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The crystal structure of *catena*-poly[(4-iodopyridine-2,6-dicarboxylato- $\kappa^4 O, N, O', O''$)(4-imidazol-1-ylpyridine- κN)copper(II)], $C_{15}H_9N_4O_4ICu$

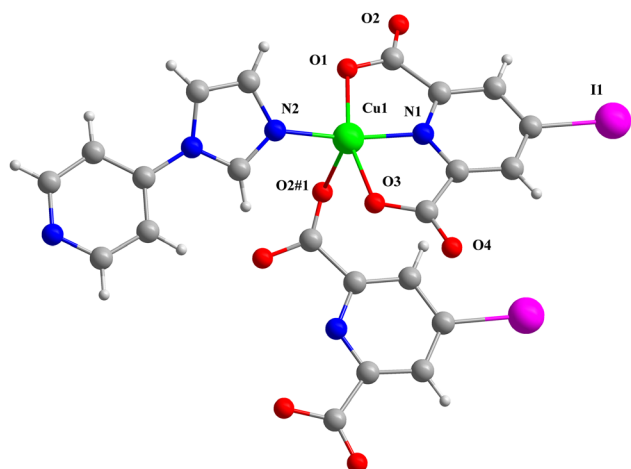


Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.31 × 0.29 × 0.25 mm
Wavelength:	MoK α radiation (0.71073 Å)
μ :	3.49 mm ⁻¹
Diffractionmeter, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.0°, 98 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	19584, 2628, 0.044
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 2391
$N(\text{param})_{\text{refined}}$:	226
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], OLEX2 [4]

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

All chemicals were of analytical grade (AR) and used as received. The title compound was prepared under hydrothermal conditions. A mixture of $Cu(OAc)_2 \cdot H_2O$ (40.0 mg, 0.2 mmol), 4-iodopyridine-2,6-dicarboxylic acid (58.4 mg, 0.2 mmol), 4-imidazol-1-ylpyridine (29.0 mg, 0.2 mmol) and deionized water (10 mL) was sealed in a 25 mL screw capped vial and heated at 90 °C for 72 h. After being cooled to RT in 12 h, blue crystals were acquired by filtration and washed with distilled water in 49 % yield.

2 Experimental details

Using OLEX2 [1], the structure was solved with the SHELXT [2] structure solution program and refined with the SHELXL [3] refinement package.

3 Comment

In recent years, the design and synthesis of coordination polymers have attracted much attention [5–7]. At present,

