Supplementary Data

A new lead-free 1D hybrid copper perovskite with structural, thermal, vibrational, optic and magnetic characterizations

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Thermal properties

The TGA plot shows that the decomposition of the precursor proceeds through two stages. The studied compound is stable up to about 182°C. At this temperature until 249°C we observe the first weight loss of 11.2%, in agreement with the departure of one chloride ion as HCl due to atmospheric moisture (theoretical weight loss of 11.5%) [1]. This decomposition process is accompanied by two endothermic peaks on the DTA curve at 213 and 237°C, respectively. The second transformation occurs in the temperature range 248–452°C (observed mass loss 54.32%, calculated mass loss 52.2%) which can be assigned to the degradation of the organic fragment ($C_5H_{12}N_2$) and the departure of one additional molecule of hydrogen chloride, leading most likely to the formation of $CuCl_2$. This decomposition process is accompanied by an intense endothermic peak on the DTA curve at 337°C.

Table S1: Experimental conditions and data collection of the $(C_5H_{14}N_2)[CuCl_4]$ crystal.

Empirical formula	$(C_5H_{14}N_2)[CuCl_4]$
Formula weight (g/mol^{-1})	307.52
Space group	$P\,2_1/n$
Crystal system	Monoclinic
a(Å)	6.0751(3)
b(Å)	15.6732(8)
c (Å)	12.0466(7)
ß (°)	98.521(2)
V(Å^3)	1134.37(10)
Z	4
Crystal size (mm^3)	0.41 × 0.03 × 0.02
Crystal color and shape	Yellow thin stick
λ (MoKα) $(Å)$	0.71073
Absorption correction	Multi-scan
Transmission factors	0.945, 0.754
hkl range	$-7 \leq h \leq 7$
	$-20 \leq k \leq 20$
	$-15 \leq l \leq 15$
Programs system	SHELXL-2018 and SHELXT-2015
θ range for data collection (deg)	3.11-27.48
Diffractometer	D8 VENTURE Bruker AXS
No. of reflection collected	9644
No. of independent reflection	2608
No. of reflections observed (I >2σ(I))	2341
Rint	0.0294
No. of parameters	121
Goodness of fit	1.09
R indices (I >2σ(I))	R_1= 0.0388 wR_2= 0.1013
R indices (all data)	R_1= 0.0433 wR_2= 0.1042

Table S2: Structural parameters of $(C_5H_{14}N_2)[CuCl_4]$, (Distances in Å and angles in °).

CuCl$_6$ octahedron anion		C$_5$H$_{14}$N$_2$ organic cation	
Cu-Cl1	2.3383(8)	C1-C2	1.452(7)
Cu-Cl2	2.2838(8)	C2-C3	1.523(6)
Cu-Cl3	2.3323(8)	C4-C6	1.506(5)
Cu-Cl4	2.2585(9)	N1-C1	1.482(5)
Cu-Cl2^i	3.0570(9)	N1-C5	1.494(4)
Cu-Cl2^{ii}	3.0442(9)	N2-C3	1.493(5)
Cl1-Cu-Cl2	88.96(3)	N2-C4	1.489(4)
Cl1-Cu-Cl3	177.83(3)	C1-C2-C3	117.8(4)
Cl1-Cu-Cl4	90.45(3)	C2-C1-N1	116.5(4)
Cl2^{ii}-Cu-Cl3	89.54(3)	C1-N1-C5	116.3(3)
Cl2-Cu-Cl4	179.25(4)	C4-N2-C3	118.9(3)
Cl3-Cu-Cl4	91.05(3)	N1-C5-C4	114.3(2)
Cl1-Cu-Cl2^i	88.80(3)	N2-C4-C5	113.3(3)
Cl2^i-Cu-Cl2	84.62(1)	N2-C3-C2	115.6(3)
Cl3-Cu-Cl2^i	89.50(3)		
Cl4-Cu-Cl2^i	95.84(3)		
Cl2^{ii}-Cu-Cl2^i	169.38(3)		
Cl1-Cu-Cl2^{ii}	90.03(3)		
Cl2^{ii}-Cu-Cl2	84.80(3)		
Cl3-Cu-Cl2^{ii}	91.40(3)		
Cl4-Cu-Cl2^{ii}	94.73(3)		

Symmetry codes : (i) 1-x, 1-y, 1-z ; (ii) -x, 1-y, 1-z

Table S3: Hydrogen bonding data

D-H...A	D-H	H...A	D...A	D-H...A
N1-H1A.... Cl1[iii]	0.91	2.34	3.165(3)	150.7
N1-H1B ....Cl1[iv]	0.91	2.36	3.219(3)	157.6
N2 - H2A....Cl3[ii]	0.91	2.27	3.169(3)	169.3
N2 - H2B....Cl1	0.91	2.81	3.277(3)	113.0
N2 - H2B....Cl2	0.91	2.55	3.117(3)	120.7
N2 - H2B....Cl3[i]	0.91	2.47	3.186(3)	135.6

Symmetry codes : (i)   1-x, 1-y, 1-z ; (ii) -x, 1-y, 1-z ; (iii) x-1/2, -y+1/2, z+1/2 ;

