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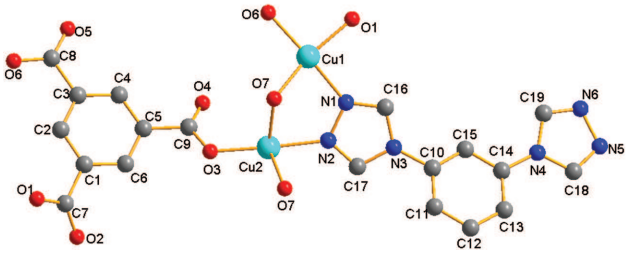
# Crystal structure of *catena*-poly[aqua-($\mu_3$-1,3,5-benzenetricarboxylato-$\kappa^3O:O':O''$)-[$\mu_3$hydroxy-(1,3-di-($\mu_2$-1,2,4-triazole-4-yl)benzoato-$\kappa^2N:N'$)copper(II)], $C_{19}H_{16}Cu_2N_6O_9$

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## Abstract

$C_{19}H_{16}Cu_2N_6O_9$, monoclinic, $P2_1/n$ (no. 14), $a = 7.9182(8)$ Å, $b = 11.7533(12)$ Å, $c = 22.7024(19)$ Å, $V = 2015.7(3)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0309$, $wR_{ref}(F^2) = 0.0692$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

## Source of material

The title compound was prepared by hydrothermal method. A mixture of $Cu(OAc)_2{\cdot}4H_2O$ (0.038 g, 0.2 mmol), 1,3,5-benzenetricarboxylic acid (0.021 mg, 0.1 mmol), 3,5-di(1,2,4-triazole-4)benzenecarboxylic acid (0.0256 g, 0.1 mmol), and $H_2O$ (10 mL) was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 140 °C for 3 days. The reaction mixture was slowly cooled to room temperature at a rate of 3 °C/h, and the blue block crystals were collected, washed with water and dried in air.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Blue block |
| Size: | 0.19 × 0.15 × 0.12 mm |
| Wavelength: | Mo $K\alpha$ radiation (0.71073 Å) |
| $\mu$: | 21.8 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART, $\varphi$ and $\omega$ |
| $2\theta_{max}$, completeness: | 51°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 15045, 3752, 0.043 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2955 |
| $N(param)_{refined}$: | 325 |
| Programs: | Bruker programs [1], SHELX [2, 3, 4] |

## Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors $U_{iso}(H) = 1.2$ times $U_{eq}$(C, aromatic ring), and $U_{iso}(H) = 1.5$ times $U_{eq}$(O, water, $OH^-$) and were refined as riding on their parent atoms.

## Discussion

The construction of coordination polymers (CPs) is of current interest not only because of their potential applications as functional materials but also, from a structural point of view, due to their intriguing variety of architectures [5]. So far, a variety of spectacular CPs have been documented, such as 1D chains and ladders, 2D grids, 3D networks, interpenetrated modes, and so on [6, 7]. It is well known that the structures of coordination polymers are strongly dependent on the nature of the organic ligands and the metal ions [8]. Among various organic ligands, aromatic polycarboxyl compounds have been proven to be excellent ones for their diverse coordination modes. On the other hand, 1,2,4-triazole and its derivatives have received much interesting because they combine the coordination geometry of both pyrazole and imidazole with regard to the arrangement of their three heteroatoms [9, 10].

