Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

## **Electronic supplementary information**

for

## Room temperature ferroelectric copper(II) coordination polymers based on amino acid hydrazide ligands

Andreas Puškarić<sup>1</sup>, Marko Dunatov<sup>1</sup>, Ivanka Jerić<sup>1</sup>, Igor Sabljić,<sup>1,2</sup> and Lidija Androš Dubraja<sup>1,\*</sup>

<sup>1</sup>Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia <sup>2</sup>Department of Molecular Sciences, Swedish University of Agricultural Sciences, Uppsala, SE-75651, Sweden

Email: Lidija.Andros@irb.hr



Figure S1. Room temperature XRD pattern and profile fitting results for  $\{Cu_3(L2)_2(TPA)\}_n \times solvent$  (2).



**Figure S2.** ATR spectra of coordination polymers  $\{Cu_3(L1)_2(TPA)\}_n \times solvent$  (1) and  $\{Cu_3(L2)_2(TPA)\}_n \times solvent$  (2)



**Figure S3.** ATR spectra of coordination polymer  $\{Cu_3(L1)_2(TPA)\}_n \times solvent (1) as-prepared and heated at 473 K.$ 



**Figure S4.** Solid state UV-visible diffuse reflectance spectrum of the  $\{Cu_3(L1)_2(TPA)\}_n \times solvent$  (1) and  $\{Cu_3(L2)_2(TPA)\}_n \times solvent$  (2)



Figure S5. DSC curves for heating and cooling cycles for compounds 1 (a) and 2 (b).



**Figure S6.** TG and DTA curves for compound **1** and **2** (orange and violet respectively) measured under a synthetic air atmosphere.



**Figure S7.** Frequency dependence of the real (closed symbols) and imaginary (open symbols) parts of the complex dielectric constant measured at different temperatures for compound **1**.

Cu1-N1	2.030(13)	Cu2–N2	1.865(15)	Cu3–N6	1.940(16)
Cu1-N4	2.003(14)	Cu2–N3	1.940(14)	Cu3–N7	2.037(14)
Cu1-N5	1.945(17)	Cu2-01	1.950(10)	Cu3-04	2.002(12)
Cu1-N8	1.943(15)	Cu2-05	1.924(11)	Cu3-07	1.874(15)

**Table S1.**Bond lengths (Å) involved in the first coordination sphere of copper(II) atoms in<br/> ${Cu_3(L1)_2(TPA)}_n \times solvent (1).$ 

**Table S2.**Selected angles (°) in the coordination spheres of copper(II) atoms in  $\{Cu_3(L1)_2(TPA)\}_n \times solvent$ (1).

N1-Cu1-N4	79.4(6)	N2-Cu2-N3	82.6(7)	N6-Cu3-N7	85.8(7)
N1-Cu1-N5	178.6(5)	N2-Cu2-O1	82.1(5)	N6-Cu3-O4	79.5(6)
N1-Cu1-N8	97.5(6)	N2-Cu2-O5	171.9(5)	N6-Cu3-O7	170.2(6)
N4–Cu1–N5	99.5(6)	N3-Cu2-O1	163.4(6)	N7-Cu3-O4	162.1(5)
N4–Cu1–N8	176.3(6)	N3-Cu2-O5	104.9(6)	N7-Cu3-O7	103.5(6)
N5–Cu1–N8	83.5(6)	01–Cu2–O5	90.8(5)	04–Cu3–O7	92.0(5)
Cu2-01-C1	110.4(11)	Cu3-04-C13	111.0(10)	C25-O5-Cu2	128.1(10)

**Table S3.** Hydrogen-bonding geometry in  $\{Cu_3(L1)_2(TPA)\}_n \times solvent (1).$ 

D-H…A	D-H/Å	H…A/Å	D…A/Å	D-H…A/°	Symm. op. on A
N3–H3C…O2	0.89	2.14	2.90(2)	142	1 + <i>x, y, z</i>
N7–H7B…O3	0.89	2.14	2.92(2)	146	-1 + <i>x, y, z</i>
N3–H3D…solvent	0.89				
N7–H7A…solvent	0.89				
N3–H3C…O6	0.89	2.51	2.88(2)	105	3 + x, -1 + y, z
C3–H3A…O1	0.97	2.57	2.914(19)	101	
C15–H15A…O4	0.97	2.52	2.87(2)	101	
C21–H21A…O3	0.97	2.56	3.24(2)	127	-1 + <i>x, y, z</i>
C28–H28…O7	0.93	2.49	2.80(2)	100	
C30–H30…O8	0.93	2.44	2.75(2)	100	