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Synthesis and crystal structure of new copper(II) metal complex: Noncovalent interactions and electrical conductance properties

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ABSTRACT

$[Cu(pydc)(apyz)(H_2O)_2]$ (**1**) (where $pydcH_2$ = pyridine-2,6-dicarboxylic acid; apyz = 2- aminopyrazine) has been synthesized and characterized by elemental analysis, IR spectroscopy and single crystal X-ray diffraction techniques. Crystallographic analysis revealed that complex **1** has distorted octahedral geometry with $pydcH_2$ coordinated as tridentate ligands to metal ion through two oxygen atoms of each carboxylate group, nitrogen atom of the pyridine ring and the auxiliary ligand pyrazine nitrogen atom form basal plane and apical positions are occupied by two oxygen atoms of water molecules. In addition, the coordination compounds are connected by a variety of non covalent interactions like OH … π, lone pair … π, π … π and hydrogen bonds. The evaluation of these noncovalent interactions is useful for rationalizing their influence in the crystal packing. In addition, electrical current measured at room temperature on thin film before and after annealed is in the order of 229 μA and 246 μA respectively with bias voltage 1 V.

1. Introduction

"Crystal engineering" has grown and developed over the past 50 years as a natural outcome of the interplay between chemistry and crystallography and it deals with the control over the organization of molecular components in the solid state [1,2]. The physical and chemical properties of crystalline material strongly depend on how the constituent components are packed with respect to one another in solid state. Recently coordination frameworks with transition metal atoms have great attention to chemists not only due to their intriguing topologies, such as molecular cage, grid, honeycomb, catenane, ladder, rotaxane, but also due to their attractive properties and potential executions, such as gas storage, ion exchange, recognition, magnetism [3]. Crystals are assembled in spontaneous process in solution named self-assembly that proceeds through a sequences of molecular recognition events. Detection of robust recognition motif or a pattern of recognition is at the heart of gaining a control over the self-assembly process. This self-assembly event between a set of molecular constituents is the outcome of the mutual interaction through variety of forces those are in operation. Though hydrogen bonding [4–8] has been extensively exploited for the construction of various supramolecular architectures in solid state, other weaker forces such as π–π, lone pair-π, CH-π forces associated with aromatic-π systems have also been successfully employed in this regard [9–11].

The carboxylate based ligands have different binding modes and each of binding modes may have a vital role in the formation of supramolecular assembly which are vastly studied and reviewed [12]. The ligands having multiple carboxylic acid functionalities are good precursor for coordination polymers and supramolecular architectures [13]. Pyridine-2,6-dicarboxylic acid ($PydcH_2$) which contain a pyridine ring and two carboxylate groups can be a good synthon to serve such purpose. There are various reports on pyridine-2,6-dicarboxylic acid ($pydcH_2$) which revealed imperative characteristics of $pydcH_2$, such as low toxicity and its diversified biological activity being present in many natural products such as oxidative degradation product of vitamins, coenzymes, alkaloids [14]. $PydcH_2$ and complexation compounds of $pydcH_2$ with different metallic ions have also attracted much attention in designing and synthesis of such compounds because of their

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interesting topologies, promising structural features, enthralling functionalities which promote wide practical utility in photoluminescence, molecular adsorption and gas storage, catalysis and magnetism [15–19]. Their complexes have been also explored as electron carriers in some model bio-systems as specific molecular tools in DNA cleavage and as NO scavengers [14].

The most commonly used practice for engineering the crystal structure of pydcH$_2$ metal complexes to explicit complexation compounds' important properties; non-covalent intermolecular forces (hydrogen bonding, aromatic ring stacking *etc*) are employed [20–22]. However, although extensive studies have been done on this ligand according to a survey of the Cambridge Structural Data base (CSD, Version 5.36, update 2015) on supramolecular systems, it still remains a challenging task to find out more and more compounds with different topological networks. Current research also deals the influence of water content on the topologies of MOFs of very similar dicarboxylic acid and pyridine-3,5-dicarboxylate and metal ions under mild conditions [23,24]. On the other hand, carboxylate anion is well known as a ligand which can play an imperative role to construct novel MOFs in coordination chemistry. They generally adopt different types of binding modes like bridging didentate in a syn-syn, syn-anti, and anti-anti configuration to metal ions, terminal monodentate, chelating to one metal ions, and bridging tridentate to two metal ions [25].

