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Supplementary Data

Optical and magnetic characterizations of one-dimensional Cu(II)-based perovskite: A high UV-Vis-NIR absorber

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Table S1. Crystal data and refinement parameters of $(C_5H_8N_3)[CuCl_3]$.

Empirical formula	$C_5H_8N_3CuCl_3$
Formula weight (g.mol-1)	560.07
Wavelength	0.71073
Temperature (K)	124.8(4)
Crystal system	Triclinic
Space group	P–1
a (Å)	3.9057(6)
b (Å)	10.3349(13)
c (Å)	11.3405(15)
α (°)	94.842(11)
β (°)	93.385(11)
γ (°)	90.039(11)
V (Å3)	455.32(11)
Z	2
Calculated density (mg/m3)	2.043
Absorption coefficient (mm-1)	3.222
F(000)	278
Crystal size (mm3)	0.3 x 0.3 x 0.3
θ range for data collection (°)	3.612 to 24.997
h,k,l range	$-4 \leq h \leq 4$; $-12 \leq k \leq 9$; $-13 \leq l \leq 13$
Reflections collected/independent	3079/3079 (Rint =0.0551)
Absorption correction	Semi-empirical from equivalents
Transmission factors	Tmin=0.74469, Tmax=1.00000
Number of parameters	110
Goodness of fit (F2)	1.034
R1	0.1049
wR2 (I>2σ(I))	0.2434
Extinction coefficient	n/a
Largest diff. peak and hole (e.Å-3)	1.687 and –0.957

Table S2. Geometric data (Å/°) of the inorganic fragment

Cu-Cl distances (Å)		**Cl-Cu-Cl angles (°)**	
Cu1–Cl1	2.269(2)	Cl1–Cu1–Cl2	96.80(8)
Cu1–Cl2	2.239(2)	Cl1–Cu1–Cl3	91.10(8)
Cu1–Cl3	2.294(2)	Cl1–Cu1–Cl3^{A}	173.55(9)
Cu1–Cl3^{A}	2.310(2)	Cl2–Cu1–Cl3	170.72(8)
Cu–Cl1^{iii}	3.013(2)	Cl2–Cu1–Cl3^{A}	89.40(8)
Cu–Cl3^{iv}	3.082(2)	Cl3–Cu1–Cl3^{A}	82.57(8)
		Cu1–Cl3–Cu1^{A}	97.43(8)

Symmetry code : (A) -x+1, -y, -z; iii: 1+x, y, z; iv: -x, -y, -z.

Table S3. Hydrogen-bond properties

D–H···A	**d(D···A)(Å)**	**d(H…A) (Å)**	**∠D–H···A(°)**
N3–H3NA···N2^{B}	3.014(10)	2.16	176
N3–H3NB···Cl1^{i}	3.257(8)	2.41	169
N1–H1N···Cl2^{i}	3.085(7)	2.29	153

Symmetry codes: B: -1-x, -1-y, 1-z; i: x, -1+y, z;

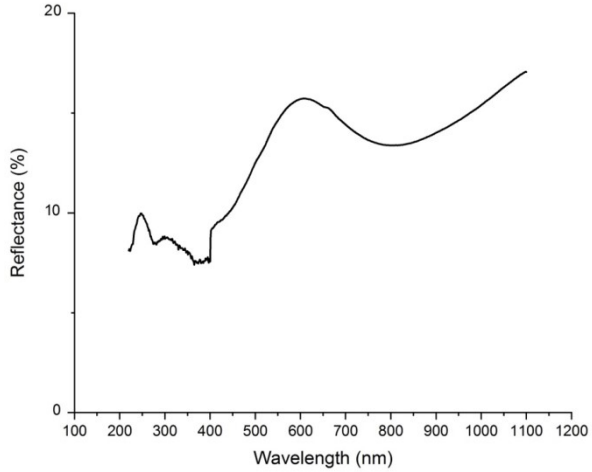

Figure S1 : Diffuse reflectance spectrum of $(C_5H_8N_3)[CuCl_3]$.

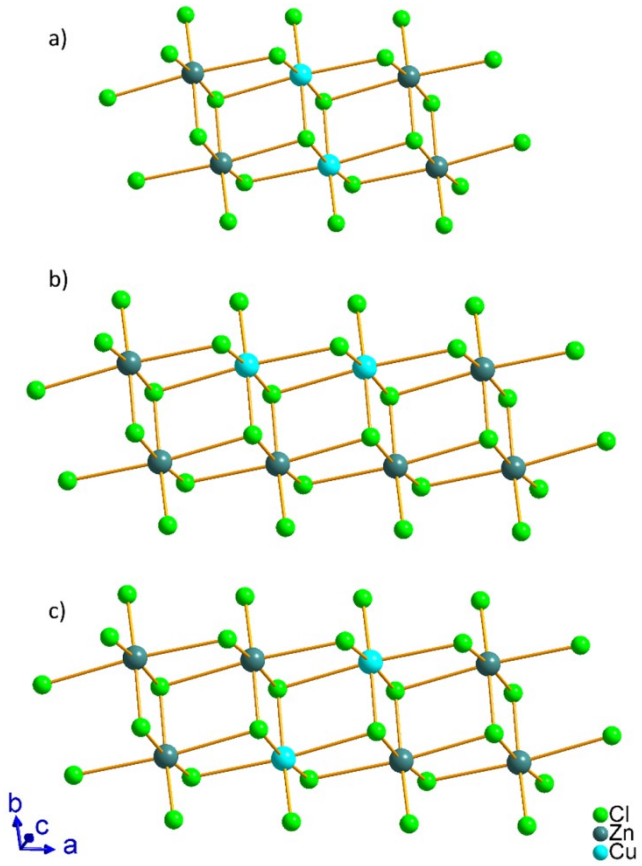

Figure S2: Model fragments used for BS DFT calculation of the rung (a), leg (b), and frustrating (c) exchange interaction in $(C_5H_8N_3)[CuCl_3]$.