that of 66.6° for the isologue Co(II) complex). The hydrogen bonds link the chains to form a plane, and then join the planes into a 3D structure.

Table 1. Data collection and handling.

Crystal:	purple rod-like, size 0.40 × 0.50 × 0.56 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	21.83 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	51.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1200, 997
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 853
$N(param)_{refined}$:	80
Programs:	SHELXTL [2], SHELXTL-plus [3]

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

Atom	Site	x	y	z	U_{iso}
H(1A)	4*e*	0.2601	–0.0397	0.5072	0.053
H(1B)	4*e*	0.1255	0.0772	0.4314	0.053
H(1C)	4*e*	0.3490	0.0848	0.4198	0.053
H(2A)	4*e*	0.3871	–0.1868	0.2608	0.039
H(2B)	4*e*	0.4897	–0.0548	0.2128	0.039
H(0A)	4*e*	0.114(5)	0.211(3)	–0.172(3)	0.07(1)
H(0B)	4*e*	0.255(2)	0.194(3)	–0.036(4)	0.050(9)

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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	2*a*	0	0	0	0.0218(3)	0.0400(3)	0.0226(3)	0.0038(2)	–0.0008(2)	0.0004(2)
O(1)	4*e*	0.2124(3)	–0.0336(2)	0.2351(2)	0.033(1)	0.055(1)	0.0269(9)	0.0085(8)	0.0000(8)	–0.0071(8)
O(2)	4*e*	0.1854(2)	–0.1063(2)	–0.1134(2)	0.0284(8)	0.052(1)	0.0266(9)	0.0049(8)	–0.0001(7)	–0.0028(8)
O(3)	4*e*	0.4721(2)	–0.2037(2)	–0.0837(2)	0.0328(9)	0.046(1)	0.0336(9)	0.0077(8)	0.0044(7)	–0.0026(8)
O(4)	4*e*	0.1415(3)	0.1777(2)	–0.0696(3)	0.033(1)	0.060(1)	0.040(1)	–0.004(1)	–0.0039(9)	0.010(1)
C(1)	4*e*	0.2389(5)	0.0270(3)	0.4126(4)	0.051(2)	0.049(2)	0.034(2)	0.004(1)	0.006(1)	–0.008(1)
C(2)	4*e*	0.3724(3)	–0.1067(3)	0.1869(3)	0.032(1)	0.038(1)	0.028(1)	0.004(1)	0.001(1)	0.001(1)
C(3)	4*e*	0.3413(3)	–0.1417(2)	–0.0188(3)	0.028(1)	0.028(1)	0.030(1)	–0.003(1)	0.004(1)	0.003(1)

Acknowledgments. The authors thank the Education Office of Hubei Province, P. R. China, for the research grant No. 2002B29002 and the Natural Science Foundation of Hubei Province, P. R. China, for the research grant No. 2003ABB010.

References

1. Zhu, H.-L.; Liu, X.; Zhu, X.-L.; Wang, D.-Q.: Crystal structure of diaqua-di(2-methoxyacetato)cobalt(II), $C_6H_{14}CoO_8$. Z. Kristallogr. NCS **218** (2003) 313-314.
2. Sheldrick, G. M.: Siemens SHELXTL (Version 5.0). Siemens Industrial Automation, Inc., Analytical Instrumentation, USA 1995.
3. Sheldrick, G. M.: SHELXTL-plus. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison Wisconsin, USA 1991.