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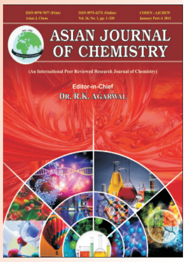

NOTE

Hydrothermal Synthesis and Crystal Structure of [Pyridine-2,6-dicarboxylato-\k: N,O,O'](pyrrole-\k:N)]copper(II)

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One new copper complex of $CuCl_2\cdot 4H_2O$, pyrrole and pyridine-2,6-dicarboxylic acid has been successfully synthesized. The complex shows a one-dimensional framework. The 1D supramolecular structure is formed *via* hydrogen bonding connection.

Keywords: Coordination polymer, Crystal structure, Copper(II).

Metal organic frameworks (MOFs) have received much attention in the field of crystal engineering and supramolecular chemistry because of their diverse structures and promising applications in functional materials such as luminescent materials, gas adsorption and magnetism[1-4]. Hydrogen bonds are well suited for the design of polymeric arrangement and crystal engineering because of their important directional interactions and because they can interlink 1-D, or 3-D structures into higher-dimensionality systems[5,6].

All reagent and solvents employed were commercially available and used as received without further purification.

A mixture of $CuCl_2\cdot 4H_2O$ (0.1 mmol), pyrrole (0.1 mmol) and pyridine-2,6-dicarboxylic acid (0.1 mmol), disodium dipicolinate (0.2 mmol) and distilled water (30 mL) was heated in a 25 mL stainless steel reactor with a teflon liner 167 °C for 24 h, followed by slow cooling to room temperature. Blue crystals of the compound formed.

Detection method: Diffraction intensity data of the single crystal of the five compounds were collected on a Bruker SMART APEXII CCD diffractometer equipped with a graphite monochromated MoK_α radiation ($\lambda = 0.71073$ Å) by using a ω-scan mode. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHEXL 97[7]. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located by geometrically calculations and their positions and thermal parameters were fixed during the structure refinement. The crystallographic data and experimental details of structural analyses for coordination polymers are summarized in Table-1. Selected bond and angle parameters are listed in Table-2.

TABLE-2
SELECTED BOND LENGTHS (Å) AND ANGLES (°) FOR COMPLEX

Cu1—O1	2.0292 (17)	N1—C1	1.330 (2)
Cu1—N1	1.899 (3)	N1—C5	1.351 (3)
Cu1—N2	1.927 (3)		
N1—Cu1—N2	180.0	C1—N1—Cu1	118.49 (13)

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$C_{11}H_7N_2O_4Cu$	Z, Calculated density (mg/m^3)	4, 1.905
Formula weight	294.73	Absorption coefficient (mm^{-1})	2.134
Crystal system space group	Monoclinic, C2/c	F(000)	592
Unit cell dimensions	a = 8.236 (4) Å	Limiting indices	$-9 \le h \le 9$
	b = 12.736 (6) Å		$-15 \le k \le 15$
	c = 9.799 (9) Å		$-11 \le l \le 11$
Volume (Å^3)	1027.4 (9)	Largest diff. peak and hole (e/Å^3)	0.541 and -0.263
θ range for data collection	2.95-25.49	Goodness-of-fit on F^2	1.102
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0258$ $wR_2 = 0.0750$	R indices (all data)	$R_1 = 0.0270$, $wR_2 = 0.0764$

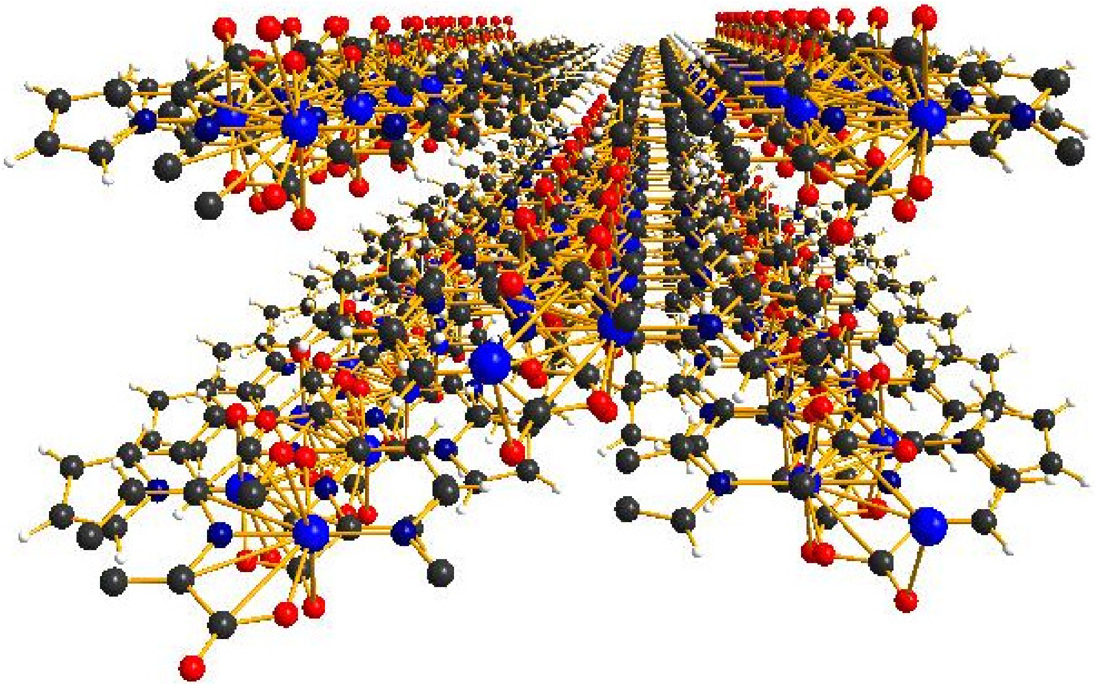

Fig. 2. 1D structure formed *via* hydrogen bonding interactions

Molecular structure of the title compound is shown in Fig. 1.

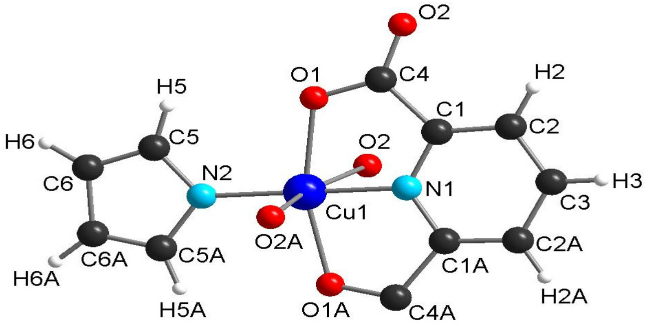

Fig. 1. Molecular structure of the title compound at 30 % probability displacement ellipsoids

X-ray diffraction analysis revealed that the fundamental building unit consists of two carboxylate groups in ortho-positions with respect to the pyridine N atom, is potentially tridentate. The copper ion is bonded to the pyridine N atom, the Cu1-N1 bond length are 1.899 (3) Å, as well as to one O atom of each carboxylate group the Cu1-O1 bond length are 2.0292 (17) Å. The chains are further assembled by the intermolecular hydrogen bonding interaction leading to the formation of a 1D framework (Fig. 2).

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