Self-assembled 3D Heterometallic Cu^{II}/Fe^{II} Coordination Polymers with Octahedral Net Skeletons: Structural Features, Molecular Magnetism, Thermal and Oxidation Catalytic Properties

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Electronic supplementary information (ESI)

ESI contains additional structural representations (Figs. S1 and S2), plots of differential thermal analyses (Fig. S3) and their summary (Table S1) for compounds **1** and **2**.

(a) (b)

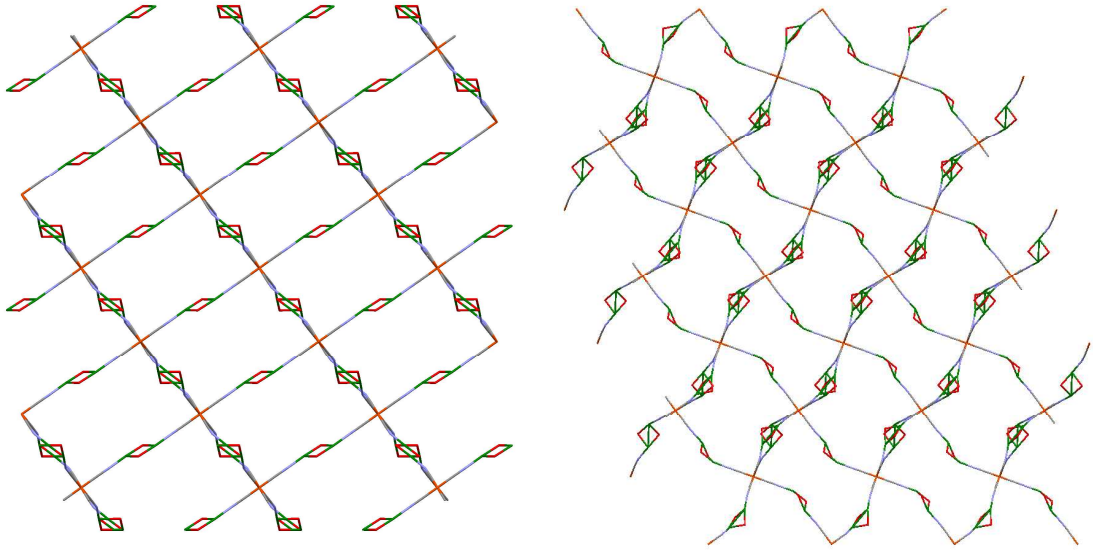
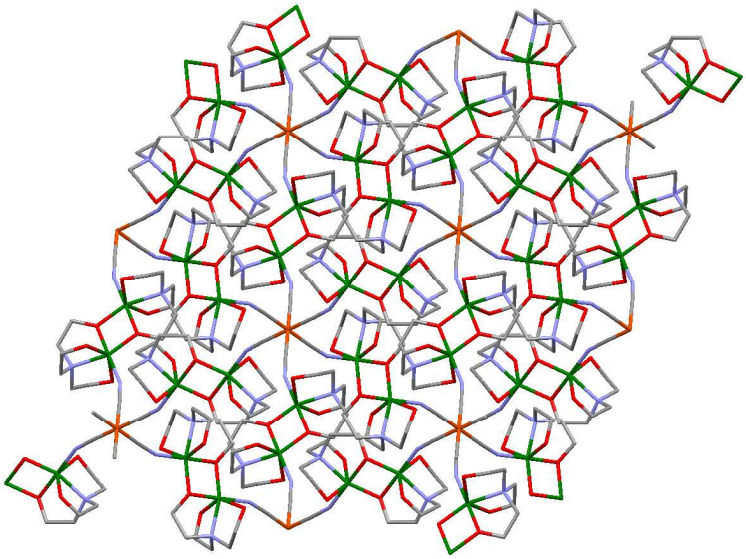


Figure S1. Simplified crystal packing diagrams (views along the *a* axis) of **1** (a) and **2** (b) showing the generation of either linear (a) or wave-like (b) ~Fe–CN–Cu_2(μ-O)$_2$–NC–Fe–CN–Cu_2(μ-O)$_2$~ cross-linking motifs. H_2tea and Hmdea moieties (except for μ-O atoms) are omitted for clarity. Fe orange, Cu green, O red, N blue and C gray.

