Crystal structure of aqua(2-(2pyridyl)benzimidazole)(methanedisulfonato)copper(II),$Cu(H_2O)(C_{12}H_8N_3)[CH_2(SO_3)_2]$

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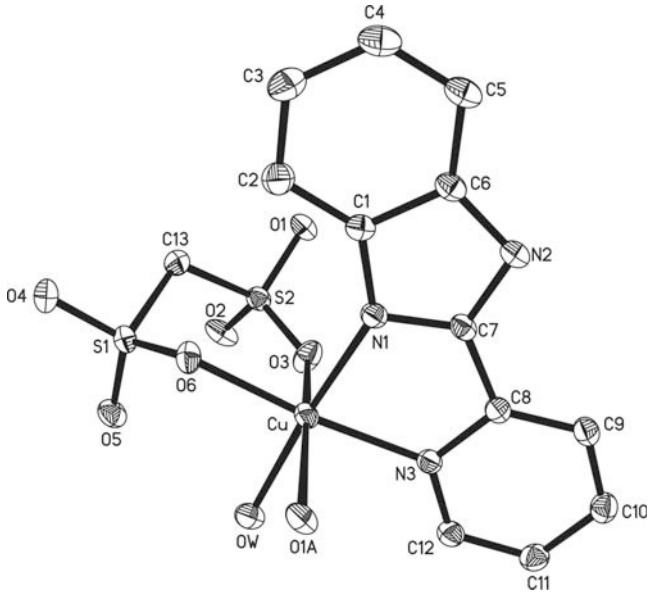

Abstract

$C_{13}H_{12}CuN_3O_7S_2$, triclinic, $P\bar{1}$ (no. 2), a = 6.9522(4) Å, b = 11.2534(6) Å, c = 11.4833(7) Å, α = 109.022(5)°, β = 99.214(5)°, γ = 101.017(5)°, V = 809.4 Å^3, Z = 2, $R_{gt}(F)$ = 0.030, $wR_{ref}(F^2)$ = 0.068, T = 293 K.

Source of material

Chemicals were purchased from commercial sources and used without further purification. A mixture containing methanedisulfonic acid (0.176 g, 1 mmol), $CuCO_3$ (0.125 g, 1 mmol), 2-(2-pyridyl)benzimidazole (0.195 g, 1 mmol) and methanol (5 mL) was sealed in a Teflon-lined reactor (15 mL), which was heated at 140 °C for 3 days, and then cooled to room temperature at 10 °C/h. Blue crystals of the title compound were collected in a 46 % yield.

Experimental details

The hydrogen atoms attached to carbons were generated geometrically with d(C—H) = 0.93 - 0.97 Å, and U_{iso}(H) = 1.2 U_{eq}(C), while the hydrogen atoms of water molecules were located from difference Fourier maps and refined with d(O—H) = 0.843 - 0.848 Å, and U_{iso}(H) = 1.5 U_{eq}(O).

Discussion

The structure of the title compound contains one Cu(II) ion, one methanedisulfonate anion, one 2-(2-pyridyl)benzimidazole lingand and one coordinating water molecule. The Cu(II) is six coordinated by three O atoms from two methanedisulfonate anion [d(Cu—O3) = 2.380 Å, d(Cu—O6) = 1.969 Å, d(Cu—O1A) = 2.527 Å], two N atoms from one 2-(2-pyridyl)benzimidazole lingand [d(Cu—N1) = 1.982 Å, d(Cu—N3) = 2.007 Å] and one O atom from water molecule with d(Cu—OW) = 1.995 Å, exhibiting a octahedral coordination geometry. One of the sulfonate groups is in a bidentate coordination mode and bridges the adjacent Cu(II) to form a chain, while the other sulfonate group displays a monodentate coordination mode.

Table 1. Data collection and handling.

Crystal:	blue block, size 0.11 × 0.14 × 0.16 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	16.52 cm^{-1}
Diffractometer, scan mode:	Oxford Diffraction Gemini R Ultra, ω
$2\theta_{max}$:	58.56°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5630, 3639
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2708
$N(param)_{refined}$:	242
Programs:	SHELXS-97, SHELXL-97 [1]

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

Atom	Site	x	y	z	U_{iso}
H(10)	2*i*	0.1875	–0.3003	–0.3719	0.042
H(13A)	2*i*	–0.1646	–0.1625	0.4195	0.042
H(13B)	2*i*	–0.0550	–0.0619	0.3690	0.042
H(5)	2*i*	0.2758	0.3556	0.1426	0.045
H(11)	2*i*	0.1833	–0.4719	–0.3015	0.041
H(9)	2*i*	0.2245	–0.0928	–0.2242	0.036
H(4)	2*i*	0.3168	0.4517	0.3583	0.053
H(12)	2*i*	0.2129	–0.4366	–0.0918	0.037
H(3)	2*i*	0.3514	0.3350	0.4895	0.052
H(2)	2*i*	0.3403	0.1157	0.4075	0.044
H(1B)	2*i*	0.378(2)	–0.386(3)	0.160(3)	0.056
H(1A)	2*i*	0.204(3)	–0.384(3)	0.211(2)	0.056

