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Crystal structure of *catena*-poly[bromido-(μ_2 -pyrazine-2-carboxylato- $\kappa^3N:N',O$)copper(II)], $C_{10}H_6N_4Cu_2O_4Br$

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.46 × 0.45 × 0.25 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	6.68 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	4841, 1095, 0.107
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 933
$N(\text{param})_{\text{refined}}$:	101
Programs:	Bruker programs [1], SHELX [2, 3]

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Abstract

$C_{10}H_6N_4Cu_2O_4Br$, orthorhombic, $Pnma$ (no. 62), $a = 6.7680(10)$ Å, $b = 23.693(2)$ Å, $c = 7.7301(11)$ Å, $V = 1239.5(3)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0473$, $wR_{\text{ref}}(F^2) = 0.1293$, $T = 298(2)$ K.

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A part of the polymeric title crystal structure is shown in the figure ($A = -x, 2 - y, 2 - z$). Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.000000	1.000000	1.000000	0.0276(4)
Br1	0.82422(14)	0.750000	0.96768(11)	0.0395(4)
N1	0.1513(7)	0.9285(2)	1.0243(5)	0.0275(11)
N2	0.3354(7)	0.8248(2)	0.9913(6)	0.0332(12)
Cu2	0.47001(19)	0.750000	0.96815(16)	0.0448(4)
O1	0.0675(6)	0.99214(16)	0.7565(5)	0.0310(9)
O2	0.2178(6)	0.93310(18)	0.5733(5)	0.0390(10)
C1	0.1608(7)	0.9476(2)	0.7192(6)	0.0269(12)
C2	0.2063(8)	0.9091(2)	0.8692(7)	0.0276(12)
C3	0.2965(8)	0.8572(2)	0.8535(8)	0.0320(13)
H3	0.331341	0.844318	0.744021	0.038*
C4	0.2860(8)	0.8455(2)	1.1470(8)	0.0348(13)
H4	0.314624	0.824568	1.245711	0.042*
C5	0.1928(8)	0.8975(2)	1.1638(7)	0.0326(13)
H5	0.159048	0.910797	1.273086	0.039*

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Source of material

A mixture of CuBr (28.69 mg, 0.4 mmol), pyrazine-2-carboxylic acid (49.64 mg, 0.4 mmol) and distilled water (10 mL) was sealed in a 23 mL Teflon-lined steel vessel (solution pH 2.5) and heated at 160 °C for 72 h, and then cooled to room temperature at a rate of 0.05 °C min⁻¹. The resulting light turquoise block crystals of the compound were obtained and washed with distilled water. The yield is ca 37%. IR(KBr): 3257(s), 1598(s), 1519(s), 1496(s), 1445(s), 1359(s), 1246(s),

1176(s), 1116(s), 1075(s), 1001(s), 927(s), 899(s), 834(m), 771(m), 714(m), 616(m), 499(m)cm⁻¹.

Experimental details

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

Discussion

Supramolecular complexes, as an emerging class of hybrid materials, have attracted numbers of attention, due to not only their charming structures, but also the potential applications. In the process of design and synthesis, the rational combination of metal ions and the organic ligands are helpful to construct the target supramolecular complexes [4–9]. Pyrazine carboxylate as a multifunctional ligand is excellent for many architectures: firstly, the multidentate organic ligands containing *N*-heterocycle and the carboxylate group possess potential coordination nodes and the strong coordination ability which can form various metal-organic constructions; secondly, pyrazine carboxylate can act as proton donors and acceptors and may build high-dimensional supramolecular frameworks by hydrogen-bonding or π - π stacking interactions. To the best of our knowledge, several literatures have reported many complexes based on pyrazine carboxylic ligands [10–13].

As shown in the figure, one formula unit consist of one pyrazine carboxyl, two half Cu atoms and one bromine atom. Cu1 ion is in a slightly distorted square planar coordination environment, with two nitrogen atoms from two pyrazine carboxylic ligands and two oxygen atoms from carboxyl group. Cu2 is coordinated by two nitrogen atoms from pyrazine groups and one bromido ligand. The bond length of Cu1–N1 is 1.99 Å, while the bond length of Cu2–N2 is 2.00 Å. The Cu1 ion is more stable than the Cu2 ion. The bond length of Cu1–O1 and Cu1–O1A is 1.945 Å. The bond lengths of C1–O1 and C2–O2 are 1.264 Å and 1.263 Å, respectively. The formula unit is linked to an one-dimensional chain through the coordination of the Cu atoms. The coordination-mode of the organic title ligand is very similar to a related Ni(II) complex [14].

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