Crystal structure of *trans*-diaqua-di(bis(pyrazolylmethane)copper(II) dinitrate, $Cu(C_7H_{10}N_4)_2(OH_2)_2(NO_3)_2$

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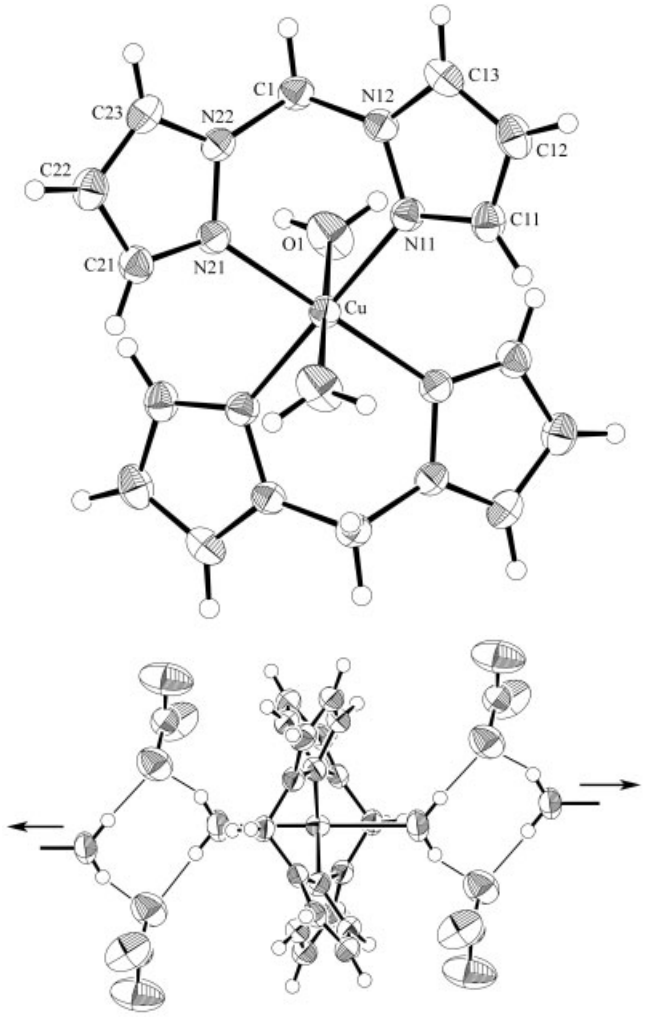

Abstract

$C_{14}H_{20}CuN_{10}O_8$, triclinic, $P\bar{1}$ (No. 2), a = 8.498(1) Å, b = 9.167(2) Å, c = 8.323(3) Å, α = 103.41(3)°, β = 101.87(3)°, γ = 117.10(1)°, V = 523.9 Å^3, Z = 1, $R_{gt}(F)$ = 0.041, $wR_{ref}(F^2)$ = 0.122, T = 293 K.

Source of material

The complex was used as a precursor to prepare mixed $(bpm)_2Cu(II)$-hexacyanoiron(III)-bridged molecule-based magnetic materials for comparison to other $Ni(II)(bpm)_2$-$Fe(CN)_6$ systems [1]. The complex was characterized by magnetic moment data (1.88 μB at 295 K), which were compatible with a mononuclear Cu(II) structure; and by IR spectroscopy which showed the characteristic bands of the ligand and anion.

Discussion

The Cu atom in the cation lies on a crystallographic centre of inversion and exists within a N_4O_2 donor set defined by two chelating bpm ligands and two oxygen atoms derived from two water molecules. The coordination is axially-distorted octahedral with the O atoms in axial positions. Key geometric parameters: d(Cu—N11) = 1.994(2) Å, d(Cu—N21) = 2.028(2) Å, d(Cu—O1) = 2.471(2) Å and a chelate angle of 88.90(9)°. Each water molecule forms two hydrogen bonds, one each to two nitrate anions that, in turn are linked to a centrosymmetrically related water molecule so that twelve-membered $[H–O–H\cdots O–N(O)–O\cdots]_2$ rings are formed as highlighted in the lower view of the Figure. Thus, the complex cations and anions are linked into chains via hydrogen bonding contacts. The parameters associated with the hydrogen bonding are d(O1–H···O2) = 2.02 Å, d(O1···O2) = 2.871(5) Å and the angle at H is 168°, and d(O1–H···O4^i) = 2.06 Å, d(O1···O4^i) = 2.839(5) Å and angle of 149°; i: $-x$, $-y$, $-1-z$.

Table 1. Data collection and handling.