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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*i*	0.26586(4)	–0.19871(3)	0.15540(3)	0.0305(2)	0.0256(2)	0.0291(2)	0.0096(1)	0.0093(1)	0.0154(1)
S(2)	2*i*	–0.22990(8)	–0.24862(6)	0.20413(6)	0.0257(3)	0.0312(3)	0.0327(4)	0.0109(3)	0.0093(3)	0.0157(3)
S(1)	2*i*	0.15090(9)	–0.18638(6)	0.40846(6)	0.0345(3)	0.0315(3)	0.0269(4)	0.0109(3)	0.0077(3)	0.0160(3)
O(1)	2*i*	–0.3595(2)	–0.1694(2)	0.1739(2)	0.0313(9)	0.0341(9)	0.043(1)	0.0122(8)	0.0080(8)	0.0221(9)
O(5)	2*i*	0.1146(2)	–0.3261(2)	0.3702(2)	0.0397(9)	0.0327(9)	0.044(1)	0.0119(8)	0.0140(9)	0.0228(9)
O(2)	2*i*	–0.3438(2)	–0.3677(2)	0.2093(2)	0.0333(9)	0.035(1)	0.067(2)	0.0128(8)	0.0123(9)	0.030(1)
O(6)	2*i*	0.2861(2)	–0.1347(2)	0.3394(2)	0.0363(9)	0.0314(9)	0.026(1)	0.0031(7)	0.0051(8)	0.0133(8)
O(3)	2*i*	–0.0906(2)	–0.2684(2)	0.1227(2)	0.0257(9)	0.059(1)	0.030(1)	0.0090(8)	0.0083(8)	0.0100(9)
OW	2*i*	0.2594(2)	–0.3780(2)	0.1516(2)	0.0307(9)	0.0317(9)	0.044(1)	0.0120(8)	0.0160(8)	0.0199(9)
O(4)	2*i*	0.2150(3)	–0.1135(2)	0.5420(2)	0.054(1)	0.048(1)	0.026(1)	0.0170(9)	0.0066(9)	0.0162(9)
C(10)	2*i*	0.2000(4)	–0.2866(2)	–0.2863(3)	0.034(1)	0.041(2)	0.029(2)	0.010(1)	0.007(1)	0.014(1)
N(2)	2*i*	0.2570(3)	0.0908(2)	0.0229(2)	0.029(1)	0.025(1)	0.035(1)	0.0084(8)	0.0063(9)	0.014(1)
C(13)	2*i*	–0.0830(4)	–0.1525(2)	0.3606(3)	0.040(1)	0.041(1)	0.029(2)	0.020(1)	0.012(1)	0.013(1)
C(5)	2*i*	0.2868(4)	0.3078(2)	0.1947(3)	0.037(1)	0.027(1)	0.052(2)	0.009(1)	0.010(1)	0.018(1)
C(6)	2*i*	0.2778(3)	0.1755(2)	0.1456(3)	0.022(1)	0.028(1)	0.039(2)	0.008(1)	0.008(1)	0.016(1)
N(3)	2*i*	0.2356(3)	–0.2486(2)	–0.0323(2)	0.025(1)	0.026(1)	0.028(1)	0.0091(8)	0.0074(9)	0.0119(9)
C(7)	2*i*	0.2597(3)	–0.0261(2)	0.0313(2)	0.022(1)	0.026(1)	0.033(2)	0.0072(9)	0.010(1)	0.017(1)
C(11)	2*i*	0.1973(4)	–0.3885(2)	–0.2442(3)	0.039(1)	0.029(1)	0.034(2)	0.009(1)	0.010(1)	0.008(1)
N(1)	2*i*	0.2799(3)	–0.0240(2)	0.1476(2)	0.026(1)	0.025(1)	0.029(1)	0.0083(8)	0.0082(9)	0.0118(9)
C(9)	2*i*	0.2215(3)	–0.1636(2)	–0.1989(3)	0.029(1)	0.033(1)	0.033(2)	0.009(1)	0.008(1)	0.018(1)
C(4)	2*i*	0.3125(4)	0.3639(3)	0.3228(3)	0.044(2)	0.027(1)	0.058(2)	0.008(1)	0.012(2)	0.011(1)
C(1)	2*i*	0.2937(3)	0.1029(2)	0.2244(2)	0.024(1)	0.024(1)	0.033(2)	0.006(1)	0.009(1)	0.010(1)
C(8)	2*i*	0.2383(3)	–0.1486(2)	–0.0744(2)	0.021(1)	0.029(1)	0.030(2)	0.007(1)	0.009(1)	0.014(1)
C(12)	2*i*	0.2151(3)	–0.3669(2)	–0.1186(3)	0.034(1)	0.027(1)	0.035(2)	0.010(1)	0.011(1)	0.014(1)
C(3)	2*i*	0.3326(4)	0.2930(3)	0.4026(3)	0.048(2)	0.036(1)	0.040(2)	0.009(1)	0.013(1)	0.005(1)
C(2)	2*i*	0.3250(4)	0.1623(2)	0.3544(3)	0.039(1)	0.036(1)	0.038(2)	0.010(1)	0.012(1)	0.015(1)

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References

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