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Crystal structure of bis(μ_2 -4-iodopyridine-2,6-dicarboxylato- $\kappa^3 O:N:O'$)-bis(4-iodopyridine-2,6-dicarboxylato- $\kappa^3 O:N:O'$)-bis(μ_2 -1-(4-pyridyl)piperazine- $\kappa^2 N:N'$)-hexa-aqua-tetra-copper(II), $C_{46}H_{46}Cu_4I_4N_{10}O_{22}$

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Abstract

$C_{46}H_{46}Cu_4I_4N_{10}O_{22}$, monoclinic, $P2_1/c$ (no. 14), $a = 10.6637(2)$ Å, $b = 18.8249(6)$ Å, $c = 14.8626(5)$ Å, $\beta = 93.853(3)^\circ$, $Z = 2$, $V = 2976.81(15)$ Å³, $R_{gt}(F) = 0.0361$, $wR_{ref}(F^2) = 0.0726$, $T = 291$ K.

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The molecular 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

The title compound was synthesized *via* the reaction of 4-iodopyridine-2,6-dicarboxylic acid (ipydc) (29.2 mg, 0.1 mmol), 1-(4-pyridyl)piperazine (pypi) (16.3 mg,

Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.32 × 0.30 × 0.28 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.57 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	17,298, 5227, 0.032
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 4340
$N(param)_{refined}$:	393
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], Olex2 [4]

0.1 mmol), $Cu(OAc)_2 \cdots H_2O$ (20.0 mg, 0.1 mmol) in 4 mL deionized water. The mixture was placed in a 23 ml Teflon lined stainless steel reactor and then heated at 343 K for two days to afford green block crystals in a yield of 81%.

Experimental details

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

Comment

The design and synthesis of inorganic-organic coordination compounds have been an active area because such compounds could exhibit a variety of unique functional applications [5–8]. At present, the appropriate choice of organic ligands and central metal ions is one of the most effective ways to construct these compounds [9, 10]. In this regard, versatile pyridine polycarboxylic acids have been widely used as excellent candidates owing to their high structural stability and versatile coordination modes. As a member of the pyridine polycarboxylate

