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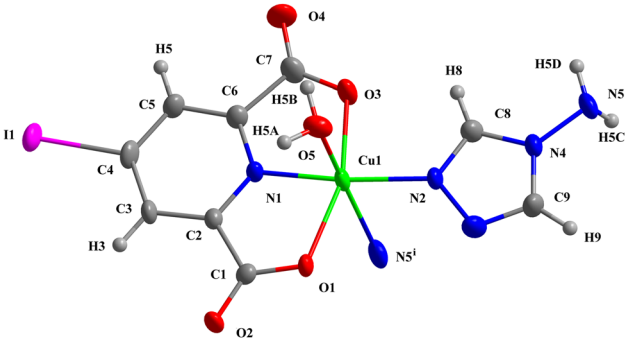
# Crystal structure of *catena*-poly[aqua-(4-iodopyridine-2,6-dicarboxylato-κ$^3$*N*,*O*,*O*′)-(μ$_2$-4-amino-4*H*-1,2,4-triazole-κ$^2$*N*:*N*′) copper(II)], $C_9H_8N_5O_5CuI$

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**Abstract**

$C_9H_8N_5O_5CuI$, orthorhombic, *Pbca* (no. 61), $a$ = 11.0801(4) Å, $b$ = 6.8489(3) Å, $c$ = 35.3975(13) Å, $Z$ = 8, $V$ = 2686.20(18) Å$^3$, $R_{gt}(F)$ = 0.0325, $wR_{ref}(F_2)$ = 0.0707, $T$ = 292 K.

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A part of the polymeric title structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

## Source of material

All chemicals were used without further purification. The title compound was prepared under hydrothermal conditions. A mixture of $Cu(OAc)_2{\cdot}H_2O$ (20.0 mg, 0.1 mmol), 4-iodopyridine-2,6-dicarboxylic acid (29.2 mg, 0.1 mmol), 4-amino-4*H*-1,2,4-triazole and 4 mL deionized water was sealed in a 20 mL screw capped vial and heated at 70 °C for three days. After cooling to room temperature naturally, blue crystals were collected by filtration and washed with distilled water in 53% yield. **Elemental analysis** calculated for $C_9H_8N_5O_5CuI$: C 23.65, H 1.75, O 17.52%; found C 23.68, H 1.82, O 17.56%.

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

| | |
|---|---|
| Crystal: | Blue block |
| Size: | 0.32 × 0.28 × 0.21 mm |
| Wavelength: | Mo *Kα* radiation (0.71073 Å) |
| $\mu$: | 3.96 mm$^{-1}$ |
| Diffractometer, scan mode: | SuperNova, $\omega$ |
| $\theta_{max}$, completeness: | 25.0°, 99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 23,030, 2332, 0.043 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 2218 |
| $N(param)_{refined}$: | 192 |
| Programs: | CrysAlis$^{PRO}$ [1], SHELX [2, 3], Olex2 [4] |

## Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

## Comment

Recently, much effort has been devoted to the synthesis of coordination polymers (CPs) owing to their potential applications in catalysis, drug delivery, chromism, gas storage, and luminescent sensors [5–10]. In the self-assembly of CPs, noncovalent interactions, such as hydrogen bonding, π···π stacking, van der Waals, halogen bonding, as well as electrostatic or dipole interaction are important as they not only help in understanding the essential nature of these interactions but also provide many clues to guide the synthesis of CPs [11–13]. On the other hand, aromatic polycarboxylates with various coordination modes have been used to synthesize target CPs. However,

