Crystal structure of aqua(2,2′-bipyridine-κ^2N,N')-bis((2,4-dichlorophenoxyacetato-κO)copper(II), $Cu(H_2O)(C_{10}H_8N_2)(C_8H_5Cl_2O_3)_2$

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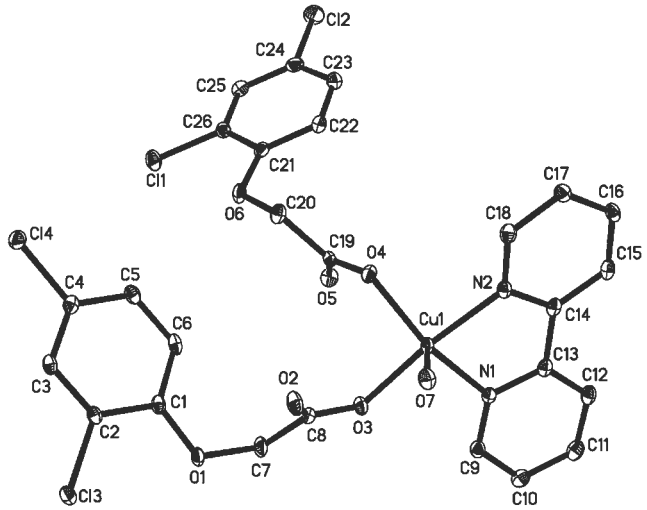

Abstract

$C_{26}H_{20}Cl_4CuN_2O_7$, monoclinic, *C*12/*c*1 (no. 15), a = 39.686(8) Å, b = 7.154(1) Å, c = 19.578(4) Å, β = 102.46(3)°, V = 5427.8 Å^3, Z = 8, $R_{gt}(F)$ = 0.039, $wR_{ref}(F^2)$ = 0.094, T = 113 K.

Source of material

A mixture of basic copper(II) carbonate (0.19 mmol, 0.043 g), 2,4-dichlorophenoxy acetic acid (0.58 mmol, 0.129 g) and 2,2′-bipyridine (0.13 mmol, 0.021g) were dissolved in 15 ml of ethanol (95 %). The pH value of the resultant mixture was adjusted to about 4.8 by adding one drop of triethylamine solution and the reaction was kept under water-bath condition at 343 K for 20 h. Afterwards the mixture was filtrated, and the filtrate was cooled to room temperature slowly. Blue block-shaped single crystals of the title compound suitable for X-ray diffraction analysis were obtained after one week.

Experimental details

Hydrogen atoms bound to carbon atoms were positioned geometrically with d(C—H) = 0.93 Å and refined as riding, with U_{iso}(H) = 1.2 U_{eq}(C). The hydrogen atom H7B of water was located from difference Fourier map and refined freely.

Discussion

It is well known that 2,2′-bipyridine is an excellent N electron donor and carboxylic acid shows versatile coordination modes with metal ions. 2,2′-Bipyridine and carboxylic acid coordinated with most transition metals to give a series of complexes possessing novel structures and properties [1-3]. Nevertheless, copper(II) complex with 2,2′-bipyridine and 2,4-dichlorophenoxyacetic acid as ligands has not been studied.

In the crystal structure of the title compound the central copper(II) ion is coordinated by two nitrogen atoms from 2,2′-bipyridine, two oxygen atoms from two 2,4-dichlorophenoxyacetates and one water to give a trigonal bipyramide, where N1, O7 and O4 locate at the equatorial positions while O3 and N2 occupy the axial positions. In addition, strong hydrogen bonds exist between uncoordinated carboxylic oxygen atom of 2,4-dichlorophenoxyacetate and neighbouring proton of water (O7–H7A···O2, 2.805(2) Å, 135°; O7–H7B···O5, 2.865(2) Å, 158°).

Table 1. Data collection and handling.

Crystal:	blue block, size 0.12 × 0.18 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	12.48 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn CCD, φ/ω
$2\theta_{max}$:	50.04°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	19154, 4765
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4259
$N(param)_{refined}$:	367
Programs:	SHELXS-97 [4], SHELXL-97 [5], SHELXTL [6]

