Exploration of Cl···Cl and π···π stacking contacts along with conductivity properties of a Cu-MOF featured with paddle-wheel SBUs

Sanobar Naaz,[a] Pubali Das,[b] Souvik Mukherjee,[c] Samim Khan,[a] Goutam Pramanik,[d] Prasanta Ghosh,[c] Antonio Frontera,*[e] Partha Pratim Ray*[b] and Mohammad Hedayetullah Mir*[a]

[a]Department of Chemistry, Aliah University, New Town, Kolkata 700 160, India.

[b]Department of Physics, Jadavpur University, Jadavpur, Kolkata 700 032, India.

[c]Department of Chemistry, R. K. M. Residential College, Narendrapur, Kolkata 700 103, India

[d]UGC-DAE CSR, Kolkata Centre, Sector III, LB-8, Bidhan Nagar, Kolkata 700 106, India.

[e]Departament de Química, Universitat de les Illes Balears, Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), Spain.

To whom correspondence should be addressed. E-mail: toni.frontera@uib.es; partha@phys.jdvu.ac.in and chmmir@gmail.com

Supporting Information

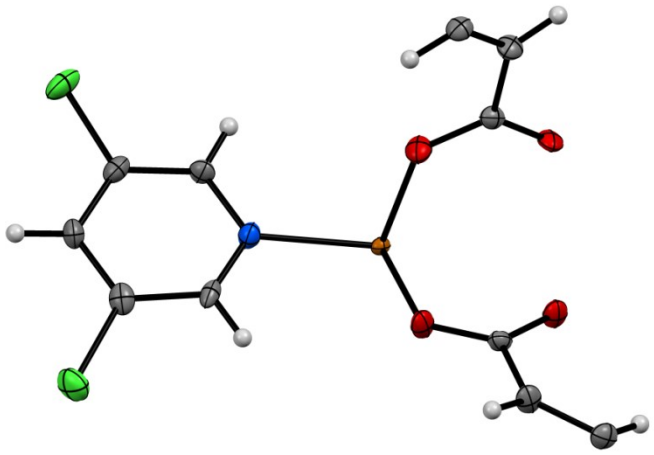

Fig. S1 Asymmetric unit of compound **1** with 30% ellipsoid plot. Carbon: black; nitrogen: blue; oxygen: red; hydrogen: grey; copper: brown.

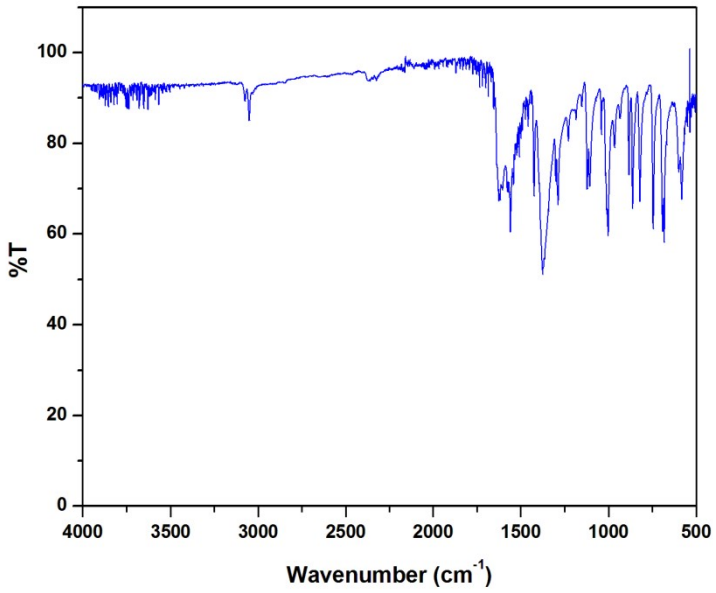

Fig. S2 IR spectrum of compound **1**.

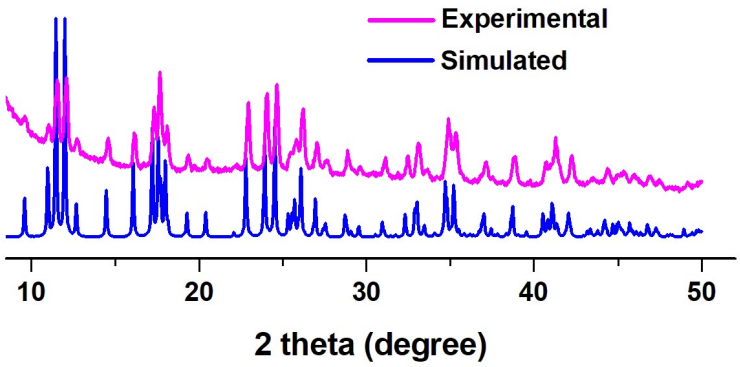

Fig. S3 PXRD data of simulated **1** (blue) and as-synthesized **1** (pink).