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| I1 | 0.60511 (3) | 0.22740 (5) | 0.48729 (2) | 0.03420 (12) |
| Cu1 | 0.46387 (4) | 0.45082 (9) | 0.66587 (2) | 0.02476 (16) |
| O1 | 0.2926 (2) | 0.4176 (4) | 0.64443 (7) | 0.0231 (7) |
| O2 | 0.1976 (3) | 0.3258 (5) | 0.59169 (8) | 0.0293 (7) |
| O3 | 0.6498 (3) | 0.4454 (5) | 0.66933 (8) | 0.0334 (8) |
| O4 | 0.8101 (3) | 0.4289 (6) | 0.63146 (10) | 0.0435 (9) |
| O5 | 0.4725 (3) | 0.7739 (5) | 0.64672 (9) | 0.0336 (8) |
| H5A | 0.4320 | 0.7914 | 0.6266 | 0.050* |
| H5B | 0.5438 | 0.8050 | 0.6401 | 0.050* |
| N1 | 0.5017 (3) | 0.3674 (5) | 0.61579 (9) | 0.0203 (8) |
| N2 | 0.4495 (3) | 0.5222 (6) | 0.71922 (9) | 0.0241 (8) |
| N3 | 0.3489 (3) | 0.5271 (7) | 0.74187 (11) | 0.0364 (10) |
| N4 | 0.5097 (3) | 0.5676 (5) | 0.77657 (10) | 0.0243 (8) |
| N5 | 0.5828 (3) | 0.6107 (6) | 0.80829 (10) | 0.0297 (9) |
| H5C | 0.5842 | 0.5108 | 0.8234 | 0.036* |
| H5D | 0.6562 | 0.6361 | 0.8013 | 0.036* |
| C1 | 0.2897 (4) | 0.3597 (6) | 0.61026 (12) | 0.0208 (9) |
| C2 | 0.4122 (4) | 0.3307 (6) | 0.59181 (12) | 0.0195 (9) |
| C3 | 0.4377 (4) | 0.2834 (7) | 0.55476 (12) | 0.0249 (10) |
| H3 | 0.3763 | 0.2539 | 0.5378 | 0.030* |
| C4 | 0.5579 (4) | 0.2812 (7) | 0.54364 (12) | 0.0266 (10) |
| C5 | 0.6498 (4) | 0.3206 (7) | 0.56921 (12) | 0.0270 (10) |
| H5 | 0.7303 | 0.3183 | 0.5619 | 0.032* |
| C6 | 0.6174 (4) | 0.3630 (7) | 0.60573 (12) | 0.0242 (10) |
| C7 | 0.7015 (4) | 0.4156 (7) | 0.63782 (13) | 0.0305 (11) |
| C8 | 0.5438 (4) | 0.5452 (7) | 0.74076 (12) | 0.0287 (11) |
| H8 | 0.6234 | 0.5460 | 0.7323 | 0.034* |
| C9 | 0.3885 (4) | 0.5551 (9) | 0.77627 (14) | 0.0395 (13) |
| H9 | 0.3397 | 0.5650 | 0.7976 | 0.047* |

the multidentate ligands containing N and O atoms are very limited [14–16]. From the point of view of structural chemistry, 4-iodopyridine-2,6-dicarboxylate (ipydc) containing N and O coordination sites is a tridentate carboxylate derivative and provides various coordination modes to synthesize both discrete and consecutive CPs under appropriate conditions. Moreover, the I atom on the pyridyl ring can be involved in halogen bonding formation. In this work, we report a CP based on Cu(II) ions, ipydc ligand and 4-amino-4*H*-1,2,4-triazole ($NH_2$trz).

In the asymmetric unit of the title structure, there are one crystallographically independent Cu(II) centre, one NH2trz molecule, one deprotonated ipydc ligand and one coordinated water molecule. The Cu(II) centre is in a distorted octahedral geometry with the $CuO_3N_3$ chromophore. The basal positions are occupied by three donor atoms from one tridentate ipydc ligand and one nitrogen atom from one $NH_2$trz ligand. The axial position is occupied by an oxygen atom of the coordinated water molecule and one nitrogen atom from one $NH_2$trz ligand. The Cu–O/N distances associated with central Cu atoms are in the range of 1.909(3)–2.556(4) Å and the bond angles about the Cu(II) centers range from 80.04(12)° to 171.34(15)°. These values match with previously reported Cu(II) compounds [17]. The NH2trz ligand link Cu(II) centers to generate a one-dimensional chain structure (see the figure).

It is worth mentioning that the compound contains water and $NH_2$ groups of NH2trz molecules, which form abundant hydrogen bonds. A number of O–H···O, and N–H···O hydrogen bonds is present, involving the water molecule, the $NH_2$ group of NH2trz and the carboxylate groups of ipydc. Besides the hydrogen-bonding interactions, the coordinated triazole rings are connected through π···π stacking interactions, with a centroid–centroid distance of 3.613(3) Å. Furthermore, there is a halogen bond as the distance between I atom and the carboxylate O atom of ipydc is 3.000(3) Å, which is shorter than the sum of the van der Waals radii of the two atoms (ca. 3.5 Å).

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