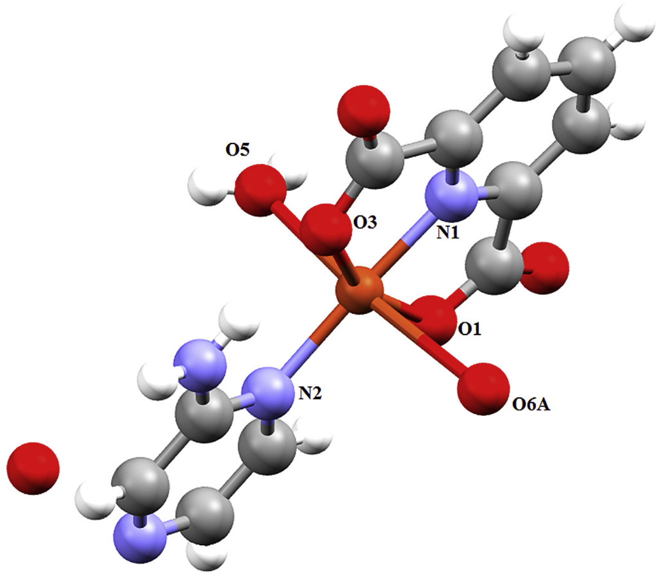


Fig. 1. The molecular structure of **1**.

Table 1
Experimental data for crystallographic analysis of complex **1**.

Compound	**1**
Empirical formula	$C_{11}H_{10}CuN_4O_6$
Formula weight	357.78
Temperature (K)	150(2)
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	6.3410(5)
b (Å)	7.0001(6)
c (Å)	15.9946(13)
α (°)	83.766(6)
β (°)	84.892(6)
γ (°)	71.106(5)
Volume (Å^3)	666.64(10)
Z	2
Density$_{cal}$ (Mg m^{-3})	1.782
Absorption coefficient (mm^{-1})	1.676
F(000)	362
Independent reflections [R$_{int}$]	2685 [R(int) = 0.041]
Data/restraints/parameters	2685, 0, 202
Reflections collected	7251
Final R indices	R1 = 0.0714,
[I > 2σ (I)]	WR2 = 0.2022
Largest difference peak and hole (eÅ^{-3})	−0.66, 2.06

Table 2
Selected bond distances (Å) and angles (°) data for **1**.

Selected Bonds	(Å)	Selected Angles	(°)
Complex 1	2.031(5)	O1–Cu1–O3	160.43(18)
Cu1–O1	2.010(5)	O1–Cu1–O5	91.22(19)
Cu1–O3	2.356(6)	O1–Cu1–N1	80.2(2)
Cu1–O5	1.904(5)	O1–Cu1–N2	98.9(2)
Cu1–N1	1.992(5)	O1–Cu1–O6A_b	86.86(17))
Cu1–N2	2.625(5)	O3–Cu1–O5	91.57(19)
Cu1–O6A_b		O3–Cu1–N1	80.5(2)
		O3–Cu1–N2	100.3(2) 88.45(17)
		O3–Cu1–O6A_b	90.0(2)
		O5–Cu1–N1	92.6(2)
		O5–Cu1–N2	174.23(18)
		O5–Cu1–O6A_b	177.3(2)
		N1–Cu1–N2	84.33(18)
		O6A_b-Cu1-N1	93.09(19)
		O6A_b-Cu1-N2	

Translation of Symmetry Code to Equiv.Pos, b = [1565.00] = x,1 + y,z.

In this endeavor, in constructing new supramolecular architectures *via* cooperative weak noncovalent interactions in the solid state, the X-ray structure analysis were undertaken. For further understanding of the structure formation principles that direct the interactions of the proposed structure and conductivity of the title structure are presented here.

2. Experimental methods

2.1. General methods and materials

All reagents and chemicals (including Cu(ClO$_4$)$_2$·6H$_2$O) were of AR grade and procured from commercial sources (SD Fine Chemicals, India; and Aldrich) and used without further purification.

