Crystal structure of monoqua-(2,2'-bipyridyl-*N,N'*)-(adipato-*O*)-copper(II) dihydrate, [Cu(H₂O)(C₁₀H₈N₂)(C₆H₈O₄)] · 2H₂O

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Abstract

C₁₆H₂₂CuN₂O₇, triclinic, *P* $\bar{1}$ (no. 2), *a* = 6.993(2) Å, *b* = 10.902(3) Å, *c* = 12.396(3) Å, α = 82.289(4)°, β = 80.859(4)°, γ = 72.673(4)°, *V* = 886.9 Å³, *Z* = 2, *R*_{gt}(*F*) = 0.055, *wR*_{ref}(*F*²) = 0.159, *T* = 293 K.

Source of material

A mixture of adipic acid (0.157 g, 1.1 mmol), Cu(NO₃)₂·3H₂O (0.276 g, 1.1 mmol), 2,2'-bipyridine (0.166 g, 1.1 mmol) was added into a mixture of 10 ml water and 10 ml methanol. The mixture was adjusted to pH = 8.0 by addition of 1 M NaOH solution, then stirred for 2 hours at 295 K. The resulting solution was filtered, the filtrate was evaporated slowly at room temperature. Blue crystals of the title compound were obtained after one week.

Discussion

The crystal structure of the title compound consists of one Cu²⁺ cation, two 2,2'-bipyridine molecules, one adipate anion, one coordinating water molecule and two water molecules of crystallization. The Cu(II) atom is five-coordinated in a distorted square pyramidal coordination, formed by two N atoms from 2,2'-bipyridine molecule, two O atoms from carboxylate groups offered by two different adipic acid ligands and one O atom of coordinating water molecule at the apical position. The bipyridine ligands chelating metal atoms exhibit nearly perfect coplanarity. The lengths of the Cu—O bonds are 1.946 Å and 1.974 Å, respectively. The lengths of Cu—N bonds (2.007 Å and 2.019 Å) are slightly different. This behavior is similar to the reported complex

structure built of Cu(II) and 2,2'-bipyridine (1.994 Å and 2.000 Å) [1]. The [Cu(C₁₀H₈N₂)(H₂O)]²⁺ units are bridged by bimonodentate adipic acid ligands to generate zigzag chains along [010]. The adjacent chains are linked to layers parallel (100) by π - π interactions between the neighboring bipyridine ligands, which the distance is 3.390 Å suggests significant inter-chain π - π stacking interactions [2,3]. The strong interlayer hydrogen bond O5—H5B...O2 with *d*(O...O) = 2.647 Å and the weak O6—H6A...O1 and O7—H7B...O3 hydrogen bonds play an important role in assembling the layers into 3D open framework.

Table 1. Data collection and handling.

Crystal:	blue column, size 0.11 × 0.112 × 0.395 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	12.73 cm ⁻¹
Diffraction, scan mode:	Bruker SMART CCD, φ/ω
2 θ _{max} :	55.14°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	5011, 4090
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 2218
<i>N</i> (<i>param</i>) _{refined} :	235
Programs:	SHELXS-97 [4], SHELXL-97 [5], SHELXTL [6]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	2i	0.8198	0.5760	0.5484	0.067
H(2)	2i	0.8660	0.5723	0.3615	0.075
H(3)	2i	0.8506	0.7628	0.2496	0.072
H(4)	2i	0.8017	0.9514	0.3289	0.065
H(7)	2i	0.7358	1.1267	0.4199	0.062
H(8)	2i	0.6659	1.2963	0.5257	0.074
H(9)	2i	0.6399	1.2547	0.7167	0.077
H(10)	2i	0.6730	1.0449	0.7933	0.064
H(12A)	2i	0.6048	0.4178	0.8334	0.073
H(12B)	2i	0.8020	0.3392	0.8840	0.073
H(13A)	2i	0.5459	0.3676	1.0251	0.078
H(13B)	2i	0.6828	0.4518	1.0420	0.078
H(15A)	2i	0.3262	0.9998	0.9693	0.058
H(15B)	2i	0.3120	0.8631	1.0205	0.058
H(16A)	2i	0.0182	0.8926	0.9423	0.062
H(16B)	2i	0.0346	1.0269	0.8848	0.062
H(5A)	2i	1.0929	0.7805	0.7685	0.073
H(5B)	2i	1.0130	0.6683	0.7918	0.073
H(6B)	2i	0.6808	1.4033	0.3219	0.156
H(6A)	2i	0.4834	1.4365	0.3218	0.156
H(7B)	2i	0.7429	0.7277	0.0043	0.113
H(7A)	2i	0.8069	0.6387	0.0851	0.113

