Dynamic Combinatorial Chemistry in a Solvothermal Process of Cu(I,II) and Organosulfur Ligands

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Supporting Information

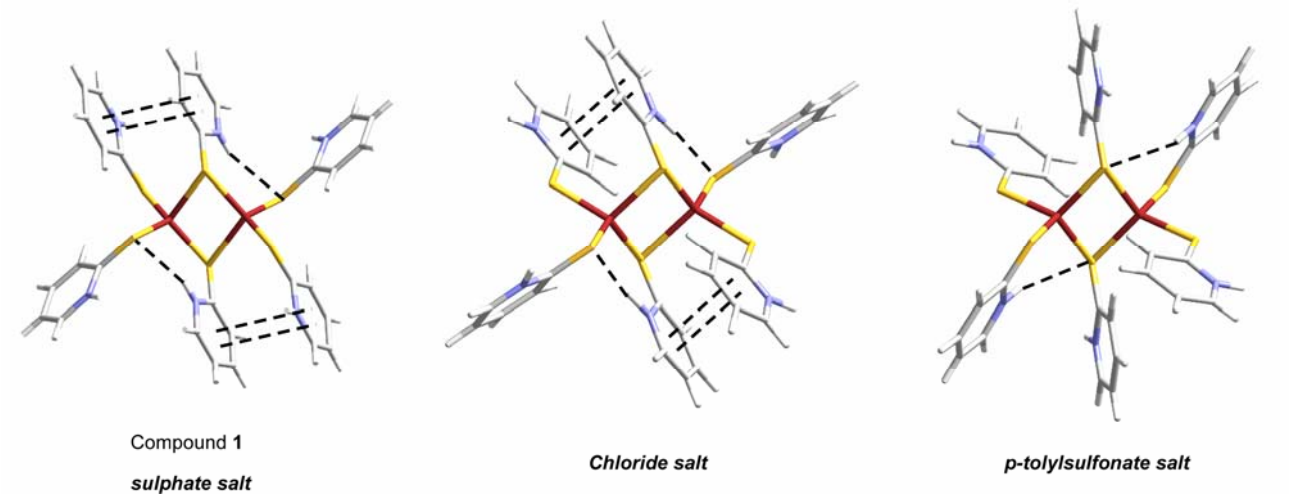

Fig. S1 Comparative intradimeric non-covalent interactions in sulphate, chloride and p-tolylsulfonate salts of the cationic $[Cu_2(\mu\text{-pyt-}\kappa S\text{:k}S)_2(\text{pyt-}\kappa S)_4]^{2+}$ complex.

