Metallosupramolecular compounds based on copper(II/I) chloride and two bis-tetrazole organosulfur ligands

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Supplementary material

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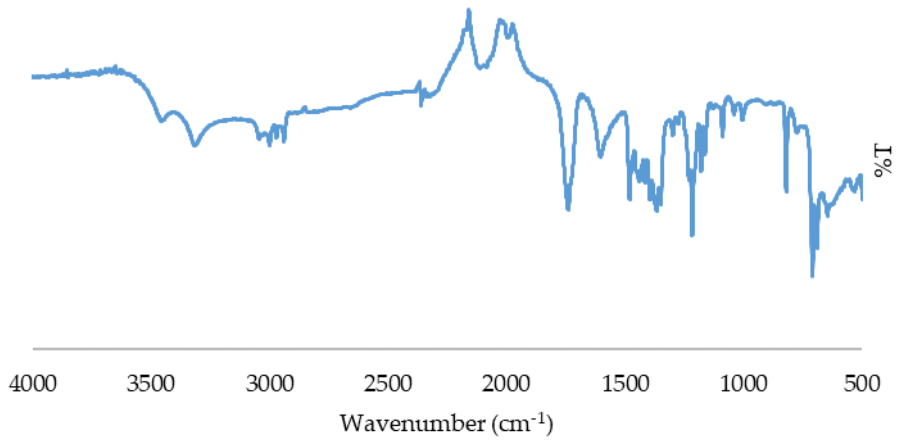
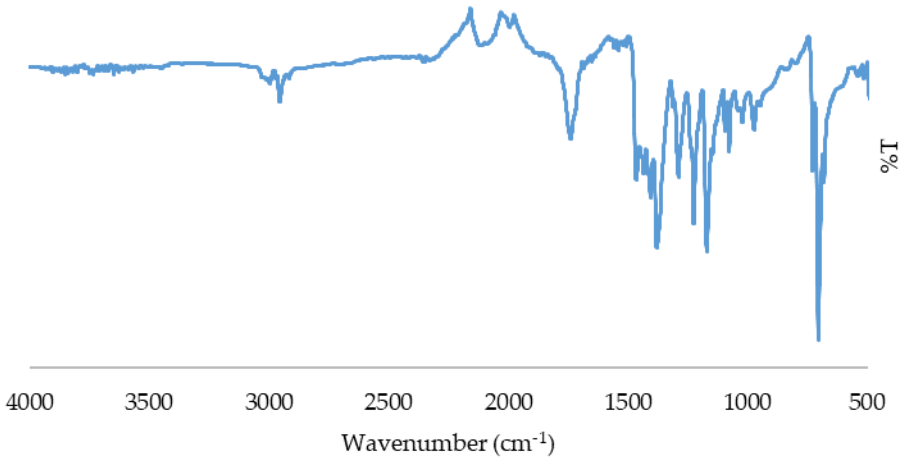
1. Characterization