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.49262(5) | 0.39861(3) | 0.629085(17) | 0.01946(11) |
| Cu2 | 0.30852(5) | 0.04604(3) | 0.983114(17) | 0.01927(11) |
| N1 | 0.3572(3) | 0.5457(2) | 0.60737(11) | 0.0196(6) |
| N2 | 0.2826(3) | 0.5667(2) | 0.54542(11) | 0.0193(6) |
| N3 | 0.2458(3) | 0.7167(2) | 0.59633(11) | 0.0210(6) |
| N4 | 0.0760(4) | 1.0118(2) | 0.71878(12) | 0.0229(6) |
| N5 | −0.0135(4) | 1.1216(3) | 0.78202(14) | 0.0384(8) |
| N6 | 0.0334(4) | 1.0166(3) | 0.80942(13) | 0.0379(8) |
| O1 | 0.4937(3) | 0.42389(18) | 0.71341(10) | 0.0260(5) |
| O2 | 0.2741(3) | 0.2996(2) | 0.70192(11) | 0.0393(7) |
| O3 | 0.3329(3) | 0.16106(17) | 0.92536(10) | 0.0235(5) |
| O4 | 0.2105(3) | 0.28685(19) | 0.97404(10) | 0.0319(6) |
| O5 | 0.3512(4) | 0.69628(19) | 0.94077(11) | 0.0387(7) |
| O6 | 0.4144(3) | 0.74386(18) | 0.85424(10) | 0.0292(6) |
| O7 | 0.5186(3) | 0.40749(17) | 0.54839(9) | 0.0198(5) |
| H7D | 0.5661 | 0.3455 | 0.5422 | 0.030* |
| O8 | 0.0726(3) | 0.0065(2) | 0.92902(10) | 0.0294(6) |
| H1W | 0.0703 | 0.0121 | 0.8915 | 0.044* |
| H2W | 0.0271 | −0.0556 | 0.9361 | 0.044* |
| O9 | 0.1431(4) | 0.3224(2) | 0.57233(12) | 0.0403(7) |
| H3W | 0.2231 | 0.2956 | 0.6031 | 0.060* |
| H4W | 0.1721 | 0.2841 | 0.5451 | 0.060* |
| C1 | 0.3686(4) | 0.4044(3) | 0.79561(13) | 0.0179(7) |
| C2 | 0.3935(4) | 0.5168(3) | 0.81571(14) | 0.0195(7) |
| H2 | 0.4284 | 0.5711 | 0.7919 | 0.023* |
| C3 | 0.3665(4) | 0.5483(3) | 0.87126(14) | 0.0184(7) |
| C4 | 0.3274(4) | 0.4650(3) | 0.90900(14) | 0.0195(7) |
| H4 | 0.3111 | 0.4856 | 0.9465 | 0.023* |
| C5 | 0.3126(4) | 0.3517(3) | 0.89101(13) | 0.0170(7) |
| C6 | 0.3276(4) | 0.3224(3) | 0.83341(14) | 0.0188(7) |
| H6 | 0.3101 | 0.2473 | 0.8200 | 0.023* |
| C7 | 0.3786(4) | 0.3714(3) | 0.73222(14) | 0.0215(7) |
| C8 | 0.3787(4) | 0.6720(3) | 0.89141(15) | 0.0229(7) |
| C9 | 0.2804(4) | 0.2613(3) | 0.93392(14) | 0.0193(7) |
| C10 | 0.2066(4) | 0.8331(3) | 0.60658(14) | 0.0197(7) |
| C11 | 0.2170(5) | 0.9115(3) | 0.56285(15) | 0.0273(8) |
| H11 | 0.2525 | 0.8898 | 0.5290 | 0.033* |
| C12 | 0.1740(5) | 1.0224(3) | 0.57030(17) | 0.0373(9) |
| H12 | 0.1758 | 1.0761 | 0.5404 | 0.045* |
| C13 | 0.1283(5) | 1.0548(3) | 0.62180(16) | 0.0341(9) |
| H13 | 0.1010 | 1.1304 | 0.6269 | 0.041* |
| C14 | 0.1228(4) | 0.9753(3) | 0.66570(14) | 0.0206(7) |
| C15 | 0.1579(4) | 0.8618(3) | 0.65805(14) | 0.0208(7) |
| H15 | 0.1489 | 0.8071 | 0.6865 | 0.025* |
| C16 | 0.3334(4) | 0.6366(3) | 0.63710(14) | 0.0209(7) |
| H16 | 0.3710 | 0.6451 | 0.6798 | 0.025* |
| C17 | 0.2175(4) | 0.6689(3) | 0.54008(14) | 0.0212(7) |
| H17 | 0.1595 | 0.7042 | 0.5028 | 0.025* |
| C18 | 0.0131(5) | 1.1157(3) | 0.72873(17) | 0.0329(9) |
| H18 | −0.0082 | 1.1752 | 0.7005 | 0.039* |
| C19 | 0.0862(5) | 0.9535(3) | 0.77126(16) | 0.0357(9) |
| H19 | 0.1254 | 0.8788 | 0.7789 | 0.043* |

The asymmetric unit of the title stucture consists of two Cu(II) ions, one 1,3,5-benzenetricarboxylic acid anion, one 1,3-di-(1,2,4-triazole-4-yl)benzene (dtb) ligand, a coordinated water molecule, a $OH^-$ anion, and one lattice water molecule (*cf.* the figure). The Cu1 center has a four-coordinated square planar geometry and is coordinated to two atoms from two symmetry-equivalent 1,3,5-benzenetricarboxylic acid anions, one nitrogen atom from 1,3-di-(1,2,4-triazole-4-yl)benzene, and one oxygen atom from $OH^-$ anion. Cu2 is five-coordinated and adopts a tetragonal pyramid geometry. The four equatorial sites are occupied by one carboxylate oxygen atom, one oxygen atom from the $OH^-$ anion, one nitrogen atom from 1,3-di-(1,2,4-triazole-4-yl)benzene, and one coordinated water molecule. The axial site is occupied by an oxygen atom from a symmetry-equivalent $OH^-$ anion. The Cu–O bond lengths are in the range of 1.907(2)–2.371(2) Å, while the Cu–N bond length varies from 1.994(2) Å to 2.016(3) Å. Cu(II) atoms are linked by 1,3,5-benzenetricarboxylic acid anion into 1D chains that run along the *b* axis, and $OH^-$ anions connect the 1D chains to generate a 2D network extending along *bc* plane.

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