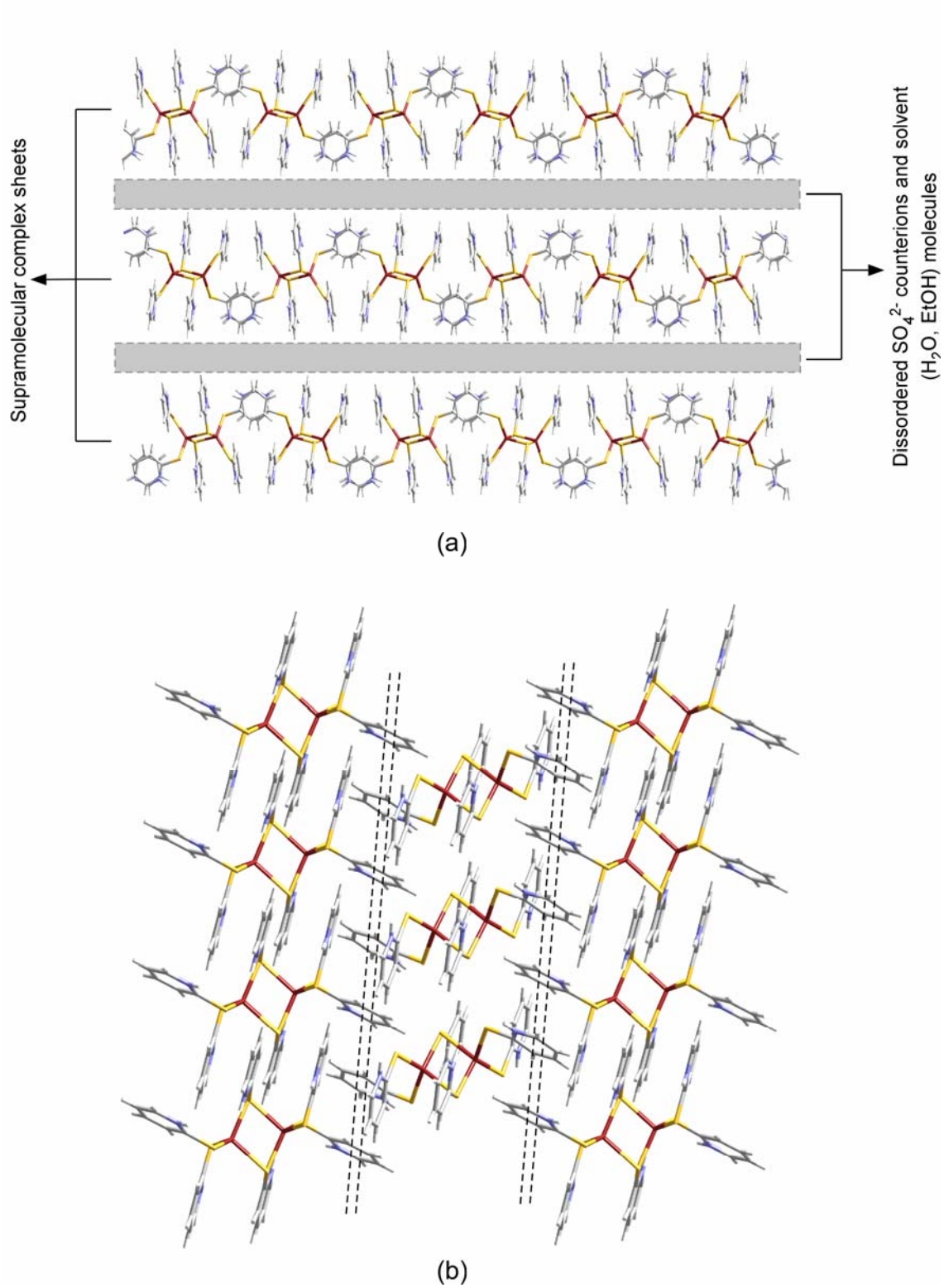

Fig. S2 (a) Lamellar crystal structure of compound **1** and (b) supramolecular sheet of cationic copper(I) dinuclear complexes. Double-dashed lines denote parallel π-stacking interactions.