Crystal:	blue block, size 0.16 × 0.19 × 0.40 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.09 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC6R, $\omega/2\theta$
$2\theta_{max}$:	55.2°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2567, 2406
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2088
$N(param)_{refined}$:	152
Programs:	teXsan [2], SAPI91 [3], SHELXL-97 [4], DIFABS [5], PLATON [6], ORTEPII [7]

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

Atom	Site	x	y	z	U_{iso}
H(1o)	2*i*	0.0741	0.1283	–0.2893	0.070
H(2o)	2*i*	0.0732	–0.0288	–0.3518	0.070
H(1a)	2*i*	–0.4898	–0.1680	–0.4138	0.070
H(1b)	2*i*	–0.2731	–0.0925	–0.3755	0.070
H(11)	2*i*	–0.0652	0.3112	0.1879	0.056
H(12)	2*i*	–0.3484	0.3217	0.0563	0.056
H(13)	2*i*	–0.5360	0.0709	–0.2328	0.056
H(21)	2*i*	–0.2155	–0.4159	–0.0420	0.056
H(22)	2*i*	–0.5539	–0.6329	–0.2310	0.056
H(23)	2*i*	–0.6575	–0.4801	–0.3966	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	1*a*	0	0	0	0.0333(2)	0.0310(2)	0.0363(3)	0.0166(2)	0.0113(2)	0.0109(2)
O(1)	2*i*	0.0813(4)	0.0468(3)	–0.2597(3)	0.095(2)	0.081(2)	0.051(1)	0.062(2)	0.046(1)	0.039(1)
O(2)	2*i*	0.0551(4)	0.3358(4)	–0.3092(5)	0.053(1)	0.075(2)	0.110(3)	0.020(1)	–0.007(2)	0.038(2)
O(3)	2*i*	–0.1683(5)	0.3787(5)	–0.4004(5)	0.102(3)	0.091(2)	0.124(3)	0.069(2)	–0.003(2)	0.003(2)
O(4)	2*i*	–0.2040(4)	0.1316(4)	–0.5204(4)	0.072(2)	0.066(2)	0.064(2)	0.027(1)	0.015(1)	0.007(1)
N(1)	2*i*	–0.1018(4)	0.2847(3)	–0.4109(3)	0.048(1)	0.047(1)	0.047(1)	0.021(1)	0.012(1)	0.017(1)
N(11)	2*i*	–0.1627(3)	0.1010(3)	–0.0337(3)	0.039(1)	0.038(1)	0.032(1)	0.0214(9)	0.0128(8)	0.0110(8)
N(12)	2*i*	–0.3243(3)	0.0213(3)	–0.1751(3)	0.038(1)	0.038(1)	0.035(1)	0.0212(9)	0.0143(8)	0.0168(9)
N(21)	2*i*	–0.2322(3)	–0.2442(3)	–0.1469(3)	0.036(1)	0.035(1)	0.035(1)	0.0167(8)	0.0120(8)	0.0144(8)
N(22)	2*i*	–0.3855(3)	–0.2699(3)	–0.2677(3)	0.036(1)	0.036(1)	0.029(1)	0.0172(8)	0.0132(8)	0.0104(8)
C(1)	2*i*	–0.3706(4)	–0.1278(3)	–0.3240(3)	0.043(1)	0.040(1)	0.031(1)	0.020(1)	0.013(1)	0.016(1)
C(11)	2*i*	–0.1599(4)	0.2339(3)	0.0778(4)	0.052(2)	0.039(1)	0.040(1)	0.025(1)	0.022(1)	0.014(1)
C(12)	2*i*	–0.3185(4)	0.2405(4)	0.0061(4)	0.059(2)	0.047(1)	0.056(2)	0.035(1)	0.034(1)	0.025(1)
C(13)	2*i*	–0.4207(4)	0.1028(4)	–0.1534(4)	0.046(1)	0.051(2)	0.056(2)	0.032(1)	0.023(1)	0.030(1)
C(21)	2*i*	–0.2909(4)	–0.3952(3)	–0.1199(4)	0.047(1)	0.037(1)	0.041(1)	0.021(1)	0.017(1)	0.018(1)
C(22)	2*i*	–0.4808(4)	–0.5178(4)	–0.2247(4)	0.045(1)	0.036(1)	0.048(2)	0.016(1)	0.023(1)	0.017(1)
C(23)	2*i*	–0.5371(4)	–0.4335(3)	–0.3160(3)	0.037(1)	0.039(1)	0.035(1)	0.015(1)	0.016(1)	0.009(1)

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