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Crystal structure of monoaquabis(imidazole)-bis(4-methoxybenzoato)-copper(II), $Cu(H_2O)(C_8H_7O_3)_2(C_3N_2H_4)_2$

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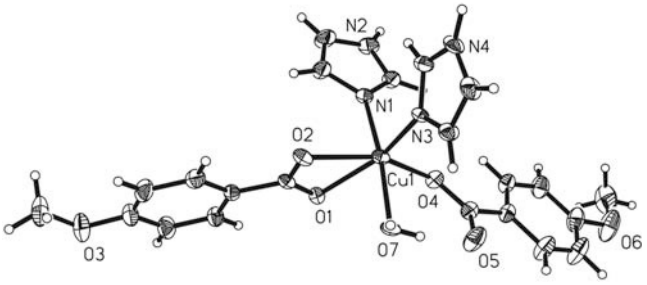

Abstract

$C_{22}H_{24}CuN_4O_7$, monoclinic, *C*12/*c*1 (no. 15), $a = 24.731(3)$ Å, $b = 7.8377(9)$ Å, $c = 24.844(3)$ Å, $\beta = 93.742(5)°$, $V = 4805.4$ Å^3, $Z = 8$, $R_{gf}(F) = 0.049$, $wR_{ref}(F^2) = 0.154$, $T = 293$ K.

Source of material

Copper(II) dichloride (171 mg, 1 mmol), imidazole (136 mg, 2 mmol), 4-methoxybenzoic acid (304 mg, 2 mmol) were dissolved in methanol (15 mL). The clear green solution gradually got celeste. It was kept still in air for one week. Large block-shaped crystals were precipitated. They were filtered and washed with ethanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 78 %). All reagents and solvents were used as obtained without further purification.

Experimental details

The hydrogen atoms attached to C atoms were placed in geometrically idealised positions and constrained to ride on their parent atoms with *d*(C—H) distance of 0.93 - 0.96 Å, and $U_{iso}(H) = 1.2\ U_{eq}(C)$ and $1.5\ U_{eq}(C)$. The hydrogen atoms of water molecule were found in the difference Fourier map and refined freely.

Discussion

Copper is an important life-required element. Due to their biological relevant important behaviors, many copper complexes with Schiff base have been reported in recent years [1-5]. In addition, metal complexes with carboxylates are among the most investigated compounds in the field of coordination chemistry [6-9].

The title crystal structure consists of mononuclear copper(II) complexe. Copper(II) atom is in a distorted octahedral environment and is six-coordinated by two N atoms from two imidazole molecules, and four O atoms, one of which from a coordinating water molecule and the other three from two 4-methoxybenzoate ligands. One of two 4-methoxybenzoate behaves as a *O*,*O'*-bidentate ligand and the other is the monodentate one. N3, O1, O2 and O4 atoms constitute the basal plane of the octahedron with the average deviation of 0.034 Å. The N1 and O7 atoms occupy the two axial positions. All the molecules participate in intermolecular hydrogen bonds (N2–H2A···O1, N4–H4A···O7, N4–H4A···O1, O7–H7C···O2, O7–H7D···O5), which join the constituents into a 3D structure.

Table 1. Data collection and handling.