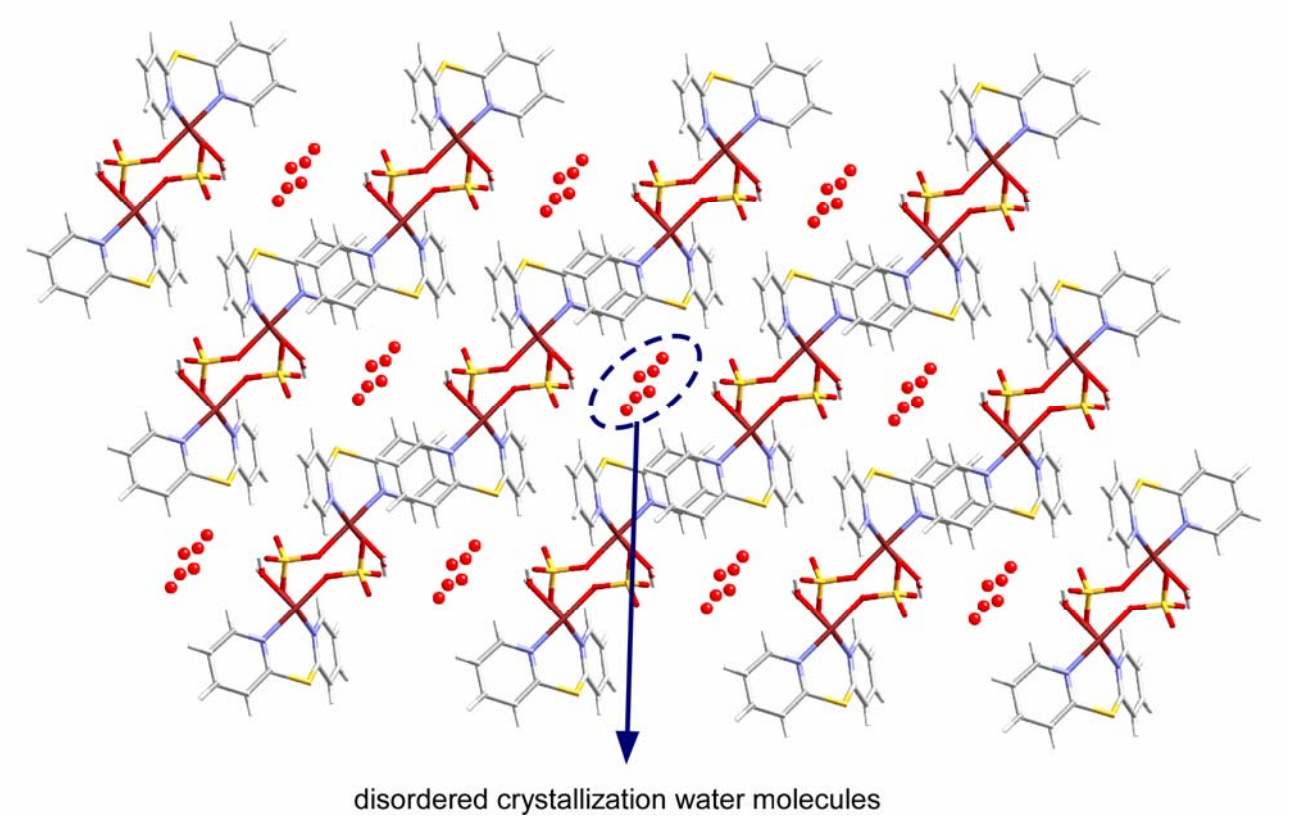

Fig. S3 Perspective view of the crystal packing of compound **3** along the *a* crystallographic axis.

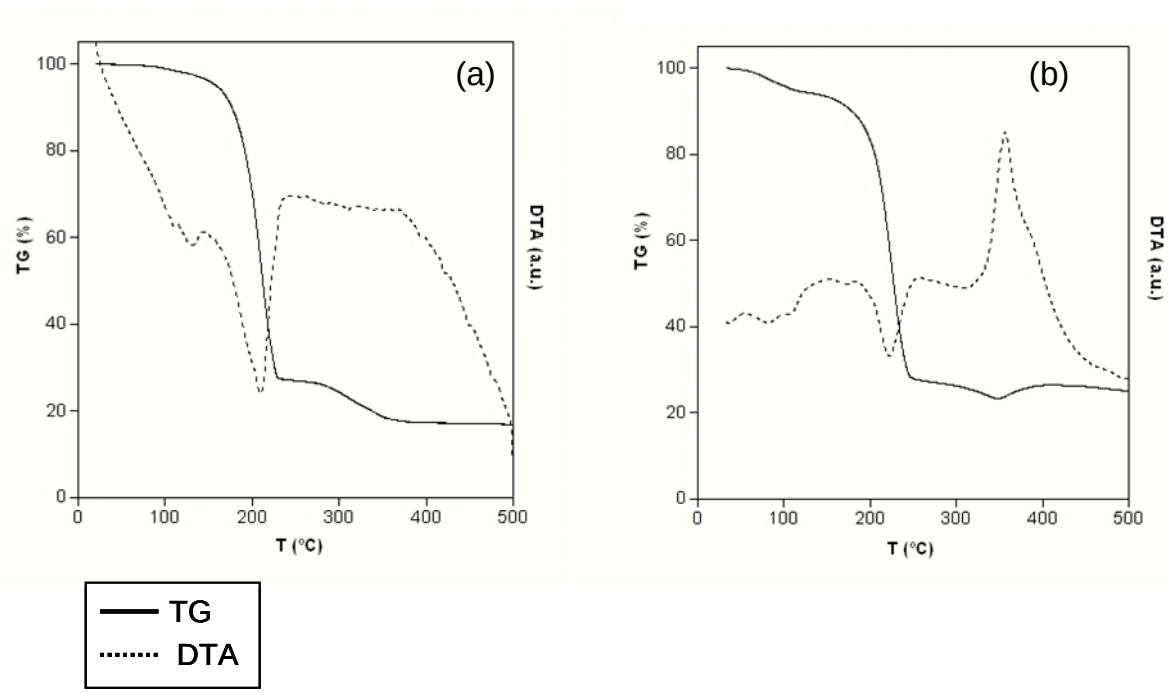

Fig. S4 Thermal behaviour of compound **1** (a) and **2** (b).