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

Atom	Site	x	y	z	U_{iso}
H(7A)	8*f*	0.0861	0.3516	0.1726	0.034
H(3)	8*f*	0.1046	1.0015	0.4972	0.023
H(5)	8*f*	0.1490	1.1242	0.3366	0.026
H(6)	8*f*	0.1002	1.0189	0.2582	0.027
H(7C)	8*f*	0.0493	0.9946	0.1995	0.030
H(7D)	8*f*	0.0167	0.8660	0.1903	0.030
H(9)	8*f*	0.0151	0.7128	0.0170	0.025
H(10)	8*f*	–0.0236	0.7187	–0.0901	0.030
H(11)	8*f*	–0.0042	0.6321	–0.1892	0.033
H(12)	8*f*	0.0525	0.5382	–0.1794	0.028
H(15)	8*f*	0.1087	0.4472	–0.1577	0.025
H(16)	8*f*	0.1644	0.3327	–0.1233	0.025
H(17)	8*f*	0.1898	0.3135	–0.0045	0.025
H(18)	8*f*	0.1598	0.4185	0.0760	0.026
H(20A)	8*f*	0.1598	0.8086	0.2609	0.026
H(20B)	8*f*	0.1873	0.7975	0.2143	0.026
H(22)	8*f*	0.2017	0.9425	0.1302	0.029
H(23)	8*f*	0.2391	1.1044	0.0762	0.033
H(25)	8*f*	0.2376	1.5388	0.2048	0.030
H(7B)	8*f*	0.1016(7)	0.244(4)	0.126(1)	0.08(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*	0.090435(7)	0.60536(4)	0.07325(1)	0.0208(2)	0.0183(2)	0.0119(2)	–0.0005(1)	0.0034(1)	–0.0016(1)
Cl(1)	8*f*	0.19532(2)	1.41576(8)	0.29407(3)	0.0401(4)	0.0207(3)	0.0278(4)	–0.0048(3)	0.0138(3)	–0.0070(2)
Cl(2)	8*f*	0.26925(2)	1.4583(1)	0.09342(4)	0.0353(4)	0.0541(5)	0.0374(4)	–0.0166(3)	0.0170(3)	0.0000(3)
Cl(3)	8*f*	0.03907(2)	0.87040(8)	0.43329(3)	0.0264(3)	0.0238(3)	0.0212(3)	0.0007(2)	0.0105(2)	–0.0022(2)
Cl(4)	8*f*	0.16870(2)	1.13927(8)	0.48223(3)	0.0256(3)	0.0248(3)	0.0247(3)	–0.0003(2)	0.0036(3)	–0.0055(2)
O(1)	8*f*	0.04321(4)	0.8799(2)	0.28784(8)	0.0241(9)	0.034(1)	0.0134(8)	0.0030(7)	0.0037(7)	–0.0057(7)
O(2)	8*f*	0.07542(5)	0.5962(2)	0.22917(9)	0.038(1)	0.031(1)	0.0145(9)	0.0097(8)	0.0064(8)	0.0021(7)
O(3)	8*f*	0.05921(4)	0.7276(2)	0.12297(8)	0.0251(9)	0.0254(9)	0.0136(8)	0.0026(7)	0.0054(7)	–0.0014(7)
O(4)	8*f*	0.13253(4)	0.6746(2)	0.14007(8)	0.0228(9)	0.0198(8)	0.0188(8)	–0.0008(7)	0.0012(7)	–0.0042(7)
O(5)	8*f*	0.12309(4)	0.9837(2)	0.12788(9)	0.0277(9)	0.0207(9)	0.0229(9)	0.0023(7)	0.0029(7)	0.0028(7)
O(6)	8*f*	0.17695(4)	1.0543(2)	0.23897(8)	0.033(1)	0.0201(8)	0.0169(9)	–0.0079(7)	0.0072(7)	–0.0051(7)
O(7)	8*f*	0.08699(4)	0.3289(2)	0.13196(8)	0.030(1)	0.0201(9)	0.0195(9)	0.0009(8)	0.0076(7)	0.0002(7)
N(1)	8*f*	0.05480(5)	0.6179(2)	–0.0164(1)	0.021(1)	0.0149(9)	0.015(1)	–0.0033(8)	0.0046(8)	0.0008(7)
N(2)	8*f*	0.11744(5)	0.4924(3)	0.0092(1)	0.024(1)	0.0145(9)	0.016(1)	–0.0019(8)	0.0048(8)	–0.0003(8)
C(1)	8*f*	0.07277(6)	0.9466(3)	0.3295(1)	0.025(1)	0.017(1)	0.017(1)	0.005(1)	0.005(1)	–0.0027(9)