2.2. Physical measurements

IR spectra were recorded in the region 4000–400 cm^{-1} using a Perkin–Elmer model 883 infrared spectrophotometer. Elemental analyses (C, H and N contents) were carried out using a Perkin–Elmer CHN analyzer 2400 at the Indian Association for the Cultivation of Science, Kolkata. Current (I) - Voltage (V) measurement at room temperature were taken before and after annealed by a Keithley 2611 A source meter and Lab Tracer 2.0 software was used to collect the electrical data.

2.3. Synthesis

(1). Synthesis of [Cu(pydc)$_2$(apym)]·3H$_2$O

An aqueous solution of Cu(ClO$_4$)$_2$·6H$_2$O (4 mmol, 1.48 g) was

Table 3
Details of hydrogen bond distances (Å) and angles (°) for **1**.

D H···A	d(D H)	d(H···A)	d(D···A)	<(DHA)
N4 – H4A ... O3	0.8800	1.8600	2.690(8)	156.00
N4 – H4B ... O6A	0.8800	2.1300	2.970(8)	158.00
O5 – H5A ... O2	0.7600	2.1900	2.817(7)	141.00
O5 – H5B ... O4	0.8700	1.9500	2.802(8)	169.00

D, donor; H, hydrogen; A, acceptor.

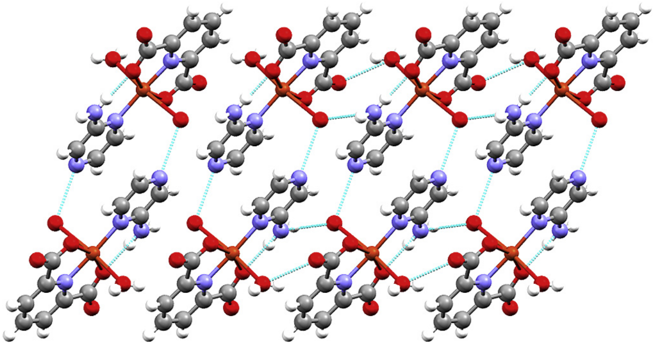


Fig. 2. 2D architecture of H bonding interaction in **1**.

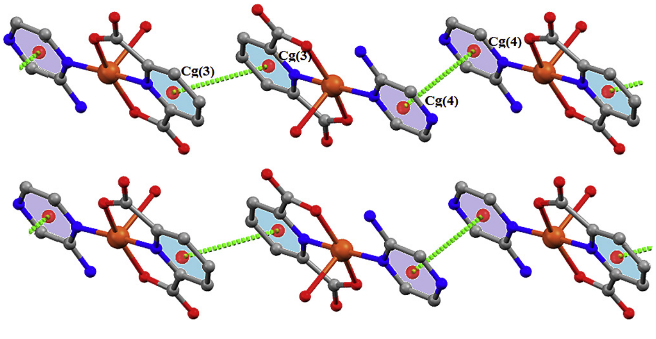


Fig. 3. 1D supramolecular chain generated through π … π interactions (H_2O molecules and H atoms are omitted for clarity).

added to an aqueous solution of pyridine-2,6-dicarboxylic acid (pydcH_2) (4 mmol, 0.67 g) and 2-aminopyrazine (apyz) (4 mmol, 0.38 g) under stirring at 60 °C for 3 h. Green colored crystals were obtained by slow evaporation of the reaction mixture at room temperature. Elemental analysis: anal. calc. for C_{11} $H_{10}CuN_4O_6$: C, 36.89; H, 2.79; N, 15.65. Found: C, 36.85; H, 2.77; N, 15.69%. IR bands (KBr pellet, cm^{-1}): 3410, 3014, 1642, 1701, 1451, 1330, 747.