(iv) x+1/2, -y+1/2, z+1/2

Table S4: IR band assignment of $(C_5H_{14}N_2)[CuCl_4]$

IR	Assignment*
3390	$\nu_a\,(NH_2)$
3036	$\nu_s(NH_2)$
2849	$\nu(CH_2)$
1634	$\delta(NH_2)$
15531	$\delta(CH_2)$
1445	$\omega(NH_2)$
1411	$\omega\,(CH_2)$
1323	$\nu(C\text{-}N)$
1125	$\nu(C\text{-}N)$
1069	$\nu_a\,(C\text{-}C)$
1027	$\nu_s\,(C\text{-}C)$
972	$\rho(NH_2)$
864	$\delta(C\text{-}C\text{-}C)$
767	$\delta(C\text{-}C\text{-}N)$
417	$\delta\,(C\text{-}N\text{-}C)$

*υ: stretching. υ_a: asymmetric stretching. υ_s: symmetric stretching. δ: scissoring. ω: wagging.

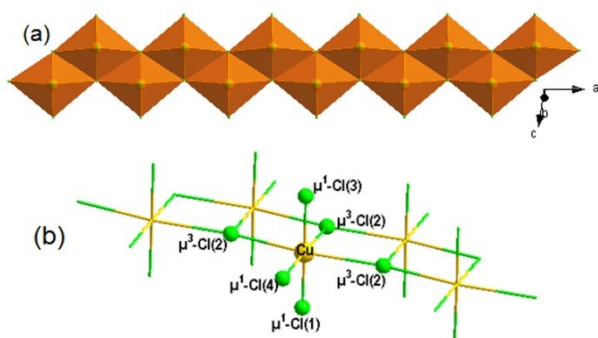1   D. B. Mitzi, *Chem. Mater.*, 1996, **8**, 791–800.

Figure S1: Description of a single inorganic chain. (a) Projection of a single chain along [010]. (b) Description of Cl ions environment
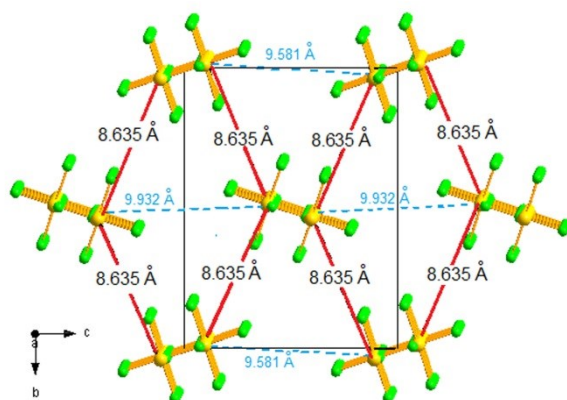

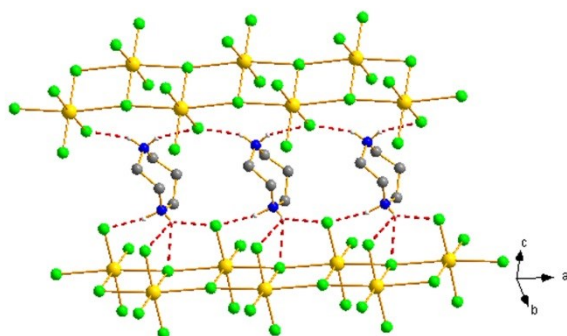**Figure S2:** Inter-chains distances in different direction in the (b, c) plan.

Figure S3: Hydrogen bonds between organic and inorganic frameworks (H...Cl represented as dashed red lines).
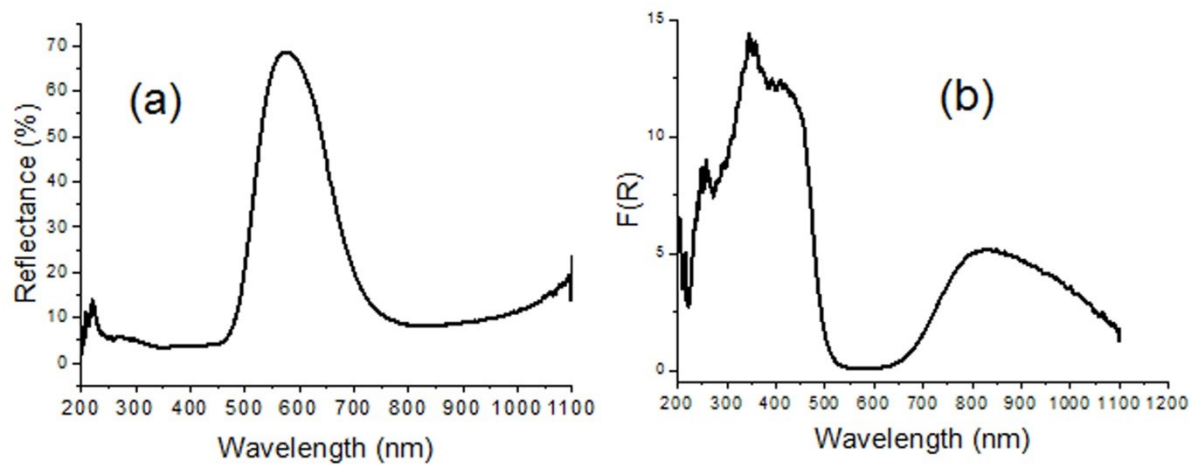
Figure S4: (a) Reflectance and (b) K-M absorption of $(C_5H_{14}N_2)[CuCl_4]$.