Crystal:	blue block, size 0.13 × 0.26 × 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	9.58 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	53°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	13754, 4958
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4070
$N(param)_{refined}$:	317
Program:	SHELXTL [10]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2A)	8*f*	0.2032	0.3392	0.2424	0.063
H(4A)	8*f*	0.4343	0.7344	0.2070	0.063
H(3)	8*f*	0.3544	–0.3573	0.3323	0.059
H(4)	8*f*	0.3619	–0.5145	0.4104	0.079
H(6)	8*f*	0.4683	–0.1747	0.4745	0.080
H(7A)	8*f*	0.4599	–0.0151	0.3969	0.063
H(8A)	8*f*	0.4825	–0.3631	0.5320	0.185
H(8B)	8*f*	0.4534	–0.4981	0.5666	0.185
H(8C)	8*f*	0.4285	–0.3152	0.5583	0.185
H(11)	8*f*	0.2644	0.0711	0.0882	0.062
H(12)	8*f*	0.2067	0.0469	0.0114	0.078
H(14)	8*f*	0.3329	–0.1051	–0.0703	0.110
H(15)	8*f*	0.3884	–0.0835	0.0065	0.090
H(16A)	8*f*	0.1625	–0.1011	–0.0656	0.163
H(16B)	8*f*	0.1638	–0.0208	–0.1232	0.163
H(16C)	8*f*	0.1718	0.0955	–0.0720	0.163
H(17)	8*f*	0.2718	0.2553	0.1841	0.055
H(18)	8*f*	0.3346	0.2277	0.3312	0.064
H(19)	8*f*	0.2414	0.3289	0.3353	0.076
H(20)	8*f*	0.3766	0.5108	0.2351	0.054
H(21)	8*f*	0.4971	0.2963	0.1676	0.057
H(22)	8*f*	0.5109	0.6043	0.1642	0.069
H(7C)	8*f*	0.4897(8)	0.028(4)	0.202(1)	0.045(9)
H(7D)	8*f*	0.453(1)	–0.028(5)	0.1617(5)	0.05(1)