$\infty^1Cu_3Cl_6(H_2O)_2(BMTTM)_2$ *(1)*



$[Cu_2Cl_2(BMTTE)]_2$ *(2)*



$\infty^2Cu_2Cl_4(BMTTE)$ *(3)*

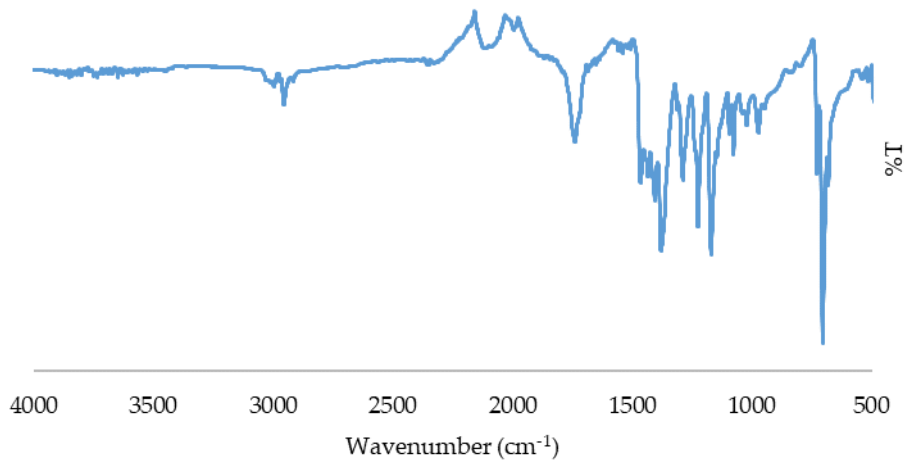
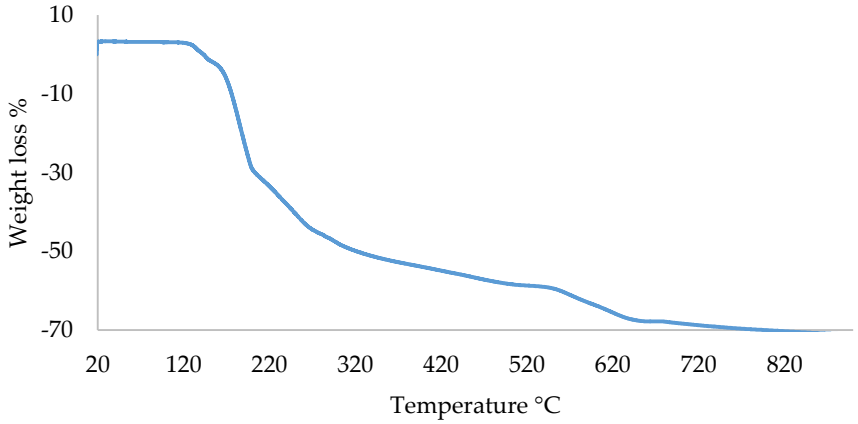
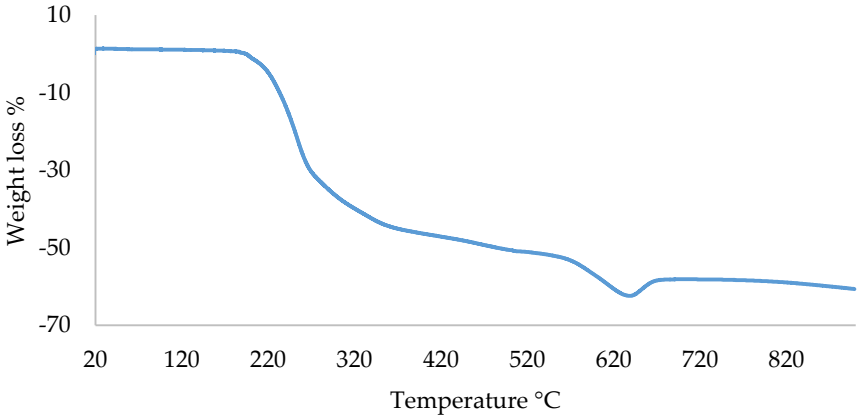


Figure S1: Infrared spectra (IR).

$\infty^1Cu_3Cl_6(H_2O)_2(BMTTM)_2$ **(1)**



$[Cu_2Cl_2(BMTTE)]_2$ **(2)**



$\infty^2Cu_2Cl_4(BMTTE)$ **(3)**

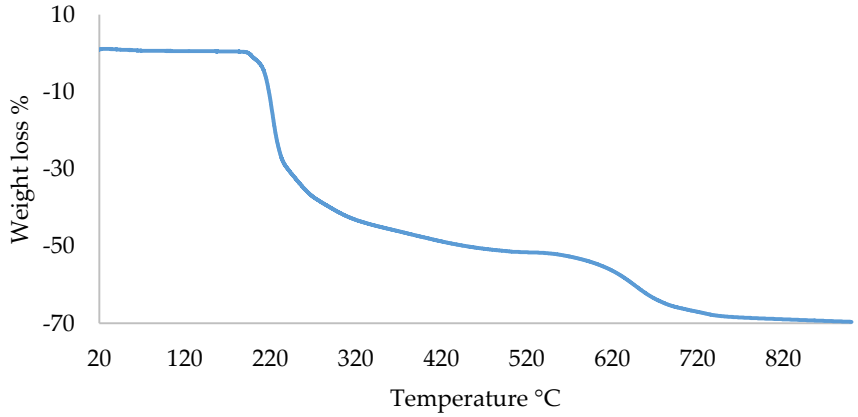
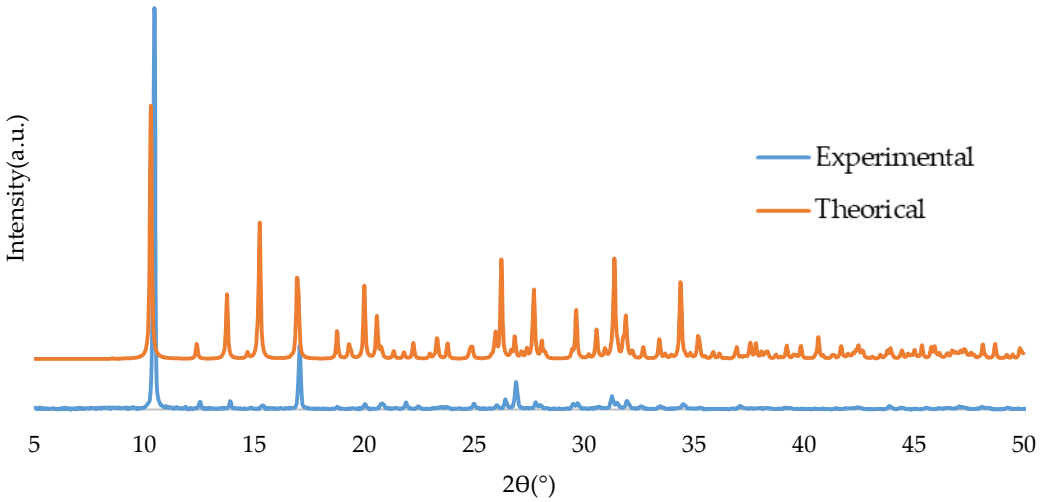


Figure S2: Thermogravimetric analysis (TGA).

