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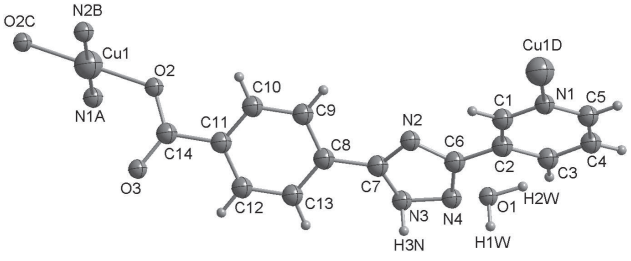
Crystal structure of catena-poly[bis(μ_2-4-(3-(pyridin-3-yl)-1H-1,2,4-triazol-5-yl)benzoato)-κ^2N:O)copper(II)] dihydrate, $C_{28}H_{22}N_8O_6Cu$



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Abstract

$C_{28}H_{22}O_6N_8Cu$, Triclinic, $P\bar{1}$, $a = 6.826(5)$ Å, $b = 9.040(7)$ Å, $c = 10.930(8)$ Å, $\alpha = 101.068(8)°$, $\beta = 95.054(8)°$, $\gamma = 96.278(8)°$, $V = 653.8(9)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0469$, $wR_{ref}(F^2) = 0.1063$, $T = 293(2)$ K.

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The crystal structure is shown in the figure, Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Cu(OAc)_2 \cdot H_2O$ (0.1 mmol, 199 mg), THF (10 mL), 4-(3-(pyridin-3-yl)-1H-1,2,4-triazol-5-yl)benzoic acid (0.3 mmol, 266 mg) was dissolved in 8 mL H_2O. Then the solution was heated in a 23 mL Teflon-lined autoclave under autogenous pressure at 393 K for five days. After cooling to room temperature crystals formed. The red crystals suitable for X-ray diffraction analysis were collected.

Experimental details

At the pyridine ring, the hydrogen atoms were assigned with $U_{iso}(H) = 1.2\ U_{eq}(C)$, and included in the final refinement by using geometrical restraints, with d(C—H) = 0.93 Å. A data completeness of only 97.2% was achieved.

Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.28×0.35×0.41 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.97 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4056, 2328
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1816
$N(param)_{refined}$:	196
Programs:	SHELX [10]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	x	y	z	U_{iso}
H(3N)	2*i*	0.5617	0.4863	0.7228	0.040
H(1W)	2*i*	0.3570	0.4683	0.0881	0.088
H(2W)	2*i*	0.4630	0.3489	0.0467	0.088
H(1)	2*i*	0.4698	0.1313	0.2659	0.039
H(3)	2*i*	0.9948	0.3515	0.4355	0.041
H(4)	2*i*	1.1321	0.2660	0.2524	0.044
H(5)	2*i*	0.9365	0.1186	0.0822	0.044
H(9)	2*i*	0.1239	0.0733	0.5792	0.041
H(10)	2*i*	−0.1456	0.0315	0.6866	0.042
H(12)	2*i*	−0.0145	0.4546	0.8958	0.040
H(13)	2*i*	0.2588	0.4946	0.7918	0.040

Discussion

Over the past few decades, supramolecular chemistry depending upon hydrogen bonding and intermolecular weak interactions have been a field of rapid growth due to potential application such as catalysis, magnetism, semiconductor, nonlinear optical materials, biological activity [1–6]. Benzimidazole and its derivatives, which are one kind of important building modules of N-containing heterocyclic ring compounds, may provide supramolecular recognition sites