2.4. X-ray crystallography study

Selected crystal data for complex **1** is given in Table 1 and selected metrical parameter of the complex is given in Table 2. For **1** data collections were made using Bruker SMART APEX II CCD area detector equipped with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) source in φ and ω scan mode at 150(2) K. Cell parameters refinement and data reduction were carried out using the Bruker SMART APEX II. Cell parameters refinement and data reduction were carried out using Bruker SMART [26] and Bruker SAINT softwares for all the complexes. The structure of all the complexes were solved by conventional direct methods and refined by full-matrix least square methods using F2 data. SHELXS-97 and SHELXL-97 programs [27] were used for structure of all the complexes solution and refinement respectively. All hydrogen atoms were located from a difference Fourier map and refined isotropically. In **1**, one oxygen atom is disordered over two positions and hydrogen atom cannot be located for O6 from the difference Fourier map.

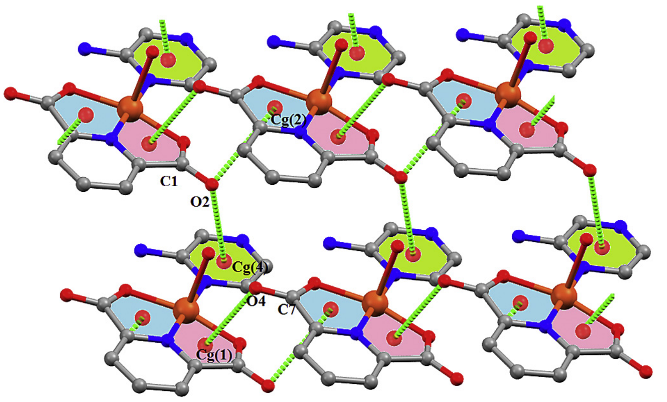


Fig. 4. 2D supramolecular architecture generated through lone pair … π interactions (H_2O molecules and H atoms are omitted for clarity).

2.5. Device fabrication for electrical conductivity measurement

To measure the electrical conductivity of the as prepared sample thin film was done by simple drop casting method on a glass substrate. This glass substrate was placed on a hot plate at the time of drop casting to evaporate the solvent to which synthesized material was dissolved. Two parallel electrodes were depicted on the thin film with average separation ~ 4 mm by silver paint (Ted Pella). To measure the I/V characteristics of the thin film, two electrodes were connected with Keithley 2611 A Source Meter and data was accumulated by Lab Tracer acquisition card.

3. Results and discussion

3.1. Crystal structure description of 1

The molecular structure of 1 is shown in Fig. 1 and selected bond lengths and angles are summarized in Table 2. The asymmetric unit consists of a neutral Cu(II) complex ligated by one hypydc unit, one 2-amino-pyrazine and two water molecules together with one uncoordinated water molecule (O_4N_2 environment).

Table 5
Geometric features (distances in Å and angles in degrees) of the lone pair…π interaction obtained for **Complex 1**.

Complex	C–H…Cg(Ring)	H…Cg (Å)	C–H…Cg (°)	C…Cg (Å)	Symmetry
Complex 1	C1–O2…Cg2	3.314(5)	102.1(3)	3.779(6)	1 + X,Y,Z
	C1–O2…Cg4	3.374(5)	3.159	3.808(7)	X,1 + Y,Z
	C7–O4…Cg1	3.358(6)	3.189	3.772(7)	−1+X,Y,Z

For complex 1, Cg(1) = centre of gravity of ring [Cu1–O1–C1–C2–N1], Cg(2) = centre of gravity of ring [Cu1–O3–C7–C6–N1], Cg(4) = centre of gravity of ring [N2–C8–C9–N3–C10–C4].

Table 4
Geometric features (distances in Å and angles in degrees) of the π…π interactions obtained for **Complex 1**.

Complex	Cg(Ring I)…Cg(Ring J)	Cg…Cg	Cg(I)…Perp	Cg(J)…Perp	α	β	γ	Symmetry
Complex 1	Cg3…Cg3	3.931(4)	3.411	3.411	0.02	29.79	29.79	-X,2-Y,-Z
	Cg4…Cg4	3.658(4)	3.628	3.628	0.02	7.33	7.33	1-X,2-Y,1-Z

α = Dihedral angle between ring I and ring J (°); β = Cg(I)– > Cg(J) or Cg(I)– > Me vector and normal to plane I (°); γ = Cg(I)– > Cg(J) vector and normal to plane J (°); Cg-Cg = Distance between ring Centroids (Å); CgI—Perp = Perpendicular distance of Cg(I) on ring J (Å); CgJ—Perp = Perpendicular distance of Cg(J) on ring I (Å); Cg(3) = centre of gravity of ring [N1-C2-C3-C4-C5-C6] and Cg(4) = centre of gravity of ring [N2-C8-C9-N3-C10-C4].