C(2)	8*f*	0.07443(6)	0.9467(3)	0.4019(1)	0.023(1)	0.014(1)	0.018(1)	0.004(1)	0.007(1)	–0.0006(9)
C(3)	8*f*	0.10362(6)	1.0052(3)	0.4494(1)	0.028(1)	0.013(1)	0.016(1)	0.005(1)	0.006(1)	–0.0007(9)
C(4)	8*f*	0.13120(6)	1.0691(3)	0.4238(1)	0.025(1)	0.012(1)	0.021(1)	0.003(1)	0.003(1)	–0.0034(9)
C(5)	8*f*	0.13032(7)	1.0775(3)	0.3527(1)	0.029(1)	0.017(1)	0.023(1)	0.001(1)	0.011(1)	–0.001(1)
C(6)	8*f*	0.10095(6)	1.0149(3)	0.3060(1)	0.034(1)	0.021(1)	0.013(1)	0.005(1)	0.008(1)	0.000(1)
C(7)	8*f*	0.04079(7)	0.8766(4)	0.2136(1)	0.028(1)	0.035(1)	0.012(1)	0.005(1)	0.002(1)	–0.003(1)
C(8)	8*f*	0.06079(6)	0.7179(3)	0.1886(1)	0.020(1)	0.026(1)	0.017(1)	–0.004(1)	0.004(1)	–0.005(1)
C(9)	8*f*	0.02247(6)	0.6751(3)	–0.0228(1)	0.026(1)	0.021(1)	0.017(1)	–0.003(1)	0.006(1)	–0.000(1)
C(10)	8*f*	–0.00089(6)	0.6809(3)	–0.0869(1)	0.025(1)	0.024(1)	0.023(1)	–0.001(1)	0.001(1)	0.003(1)
C(11)	8*f*	0.01073(7)	0.6288(4)	–0.1456(1)	0.031(1)	0.030(1)	0.018(1)	–0.002(1)	–0.003(1)	0.002(1)
C(12)	8*f*	0.04448(7)	0.5718(3)	–0.1399(1)	0.032(1)	0.022(1)	0.016(1)	–0.003(1)	0.004(1)	–0.001(1)
C(13)	8*f*	0.06605(6)	0.5656(3)	–0.0742(1)	0.027(1)	0.012(1)	0.018(1)	–0.005(1)	0.006(1)	0.0013(9)
C(14)	8*f*	0.10204(6)	0.4982(3)	–0.0598(1)	0.027(1)	0.010(1)	0.017(1)	–0.007(1)	0.005(1)	0.0008(9)
C(15)	8*f*	0.11926(6)	0.4401(3)	–0.1105(1)	0.034(1)	0.015(1)	0.014(1)	–0.006(1)	0.007(1)	–0.0002(9)
C(16)	8*f*	0.15238(6)	0.3718(3)	–0.0900(1)	0.028(1)	0.015(1)	0.024(1)	–0.003(1)	0.014(1)	–0.003(1)
C(17)	8*f*	0.16769(6)	0.3616(3)	–0.0193(1)	0.023(1)	0.018(1)	0.023(1)	–0.000(1)	0.007(1)	–0.000(1)
C(18)	8*f*	0.14949(6)	0.4240(3)	0.0286(1)	0.026(1)	0.020(1)	0.018(1)	0.001(1)	0.003(1)	0.000(1)
C(19)	8*f*	0.13841(6)	0.8459(3)	0.1567(1)	0.020(1)	0.021(1)	0.013(1)	–0.000(1)	0.0068(9)	–0.0015(9)
C(20)	8*f*	0.16722(6)	0.8656(3)	0.2216(1)	0.030(1)	0.016(1)	0.019(1)	–0.003(1)	0.003(1)	0.0000(9)
C(21)	8*f*	0.19769(6)	1.1399(3)	0.2019(1)	0.018(1)	0.023(1)	0.017(1)	–0.002(1)	0.001(1)	–0.000(1)
C(22)	8*f*	0.20907(6)	1.0615(3)	0.1458(1)	0.024(1)	0.026(1)	0.020(1)	–0.002(1)	0.003(1)	–0.005(1)
C(23)	8*f*	0.23123(6)	1.1586(4)	0.1131(1)	0.026(1)	0.038(2)	0.020(1)	0.001(1)	0.006(1)	–0.004(1)
C(24)	8*f*	0.24161(6)	1.3351(4)	0.1353(1)	0.018(1)	0.037(2)	0.022(1)	–0.007(1)	0.004(1)	0.004(1)
C(25)	8*f*	0.23056(6)	1.4184(3)	0.1904(1)	0.023(1)	0.026(1)	0.025(1)	–0.002(1)	0.002(1)	–0.000(1)
C(26)	8*f*	0.20894(6)	1.3192(3)	0.2235(1)	0.021(1)	0.021(1)	0.017(1)	0.003(1)	0.003(1)	–0.001(1)

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