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Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	1*d*	−0.5	0.0	1.0	0.0332(4)	0.0396(4)	0.0262(3)	−0.0075(3)	0.0140(3)	0.0034(3)
N(1)	2*i*	0.6834(4)	0.1111(3)	0.1560(3)	0.029(2)	0.040(2)	0.028(2)	0.000(1)	0.014(1)	0.005(1)
N(2)	2*i*	0.4320(4)	0.2310(3)	0.5001(2)	0.029(2)	0.037(2)	0.030(2)	−0.007(1)	0.012(1)	0.003(1)
N(3)	2*i*	0.5533(4)	0.4213(3)	0.6533(2)	0.028(2)	0.040(2)	0.026(2)	−0.007(1)	0.010(1)	−0.004(1)
N(4)	2*i*	0.6936(4)	0.4152(3)	0.5727(3)	0.028(2)	0.041(2)	0.029(2)	−0.005(1)	0.010(1)	0.001(1)
O(1)	2*i*	0.3636(4)	0.3795(3)	0.1019(3)	0.046(2)	0.086(2)	0.047(2)	0.007(2)	0.019(1)	0.015(2)
O(2)	2*i*	−0.3171(4)	0.0677(3)	0.8913(2)	0.041(2)	0.044(2)	0.032(1)	−0.013(1)	0.018(1)	−0.000(1)
O(3)	2*i*	−0.3415(4)	0.3171(3)	0.9443(3)	0.050(2)	0.060(2)	0.058(2)	0.018(1)	0.036(2)	0.018(1)
C(1)	2*i*	0.6043(5)	0.1595(4)	0.2634(3)	0.028(2)	0.040(2)	0.027(2)	−0.003(2)	0.010(2)	0.004(2)
C(2)	2*i*	0.7134(5)	0.2489(4)	0.3699(3)	0.028(2)	0.034(2)	0.028(2)	0.000(2)	0.011(2)	0.008(1)
C(3)	2*i*	0.9167(5)	0.2909(4)	0.3661(3)	0.028(2)	0.038(2)	0.034(2)	−0.004(2)	0.007(2)	0.005(2)
C(4)	2*i*	0.9977(5)	0.2404(4)	0.2570(3)	0.022(2)	0.045(2)	0.043(2)	0.000(2)	0.014(2)	0.010(2)
C(5)	2*i*	0.8791(5)	0.1518(4)	0.1549(3)	0.030(2)	0.047(2)	0.035(2)	0.002(2)	0.017(2)	0.009(2)
C(6)	2*i*	0.6139(5)	0.2991(3)	0.4818(3)	0.026(2)	0.032(2)	0.026(2)	−0.000(1)	0.007(1)	0.006(1)
C(7)	2*i*	0.3986(5)	0.3115(4)	0.6097(3)	0.028(2)	0.030(2)	0.027(2)	−0.003(1)	0.006(2)	0.006(1)
C(8)	2*i*	0.2237(5)	0.2880(4)	0.6760(3)	0.027(2)	0.033(2)	0.025(2)	−0.001(1)	0.010(1)	0.004(1)
C(9)	2*i*	0.0979(5)	0.1489(4)	0.6441(3)	0.036(2)	0.032(2)	0.033(2)	−0.002(2)	0.016(2)	0.000(2)
C(10)	2*i*	−0.0637(5)	0.1239(4)	0.7085(3)	0.038(2)	0.030(2)	0.036(2)	−0.006(2)	0.017(2)	0.004(2)
C(11)	2*i*	−0.1053(5)	0.2362(4)	0.8065(3)	0.028(2)	0.038(2)	0.025(2)	0.001(2)	0.011(1)	0.008(1)
C(12)	2*i*	0.0156(5)	0.3769(4)	0.8340(3)	0.033(2)	0.035(2)	0.029(2)	0.001(2)	0.012(2)	−0.003(1)
C(13)	2*i*	0.1785(5)	0.4015(4)	0.7709(3)	0.028(2)	0.033(2)	0.036(2)	−0.006(2)	0.008(2)	0.002(2)
C(14)	2*i*	−0.2686(5)	0.2083(4)	0.8857(3)	0.031(2)	0.050(2)	0.023(2)	0.000(2)	0.008(2)	0.006(2)

for N–H$\cdots$O, C–H$\cdots$O, C–H$\cdots\pi$ and π–π interactions to construct supramolecular architectures. On account of its various coordination modes, multi-carboxylate ligands are extremely popular as efficient linkers in the construction of supramolecular compounds. Thereinto, the 4-(3-(pyridin-3-yl)-1H-1,2,4-triazol-5-yl)benzoate (bta) as unsymmetrical carboxylate bridging ligands possess two or more coordination sites with differing donor abilities. Its carboxylate group can be used as hydrogen-bond acceptor. Discrete subunits or low-dimensional entities have been linked highdimensional supramolecular compounds through hydrogen bonds, $\pi\ldots\pi$ stacking and host-guest interactions [6–9].

The asymmetric unit of the title structure contains one half of a Cu(II) ion, and 4-(3-(pyridin-3-yl)-1H-1,2,4-triazol-5-yl)benzoate as a bridging ligand to construct a coordination polymer. The copper atom is four-coordinated by two oxygen atoms and two nitrogen atoms from four ligands to give a chain structure. The Cu–O bond lengths range is 1.928(2) Å, the Cu–N bond lengths range is 2.043(3) Å. In addition, there are intermolecular hydrogen bonds d(O(1)—H(1W)$\cdots$O(3)#6) = 2.900(5) Å, d(O(1)—H(2W)$\cdots$O(3)#4) = 2.798(4) Å; d(N(3)—H(3N)$\cdots$O(1)#5) = 2.895(4) Å. Symmetry codes: #4 $x+1$, y, $z-1$; #5 $-x+1$, $-y+1$, $-z+1$; #6 $-x$, $-y+1$, $-z+1$. Thus these interactions result in a hydrogen bonded three dimensional architecture.

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