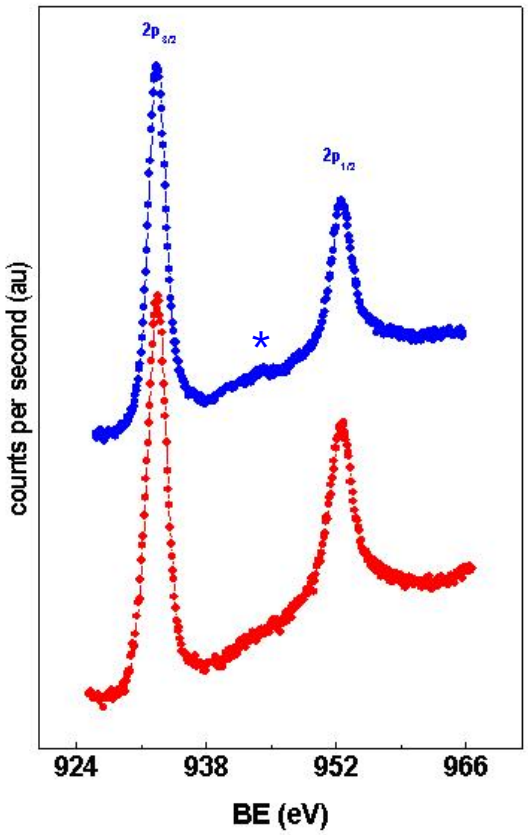

Fig. S5 XPS spectra of Cu2p region at room temperature of **1** (in red) and 2 (in blue; * indicate the satellite).