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Abstract

$C_{15}H_9N_4O_4ICu$, monoclinic, $P2_1/c$ (no. 14), $a = 13.6216(4)$ Å, $b = 13.4754(4)$ Å, $c = 8.5023(3)$ Å, $\beta = 102.610(3)^\circ$, $V = 1522.99(9)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0297$, $wR_{\text{ref}}(F^2) = 0.0781$, $T = 293$ K.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
C1	0.6545 (3)	0.3373 (3)	−0.0328 (4)	0.0232 (8)
C2	0.7606 (3)	0.3532 (2)	0.0580 (4)	0.0213 (8)
C3	0.8483 (3)	0.3543 (2)	−0.0001 (5)	0.0236 (8)
H3	0.8464	0.3473	−0.1095	0.028*
C4	0.9390 (3)	0.3663 (3)	0.1107 (5)	0.0269 (9)
C5	0.9414 (3)	0.3786 (3)	0.2731 (5)	0.0298 (9)
H5	1.0022	0.3878	0.3467	0.036*
C6	0.8520 (3)	0.3769 (3)	0.3235 (4)	0.0236 (8)
C7	0.8335 (3)	0.3896 (3)	0.4926 (5)	0.0307 (9)
C8	0.4367 (3)	0.4411 (3)	0.2492 (4)	0.0301 (9)
H8	0.4362	0.4687	0.1487	0.036*
C9	0.3596 (3)	0.4427 (3)	0.3229 (4)	0.0312 (9)
H9	0.2965	0.4706	0.2840	0.037*
C10	0.4870 (3)	0.3661 (3)	0.4770 (5)	0.0268 (9)
H10	0.5262	0.3323	0.5638	0.032*
C11	0.3357 (3)	0.3791 (3)	0.5904 (5)	0.0238 (8)
C12	0.2319 (3)	0.3860 (3)	0.5530 (5)	0.0300 (9)
H12	0.1971	0.3978	0.4477	0.036*
C13	0.1815 (3)	0.3751 (3)	0.6759 (5)	0.0323 (9)
H13	0.1118	0.3810	0.6514	0.039*
C14	0.3266 (3)	0.3467 (3)	0.8587 (5)	0.0354 (10)
H14	0.3596	0.3311	0.9635	0.043*
C15	0.3837 (3)	0.3583 (3)	0.7456 (5)	0.0311 (9)
H15	0.4534	0.3521	0.7737	0.037*
Cu1	0.64444 (3)	0.36465 (3)	0.28821 (6)	0.02408 (14)
I1	1.07119 (2)	0.36391 (2)	0.02390 (4)	0.03558 (13)
N1	0.7656 (2)	0.3641 (2)	0.2149 (4)	0.0213 (7)
N2	0.5175 (2)	0.3923 (2)	0.3446 (4)	0.0270 (7)
N3	0.3922 (2)	0.3950 (2)	0.4676 (3)	0.0232 (7)
N4	0.2275 (3)	0.3564 (2)	0.8283 (5)	0.0364 (9)
O1	0.58789 (19)	0.35314 (19)	0.0493 (3)	0.0278 (6)
O2	0.63743 (18)	0.3104 (2)	−0.1752 (3)	0.0280 (6)
O3	0.7400 (2)	0.3838 (2)	0.4993 (3)	0.0302 (6)
O4	0.9041 (2)	0.4039 (3)	0.6046 (3)	0.0475 (8)

it is a great challenge to reliably predict structures of coordination polymers because several factors could dramatically influence their structures [8–11]. Therefore, utilizing suited organic ligands to produce new coordination polymers is considered to be a rational way. Among, pyridine-based multicarboxylate ligands have been demonstrated to be interesting and versatile building blocks for constructing coordination polymers now. The rigid 4-iodopyridine-2,6-dicarboxylate (ipydc) ligand is an efficient ligand, which contains a nitrogen and several oxygen coordination sites and various coordination modes [12–14]. Moreover, the electrophilic iodine atom on the para position of ipydc ligand as the donor may be involved in halogen bonds with the acceptors. Herein,

we report a Cu(II) coordination polymer based on ipydc and 4-imidazol-1-yl-pyridine mixed ligands.

The asymmetric unit of the crystal structure consists of one crystallographically independent Cu(II) center, one deprotonated ipydc ligand and one 4-imidazol-1-yl-pyridine molecule (upper part of the figure). The central Cu(II) center is five-coordinated with a tetragonal-pyramidal geometry, in which the equatorial plane is occupied by one nitrogen atom and two oxygen atoms from one ipydc ligand (N1, O1 and O3) and one imidazole nitrogen atom of 4-imidazol-1-yl-pyridine (N2), and the axial position is occupied by oxygen atoms from one ipydc ligand (O2#1). The Cu–O/N distances associated with Cu(II) center range from 1.887 (3) to 2.384 (3) Å and the bond angles about Cu(II) center are in the range of 80.57(12)°–168.22(13)°. In the compound, the ipydc ligand adopts a μ_2 -coordination mode to connect Cu(II) centers, generating a chain structure (lower part of the figure). Noted, 4-imidazol-1-yl-pyridine uses only one terminal nitrogen (N2) atom to coordinate the Cu(II) center. In the compound, there is a noncovalent interaction involving iodine atom as electrophilic species and pyridine nitrogen atom as Lewis bases, giving rise to the I⋯N halogen bond with the distance of 2.976(4) Å [15–17].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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