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	U_{iso}^*/U_{eq}
I1	1.60627 (3)	0.38574 (2)	0.92771 (2)	0.04945 (12)
I2	−0.43199 (3)	0.81703 (2)	0.33537 (3)	0.04988 (12)
Cu1	1.02672 (5)	0.48060 (3)	0.76534 (4)	0.02909 (14)
Cu2	0.13075 (5)	0.68971 (3)	0.48657 (4)	0.03172 (15)
O1	1.0033 (3)	0.37132 (16)	0.7825 (2)	0.0328 (7)
O2	1.1106 (3)	0.27713 (17)	0.8399 (3)	0.0479 (9)
O3	1.1155 (3)	0.57880 (16)	0.7648 (2)	0.0327 (7)
O4	1.2975 (3)	0.63106 (17)	0.8096 (2)	0.0457 (9)
O5	0.9234 (3)	0.50655 (17)	0.8874 (2)	0.0386 (8)
H5A	0.9650	0.5339	0.9239	0.058*
H5B	0.9143	0.4700	0.9198	0.058*
O6	0.0417 (3)	0.59759 (15)	0.4487 (2)	0.0341 (8)
O7	−0.1372 (3)	0.55836 (16)	0.3778 (2)	0.0375 (8)
O8	0.1642 (3)	0.79722 (15)	0.5026 (2)	0.0331 (7)
O9	0.0676 (3)	0.90154 (16)	0.4864 (2)	0.0437 (9)
O10	0.0916 (3)	0.69317 (19)	0.6399 (2)	0.0509 (10)
H10A	0.0837	0.6516	0.6612	0.076*
H10B	0.0205	0.7118	0.6471	0.076*
O11	0.2037 (4)	0.7115 (2)	0.3271 (3)	0.0626 (11)
H11A	0.2230	0.7533	0.3114	0.094*
H11B	0.1467	0.6952	0.2899	0.094*
N1	1.1879 (3)	0.45622 (19)	0.8222 (2)	0.0276 (8)
N2	0.8732 (3)	0.5010 (2)	0.6888 (2)	0.0324 (9)
H2	0.8840	0.4729	0.6343	0.039*
N3	0.6344 (3)	0.5600 (2)	0.6248 (3)	0.0340 (9)
N4	0.2911 (3)	0.6482 (2)	0.5263 (3)	0.0346 (9)
N5	−0.0283 (3)	0.72679 (18)	0.4421 (2)	0.0245 (8)
C1	1.0985 (4)	0.3405 (3)	0.8206 (3)	0.0324 (11)
C2	1.2113 (4)	0.3889 (2)	0.8416 (3)	0.0288 (10)
C3	1.3303 (4)	0.3674 (3)	0.8729 (3)	0.0349 (11)
H3	1.3471	0.3200	0.8864	0.042*
C4	1.4242 (4)	0.4187 (3)	0.8837 (3)	0.0333 (11)
C5	1.3975 (4)	0.4889 (2)	0.8635 (3)	0.0329 (11)
H5	1.4596	0.5235	0.8707	0.039*
C6	1.2761 (4)	0.5068 (2)	0.8321 (3)	0.0278 (10)
C7	1.2284 (4)	0.5789 (2)	0.8011 (3)	0.0299 (10)
C8	0.8619 (4)	0.5718 (3)	0.6560 (4)	0.0474 (14)
H8A	0.9360	0.5825	0.6240	0.057*
H8B	0.8625	0.6034	0.7075	0.057*
C9	0.7516 (4)	0.5883 (3)	0.5965 (4)	0.0507 (15)
H9A	0.7440	0.6395	0.5917	0.061*
H9B	0.7649	0.5701	0.5368	0.061*
C10	0.6429 (4)	0.4894 (3)	0.6615 (4)	0.0436 (13)
H10C	0.6391	0.4558	0.6120	0.052*
H10D	0.5703	0.4811	0.6960	0.052*
C11	0.7569 (4)	0.4752 (3)	0.7197 (3)	0.0399 (12)
H11C	0.7459	0.4960	0.7784	0.048*
H11D	0.7642	0.4243	0.7280	0.048*
C12	0.5229 (4)	0.5868 (2)	0.5885 (3)	0.0253 (10)
C13	0.4070 (4)	0.5542 (3)	0.6027 (3)	0.0362 (12)
H13	0.4051	0.5122	0.6356	0.043*
C14	0.2961 (4)	0.5845 (2)	0.5678 (3)	0.0331 (11)
H14	0.2215	0.5598	0.5731	0.040*
C15	0.4011 (4)	0.6790 (3)	0.5087 (4)	0.0420 (13)
H15	0.3999	0.7194	0.4726	0.050*

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C16	0.5166 (4)	0.6521 (3)	0.5429 (3)	0.0430 (13)
H16	0.5899	0.6776	0.5355	0.052*
C17	−0.0694 (4)	0.6049 (2)	0.4119 (3)	0.0280 (10)
C18	−0.1161 (4)	0.6813 (2)	0.4100 (3)	0.0239 (9)
C19	−0.2322 (4)	0.7057 (2)	0.3777 (3)	0.0297 (10)
H19	−0.2943	0.6744	0.3555	0.036*
C20	−0.2539 (4)	0.7782 (2)	0.3791 (3)	0.0304 (11)
C21	−0.1606 (4)	0.8250 (2)	0.4108 (3)	0.0321 (11)
H21	−0.1746	0.8737	0.4111	0.039*
C22	−0.0455 (4)	0.7966 (2)	0.4420 (3)	0.0264 (10)
C23	0.0713 (4)	0.8358 (2)	0.4800 (3)	0.0292 (10)

ligands, ipydc contains several coordination sites, which can generate unusual structures *via* its multiple bonding interactions [11, 12].

The crystallographic independent unit contains two Cu(II) ions and the coordination polyhedron for each metal is best described as a slightly distorted octahedron. The basal plane is occupied by the chelating tridentate ipydc donors, and by the pyipi nitrogen atoms. The Cu(1) atom has a carboxylate oxygen atom and a water molecule at the apex of the octahedron, respectively. On the other hand, the Cu(2) atom has two water molecules at the apex of the octahedron. In the complex, ipydc ligand with a chelating/bridging tridentate/monodentate coordination mode and the pyipi ligand link Cu^{2+} centers to generate a tetranuclear structure (see the figure). Moreover, there are hydrogen bonding interactions between coordinated water molecules and carboxyl oxygen atoms, between nitrogen atom of piperazine and carboxyl oxygen atoms. In addition, the structure also contains $O \cdots I$ halogen bond interactions between carboxyl oxygen atoms and iodine atoms. All non-covalent interactions mentioned above contribute to the formation of the supramolecular architecture.

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