Table S1 Crystal data and refinement parameters of compound **1**

Formula	$C_{11}H_7Cl_2CuNO_4$ **(1)**
fw	351.63
cryst syst	Triclinic
space group	$P\bar{1}$
a (Å)	7.8327(11)
b (Å)	8.7671(13)
c (Å)	10.3665(15)
α(deg)	109.953(6)
β(deg)	105.723(6)
γ (deg)	95.799(7)
V (Å^3)	629.20(16)
Z	2
D_{calcd}(g/cm^3)	1.856
μ(mm^{-1})	2.167
λ(Å)	0.71073
GOF on F^2	1.021
Final*R* indices [$I > 2\sigma(I)$][a,b]	*R*1= 0.0841 *wR*2= 0.2653

[a]$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b]$wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths and bond angles of **1**

Bond length (Å)	
Cu(1)-O(1)	1.971(8)
Cu(1)-O(3)	1.977(9)
Cu(1)-N(1)	2.173(9)
Cu(1)-O(2)a	1.991(8)
Cu(1)-O(4)a	1.973(9)
Bond angle (°)	
O(1)-Cu(1)-O(3)	90.0(4)
O(1)-Cu(1)-N(1)	100.2(4)
O(1)-Cu(1)-O(2)a	168.7(3)
O(1)-Cu(1)-O(4)a	89.8(4)
O(3)-Cu(1)-N(1)	94.6(4)
O(2)a-Cu(1)-O(3)	89.4(4)
O(3)-Cu(1)-O(4)a	168.2(4)
O(2)a-Cu(1)-N(1)	91.1(3)
O(4)a-Cu(1)-N(1)	97.0(4)
O(2)a-Cu(1)-O(4)a	88.5(4)

Symmetric transformation: a = 1-x, 1-y, 1-z

Table S3 π···π interactions in **1**

Ring(I) → Ring(J)	Distance between the (i,j) ring centroids (Å) in the crystal
R(1)→R(1)a	3.549(7)

R(J) denotes the j-th ring: R(1) = N(1)-C(1)-C(2)-C(3)-C(4)-C(5);
Symmetry transformation: a = 1-x, 2-y, 2-z

Table S4 Cl···Cl interactions in **1**

X···X	(Å)
Cl(1)....Cl(2)a	3.670
Cl(2)....Cl(1)a	3.670
Cl(2)....Cl(2)b	3.670

Symmetry transformation: a = 1-x, 2-y, 2-z; b = -x, 2-y, 2-z

Table S5 A comparison of conductivity result of **1** with reported CPs.

MOFs	**Conductivity (S m^{-1})**	**Reference**
[Cu(muco)(3,5-DCP)]$_n$	6.02×10^{-3}	**This work**
[Cd(4-bpd)(SCN)$_2$]$_n$	2.90×10^{-4}	1
{[Cd$_2$(azbpy)$_2$(HO-1,3-bdc)$_2$](azbpy)·(H$_2$O)}$_n$	186	2
Zn(OPE-C$_{12}$)·2H$_2$O	9.6×10^{-4}	3
{[Zn(5-NIP)$_2$(INH)$_2$].(DMF)(H$_2$O)$_2$}$_n$	3.35×10^{-4}	4
{[Cd(5-NIP)$_2$(INH)$_2$].(DMF)$_2$(H$_2$O)]}$_n$	5.04×10^{-4}	4
[Zn$_4$(μ$_4$-O)(DABA)$_6$]	2.29×10^{-7}	5
[Zn$_2$(DABA)$_4$(4,4′-BPY)]$_n$	2.54×10^{-3}	5
[Cu(5-nip)(3-Clpy)$_2$]$_n$	1.58×10^{-3}	6
[Cu(5-nip)(3-Brpy)$_2$]$_n$	7.25×10^{-4}	6

References

1. S. Halder, A. Dey, A. Bhattacharjee, J. Ortega-Castro, A. Frontera, P. P. Ray and P. Roy, *Dalton Trans.,* 2017, **46**, 11239-11249.
2. B. Bhattacharya, A. Layek, M. M. Alam, D. K. Maity, S. Chakrabarti, P. P. Ray and D. Ghoshal, *Chem. Commun*., 2014, **50**, 7858-7861.
3. S. Roy, M. Das, A. Bandyopadhyay, S. K. Pati, P. P. Ray and T. K. Maji, *J. Phys. Chem. C*, 2017, **121**, 23803-23810.
4. K. Naskar, A. Dey, S. Maity, P. P. Ray and C. Sinha, *Cryst. Growth Des*., 2021, **21**, 4847-4856.
5. S. Jana, J. Datta, S. Maity, B. Thakurta, P. P. Ray and C. Sinha, *Cryst. Growth Des.*, 2021, **21**, 5240–5250.
6. S. Naaz, P. Das, A. Frontera, B. Dutta, S. Khan, P. P. Ray and M. H. Mir, *Cryst. Growth Des*., 2022, **22**, 5189-5197.