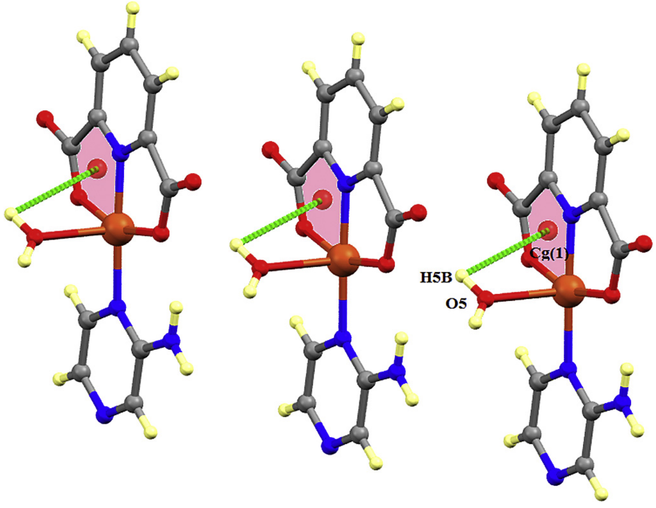


Fig. 5. OH … π interaction involved in discrete molecule.

Table 6
Geometric features (distances in Å and angles in degrees) of the OH…π interaction obtained for **Complex 1**.

Complex	C–H…Cg(Ring)	H…Cg (Å)	C–H…Cg (°)	C…Cg (Å)	Symmetry
Complex 1	O5–H5B…Cg1	2.82	86	2.893(6)	X,Y,Z

For complex 1, Cg(1) = centre of gravity of ring [Cu1–O1–C1–C2–N1].

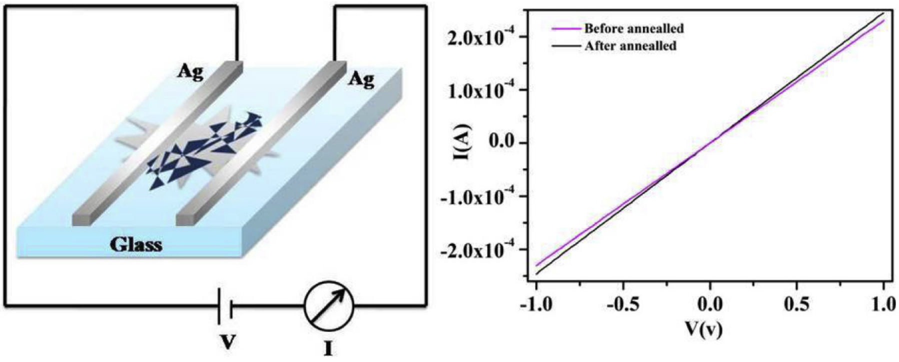
The coordination geometry of the Cu-atom can be described as distorted octahedral geometry with the basal plane defined by one N atom and two O atoms from the deprotonated pyridine-2,6-dicarboxylate ligand and one ring N atom from the 2-amino-pyrazine ligand and two water molecules in the apical position. Intra ligand bond lengths and angles are in the range expected for these coordinated ligands. As we expected the axial bond (average 2.485 Å) is longer than the others and it can be attributed to Jahn–Teller effect. It should be noted that the Cu1–N2 bond (1.992 Å) is longer than the Cu1–N1 bond (1.904 Å) which is likely due to the geometrical constraints of the hypydc ligand. A detailed analysis of the crystal structure of **1** revealed the presence of hydrogen bonding interactions in the solid state leading to the formation of extended 2D chains (Table 3) (Fig. 2. Complex **1** exhibits strong intramolecular N–H⋯O hydrogen-bonding interactions between the coordinated carboxylate oxygen atom and the noncoordinated $-NH_2$ group of amino pyrimidine ligand. In the 2D chain, each 1D chain is further connected to the neighbouring 1D chain by intermolecular hydrogen-bonding interactions.