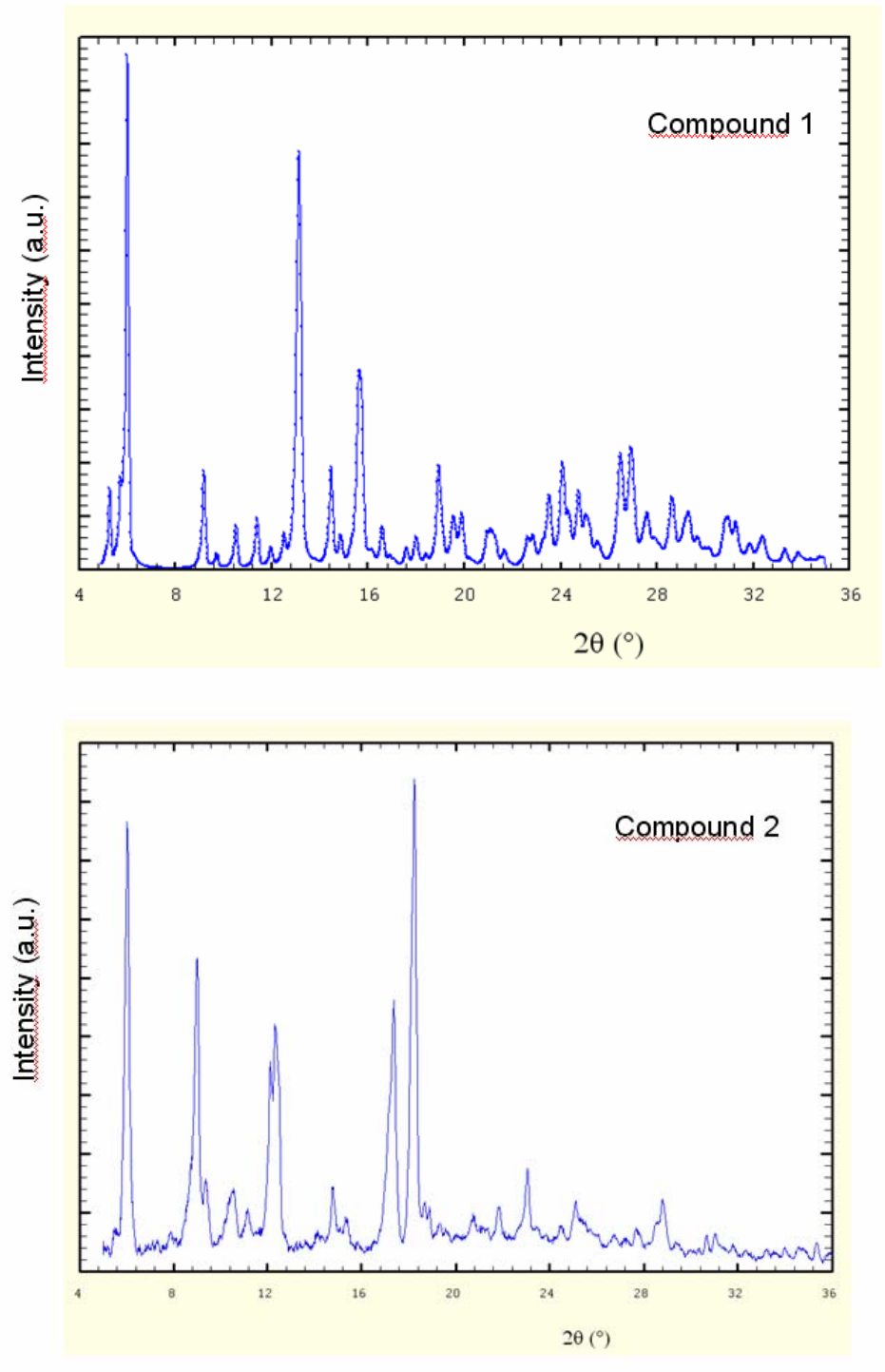

Fig. S6 Experimental Powder X-ray diffraction patterns of compounds **1** and **2**.

Table S1. Selected bond angles (º) for compounds **1**-**3**.

Compound 1			
S1–Cu1–S2	124.13(5)	S4–Cu2–S5	124.21(5)
S1–Cu1–S3	115.95(5)	S4–Cu2–S6	116.10(5)
S1–Cu1–S3^{i}	94.87(4)	S4–Cu2–S6^{i}	95.62(4)
S2–Cu1–S3	104.01(4)	S5–Cu1–S6	103.19(4)
S2–Cu1–S3^{i}	107.28(4)	S5–Cu1–S6^{i}	107.24(5)
S3–Cu1–S3^{i}	109.42(3)	S6–Cu1–S6^{i}	109.47(4)
Compound 2			
S1–Cu1–S2	106.65(5)	S1–Cu2–S2	108.11(5)
S3–Cu3–S4	116.73(5)	S3–Cu3–S5	116.51(5)
S3–Cu3–S6	101.98(5)	S4–Cu3–S5	112.60(5)
S4–Cu3–S6	90.65(5)	S5–Cu3–S6	115.00(5)
S1–Cu1–S5^{ii}	107.06(5)	S1–Cu2–S3	109.73(5)
S1–Cu1–S6^{ii}	96.84(5)	S1–Cu2–S4	99.98(5)
S2–Cu1–S5^{ii}	116.32(5)	S2–Cu2–S3	114.41(5)
S2–Cu1–S6^{ii}	111.38(5)	S2–Cu2–S4	109.52(5)
S5^{i}–Cu1–S6^{ii}	116.14(5)	S3–Cu2–S4	113.99(5)
Compound 3			
N1–Cu1–N2	89.48(15)	N3–Cu2–N4	90.15(15)
N1–Cu1–O1	115.95(5)	N3–Cu2–O2	90.16(14)
N1–Cu1–O5	178.32(14)	N3–Cu2–O6	167.44(12)
N1–Cu1–O1w	92.52(13)	N3–Cu2–O2w	104.71(11)
N2–Cu1–O1	163.53(12)	N4–Cu2–O2	177.63(13)
N2–Cu1–O5	89.74(14)	N4–Cu2–O6	86.22(13)
N2–Cu1–O1w	106.30(12)	N4–Cu2–O2w	94.09(12)
O1–Cu1–O5	95.23(12)	O2–Cu2–O6	93.96(12)
O1–Cu1–O1w	89.71(11)	O2–Cu2–O2w	83.56(11)
O5–Cu1–O1w	86.28(11)	O6–Cu2–O2w	87.56(11)

Symmetry codes: (i) 1 – x, 1 – y, 1 – z; (ii) ½ + x, y, ½ – z.