$\infty^1Cu_3Cl_6(H_2O)_2(BMTTM)_2$ *(1)*



$\infty^2Cu_2Cl_4(BMTTE)$ *(3)*

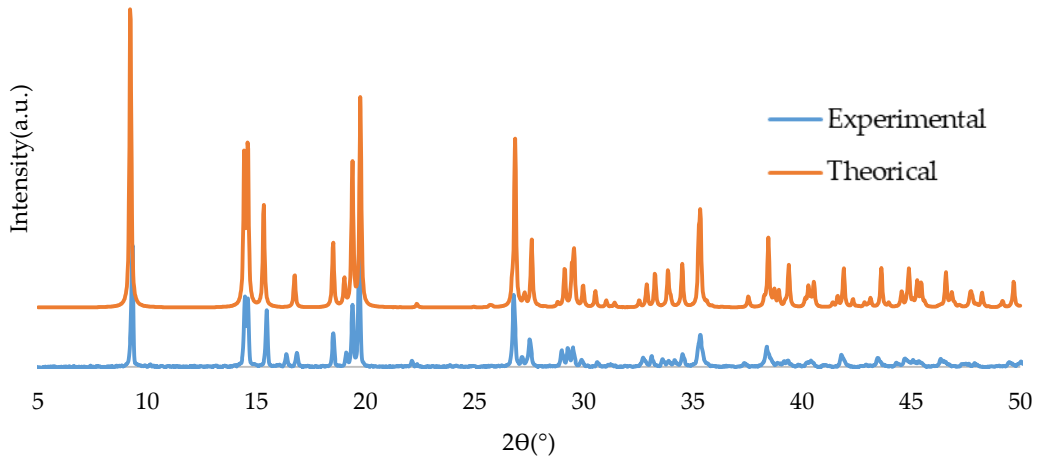


Figure S3: Powder X-Ray Diffraction (PXRD) comparison.

2. Crystallography

Table S1: Crystal data and structure refinement.

Compound		**1**	**1·solv**	**2**	**3**
Empirical formula		$C_{10}H_{20}Cl_6Cu_3N_{16}O_2S_4$	$C_{18}H_{32}Cl_6Cu_3N_{20}O_2S_4$	$C_{12}H_{20}Cl_4Cu_4N_{16}S_4$	$C_3H_5Cl_2CuN_4S$
Formula weight		927.98	1092.19	912.64	263.61
Crystal system		Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group		*P2₁/n*	*P-1*	*P2₁/n*	*C2/c*
Unit cell dimensions	a/Å	6.6586(7)	6.7181(5)	10.1237(5)	20.3164(18)
	b/Å	12.8635(14)	12.9961(9)	9.5414(5)	6.5444(6)
	c/Å	17.4187(19)	12.9971(9)	14.4784(8)	12.8543(11)
	α/°	-	64.067(2)	-	-
	β/°	99.657(3)	79.492(2)	93.650(2)	109.493(3)
	γ/°	-	82.134(2)	-	-
Volume/A^3		1470.8(3)	1001.29(12)	1395.69(13)	1611.1(2)
Z, ρ_{calc}/g·cm^{-3}		2/2.095	1/1.811	2/2.172	8/2.174
F(000)		922	549	904	1040
Crystal size (mm^3)		0.126x0.023x0.021	0.269x0.119x0.071	0.411x0.186x0.051	0.071x0.051x0.045
Abs. coeff. (mm^{-1})		3.024	2.239	3.729	3.567
θ Range (°)		2.372-28.434	2.958-30.576	2.385-28.339	3.290-28.354
Max./min. transmission		0.7454/0.6425	0.7461/0.6127	0.7457/0.4839	0.7457/0.7024
Reflections collected		18273	29257	29340	19117
Independent reflections (R_{int})		3688 (0.0523)	6158(0.0256)	3486 (0.0386)	2015 (0.0255)
Final R indices [I>2σ(I)]		R1 = 0.0494 wR2 = 0.1077	R1 = 0.0209 wR2 = 0.0501	R1 = 0.0212 wR2 = 0.0467	R1 = 0.0196 wR2 = 0.0453