3.2. *Noncovalent interactions*

The complex shows different kinds of weak interactions apart from H-bonding are π … π, lone pair … π and O–H … π in solid state structure that contributes to the self assembly process. The formation of a supramolecular 1D chain is ensured mainly by two additional π … π interactions (Fig. 3)) (Table 4). Firstly, the aromatic ring N1–C2–C3–C4–C5–C6 is stacked over the same aromatic ring of a neighbouring molecule of symmetry -X, 2-Y,-Z (3.931(4) Å). Secondly, the aromatic ring N2–C8–C9–N3–C10–C4 is stacked over same the aromatic ring of neighbouring molecule of symmetry 1-X,2-Y, 1-Z (3.658(4) Å). The solid state packing of compound **1** presents a relevant lp … π noncovalent interactions (Fig. 4) (Table 5) that is formed between the non coordinating carboxylate oxygen atom (O2) with the chelate ring Cg(2) Cu1–O3–C7–C6–N1 (Symmetry 1 + X,Y,Z) and the aromatic ring Cg(4) N2–C8–C9–N3–C10–C4 (Symmetry X, 1 + Y,Z.) of symmetry related moiety. Secondly, another the non coordinating carboxylate oxygen atom (O4) creates interaction with the chelate ring Cg(1) Cu1–O1–C1–C2–N1 (Symmetry −1+X,Y,Z). Two types of interactions create a 2D crystalline supramolecular architecture. These distances are very short indicating a strong interaction. Another kind of noncovealent interaction like O–H … π is involved in **1** (between noncoordinating N5–H5B group and chelate ring Cg(12) defined by Cu1–O1–C1–C2–N1 (symmetry X,Y,Z) to form discrete molecule with closest distance of 2.82 Å (Fig. 5) (Table 6).

3.3. *Device fabrication and the measurement of electrical conductivity*

I–V characteristic of the thin film from −1 to +1 V shown perfect symmetric and linear characteristics is depicted in Fig. 6 (a) and (b). I–V characteristics of the film was recorded before and after annealed at 60 °C for half an hour and no significant change was observed which prove that the conductivity of the material is responsible only due to bulk of the polymer not depends on contact bias. Even no improvement was found further continuation of annealing process that again confirmed the conductivity of the coordination polymer only. The Current level increases from 229 μA to 246 μA after annealed having shown in Fig. 6 (b). These values of conductivity level relatively better than that of metal-metal based coordination type polymer and this conductivity of the polymer arises due to the delocalised of carboxylate anions at ambient temperature involved with it [25,28].



(a) (b)

Fig. 6. (a) Schematic diagram of the device for measurement of electron transport, (b) Current – Voltage characteristics of the film realized with the compound **1**.

4. Conclusion

In summary, $[Cu(pydc)_2(apyz)]\cdot 3H_2O$ (**1**) (where, $pydcH_2$ = pyridine-2,6-dicarboxylic acid; apyz = 2-aminopyrazine) coordination polymer based on pyridine-2,4-dicarboxylic acid are synthesized and its supramolecular aspects are studied. In the synthesized metal ligand framework various supramolecular interactions, like H-bonding, lone pair … π, OH … π and π … π interactions are present and these imperative interactions play crucial roles in the construction of extended networks in the synthesized metal ligand framework. The above study of non covalent interactions of metal ligand frame work along with water molecules may disclose to analyze various biological processes. It may also reveal the role of ordered water in biological systems that often bear carboxylate and amino groups. Electrical conductivity of the coordination complex is prepared on glass substrate as a thin film show ohmic in nature and conductivity is responsible only due to coordination of proper metal ligand connectivity. We may also conclude that a significant part of conductivity level arises from metal ions of compound. Many features of this coordination compound, such as biological studies and magnetic properties, remain to be investigated as we intend to do in the near future.

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Appendix A. Supplementary data

CCDC 1551756 contains the supplementary crystallographic data for **1**. These data can be obtained free of charge *via* http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

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