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(1)	2i	0.8168(7)	0.6523(5)	0.5040(4)	0.053(3)	0.051(3)	0.055(3)	0.000(2)	−0.006(2)	−0.008(3)
C(2)	2i	0.8432(8)	0.6495(5)	0.3921(4)	0.060(3)	0.065(4)	0.054(3)	0.003(3)	−0.003(3)	−0.026(3)
C(3)	2i	0.8354(7)	0.7627(6)	0.3255(4)	0.050(3)	0.083(4)	0.038(3)	−0.002(3)	−0.002(2)	−0.014(3)
C(4)	2i	0.8052(7)	0.8746(6)	0.3726(4)	0.042(3)	0.070(3)	0.039(3)	−0.003(2)	0.001(2)	−0.004(3)
C(5)	2i	0.7795(6)	0.8725(5)	0.4868(3)	0.030(2)	0.056(3)	0.035(2)	−0.005(2)	−0.004(2)	0.000(2)
C(6)	2i	0.7424(6)	0.9861(5)	0.5458(4)	0.030(2)	0.051(3)	0.044(3)	−0.006(2)	−0.004(2)	−0.003(2)
C(7)	2i	0.7219(7)	1.1118(5)	0.4960(4)	0.043(3)	0.058(3)	0.048(3)	−0.010(2)	−0.006(2)	0.011(3)
C(8)	2i	0.6817(8)	1.2126(5)	0.5585(5)	0.057(3)	0.050(3)	0.080(4)	−0.016(3)	−0.020(3)	0.003(3)
C(9)	2i	0.6648(8)	1.1882(5)	0.6721(5)	0.067(3)	0.052(3)	0.075(4)	−0.014(3)	−0.018(3)	−0.012(3)
C(10)	2i	0.6861(7)	1.0615(5)	0.7173(4)	0.056(3)	0.056(3)	0.050(3)	−0.018(3)	−0.005(2)	−0.010(3)
C(11)	2i	0.7987(8)	0.5266(5)	0.8332(4)	0.056(3)	0.042(3)	0.046(3)	−0.006(2)	0.010(2)	−0.009(2)
C(12)	2i	0.6994(8)	0.4217(5)	0.8813(4)	0.068(3)	0.051(3)	0.058(3)	−0.018(3)	0.011(3)	−0.005(3)
C(13)	2i	0.5884(9)	0.4437(5)	0.9957(5)	0.074(4)	0.045(3)	0.067(4)	−0.016(3)	0.015(3)	−0.005(3)
C(14)	2i	0.4161(6)	0.8668(4)	0.8579(4)	0.032(2)	0.038(2)	0.039(3)	−0.004(2)	−0.001(2)	0.003(2)
C(15)	2i	0.2861(6)	0.9254(5)	0.9571(4)	0.036(2)	0.049(3)	0.053(3)	−0.003(2)	0.001(2)	−0.010(2)
C(16)	2i	0.0613(6)	0.9675(5)	0.9498(4)	0.035(2)	0.057(3)	0.054(3)	−0.002(2)	0.004(2)	−0.015(2)
Cu(1)	2i	0.73673(8)	0.77939(5)	0.71374(4)	0.0380(3)	0.0442(4)	0.0392(4)	−0.0025(2)	0.0000(2)	−0.0029(3)
N(1)	2i	0.7242(5)	0.9637(4)	0.6566(3)	0.032(2)	0.051(2)	0.038(2)	−0.005(2)	−0.002(2)	−0.005(2)
N(2)	2i	0.7866(5)	0.7615(4)	0.5519(3)	0.037(2)	0.048(2)	0.042(2)	0.001(2)	0.001(2)	−0.007(2)
O(1)	2i	0.7184(5)	0.6040(3)	0.7533(3)	0.053(2)	0.049(2)	0.051(2)	−0.011(2)	0.000(2)	−0.004(2)
O(2)	2i	0.9445(6)	0.5350(4)	0.8705(3)	0.074(3)	0.073(3)	0.071(3)	−0.027(2)	−0.025(2)	0.021(2)
O(3)	2i	0.6079(4)	0.8322(3)	0.8603(2)	0.037(2)	0.045(2)	0.044(2)	−0.004(1)	−0.002(1)	−0.003(1)
O(4)	2i	0.3420(4)	0.8526(3)	0.7772(2)	0.039(2)	0.055(2)	0.044(2)	−0.005(2)	−0.001(1)	−0.007(2)
O(5)	2i	1.0688(5)	0.7206(3)	0.7462(3)	0.044(2)	0.061(2)	0.078(3)	−0.018(2)	−0.014(2)	0.008(2)
O(6)	2i	0.5681(8)	1.4557(6)	0.3553(5)	0.106(4)	0.143(5)	0.146(5)	−0.039(4)	−0.014(4)	−0.027(4)
O(7)	2i	0.7761(8)	0.7255(4)	0.0706(3)	0.141(4)	0.069(3)	0.067(3)	−0.008(3)	−0.040(3)	−0.009(2)

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