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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(1)	8*f*	0.39132(1)	0.11494(4)	0.22012(2)	0.0261(2)	0.0309(2)	0.0495(3)	0.0013(1)	0.0020(2)	0.0003(1)
N(1)	8*f*	0.32084(9)	0.2197(3)	0.2493(1)	0.023(1)	0.040(1)	0.044(1)	0.0067(9)	0.0014(9)	–0.000(1)
N(2)	8*f*	0.2372(1)	0.3080(4)	0.2532(1)	0.030(1)	0.059(2)	0.069(2)	0.014(1)	0.005(1)	–0.005(2)
N(3)	8*f*	0.4268(1)	0.3453(3)	0.2044(1)	0.036(1)	0.021(1)	0.043(1)	–0.0002(9)	0.000(1)	0.0009(9)
N(4)	8*f*	0.4399(1)	0.6220(3)	0.2024(1)	0.076(2)	0.024(1)	0.056(2)	–0.005(1)	–0.014(2)	0.000(1)
O(1)	8*f*	0.37216(7)	–0.1245(2)	0.26547(8)	0.0254(9)	0.041(1)	0.039(1)	–0.0024(7)	0.0013(8)	0.0044(8)
O(2)	8*f*	0.42726(8)	0.0674(3)	0.30130(9)	0.0260(9)	0.033(1)	0.059(1)	–0.0006(8)	–0.0027(9)	0.0057(9)
O(3)	8*f*	0.4179(2)	–0.4622(5)	0.4951(1)	0.144(4)	0.110(3)	0.053(2)	0.011(3)	0.002(2)	0.034(2)
O(4)	8*f*	0.35057(8)	0.0495(3)	0.14912(8)	0.032(1)	0.051(1)	0.042(1)	–0.0032(9)	0.0005(9)	–0.006(1)
O(5)	8*f*	0.4190(1)	–0.0187(5)	0.0994(1)	0.040(1)	0.127(3)	0.055(2)	0.009(2)	0.009(1)	–0.014(2)
O(6)	8*f*	0.2351(2)	–0.0421(7)	–0.0855(1)	0.108(3)	0.186(4)	0.042(2)	–0.027(3)	–0.015(2)	–0.016(2)
O(7)	8*f*	0.46081(8)	–0.0243(2)	0.19476(9)	0.0234(9)	0.027(1)	0.059(1)	0.0012(7)	0.0050(9)	–0.0012(9)
C(1)	8*f*	0.4016(1)	–0.0703(4)	0.3050(1)	0.018(1)	0.034(1)	0.047(2)	0.006(1)	0.004(1)	0.005(1)
C(2)	8*f*	0.4058(1)	–0.1700(4)	0.3560(1)	0.029(1)	0.041(2)	0.039(2)	0.005(1)	0.003(1)	0.002(1)
C(3)	8*f*	0.3772(1)	–0.3198(5)	0.3611(1)	0.054(2)	0.050(2)	0.044(2)	–0.006(2)	0.002(1)	0.006(2)
C(4)	8*f*	0.3817(2)	–0.4145(6)	0.4075(2)	0.083(3)	0.061(2)	0.054(2)	–0.008(2)	0.008(2)	0.014(2)
C(5)	8*f*	0.4162(2)	–0.3587(6)	0.4501(2)	0.085(3)	0.079(3)	0.044(2)	0.020(2)	0.003(2)	0.017(2)
C(6)	8*f*	0.4451(2)	–0.2109(6)	0.4458(2)	0.064(2)	0.091(3)	0.043(2)	0.012(2)	–0.013(2)	–0.006(2)
C(7)	8*f*	0.4403(2)	–0.1157(5)	0.3994(2)	0.047(2)	0.058(2)	0.051(2)	0.003(2)	–0.004(2)	–0.008(2)
C(8)	8*f*	0.4480(3)	–0.405(1)	0.5417(2)	0.161(6)	0.161(7)	0.046(3)	0.049(5)	–0.010(3)	0.023(3)
C(9)	8*f*	0.3702(1)	0.0087(4)	0.1050(1)	0.043(2)	0.044(2)	0.045(2)	–0.006(1)	0.007(1)	–0.002(1)
C(10)	8*f*	0.3320(1)	–0.0045(5)	0.0560(1)	0.052(2)	0.051(2)	0.039(2)	–0.010(2)	0.008(1)	–0.003(1)
C(11)	8*f*	0.2782(1)	0.0347(5)	0.0562(1)	0.051(2)	0.066(2)	0.038(2)	–0.002(2)	0.003(1)	–0.004(2)
C(12)	8*f*	0.2434(2)	0.0221(6)	0.0100(2)	0.057(2)	0.087(3)	0.049(2)	–0.005(2)	–0.004(2)	0.002(2)
C(13)	8*f*	0.2641(2)	–0.0278(7)	–0.0377(2)	0.081(3)	0.093(3)	0.040(2)	–0.019(2)	–0.009(2)	–0.003(2)
C(14)	8*f*	0.3188(2)	–0.0690(9)	–0.0384(2)	0.089(3)	0.142(5)	0.045(2)	–0.013(3)	0.015(2)	–0.024(3)
C(15)	8*f*	0.3519(2)	–0.0566(7)	0.0075(2)	0.059(2)	0.115(4)	0.051(2)	–0.003(2)	0.012(2)	–0.017(2)
C(16)	8*f*	0.1788(3)	–0.0150(9)	–0.0867(2)	0.120(5)	0.129(5)	0.069(3)	–0.021(4)	–0.045(3)	0.006(3)
C(17)	8*f*	0.2761(1)	0.2598(4)	0.2215(1)	0.033(1)	0.056(2)	0.049(2)	0.009(1)	–0.001(1)	–0.003(2)
C(18)	8*f*	0.3102(1)	0.2455(5)	0.3017(1)	0.042(2)	0.073(2)	0.046(2)	0.023(2)	0.002(1)	–0.005(2)
C(19)	8*f*	0.2586(2)	0.3011(6)	0.3043(2)	0.050(2)	0.079(3)	0.063(2)	0.019(2)	0.020(2)	–0.009(2)
C(20)	8*f*	0.4082(1)	0.4948(4)	0.2174(1)	0.050(2)	0.033(2)	0.052(2)	0.006(1)	–0.002(1)	–0.003(1)
C(21)	8*f*	0.4741(2)	0.3784(4)	0.1805(2)	0.053(2)	0.033(2)	0.057(2)	–0.005(1)	0.012(2)	0.001(1)
C(22)	8*f*	0.4821(2)	0.5483(5)	0.1787(2)	0.067(2)	0.040(2)	0.064(2)	–0.021(2)	0.003(2)	0.010(2)

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