(a)



(b)

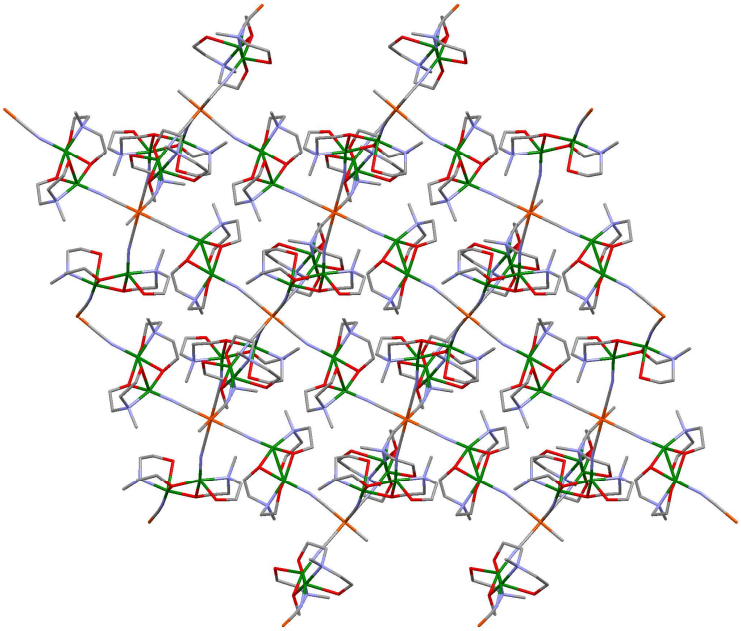
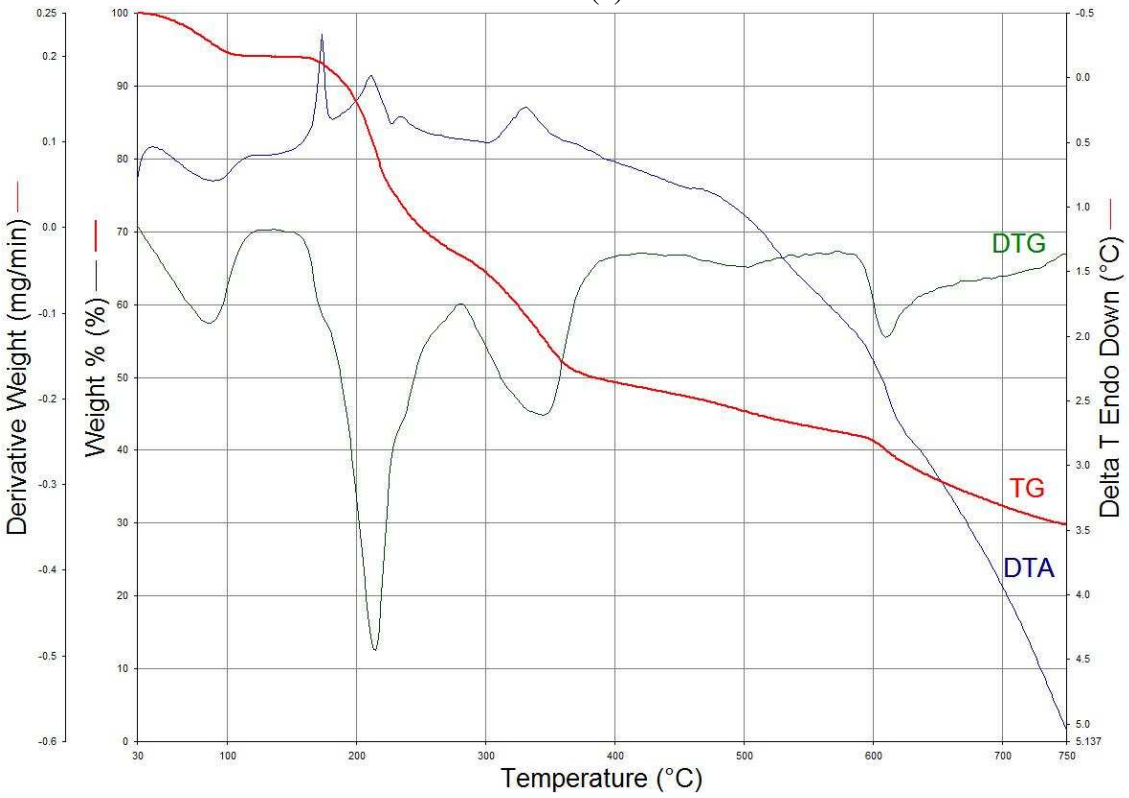


Figure S2. Crystal packing diagrams of **1** (a) and **2** (b) along the *c* axis (H atoms are omitted for clarity). Fe orange, Cu green, O red, N blue and C gray.

(a)



(b)

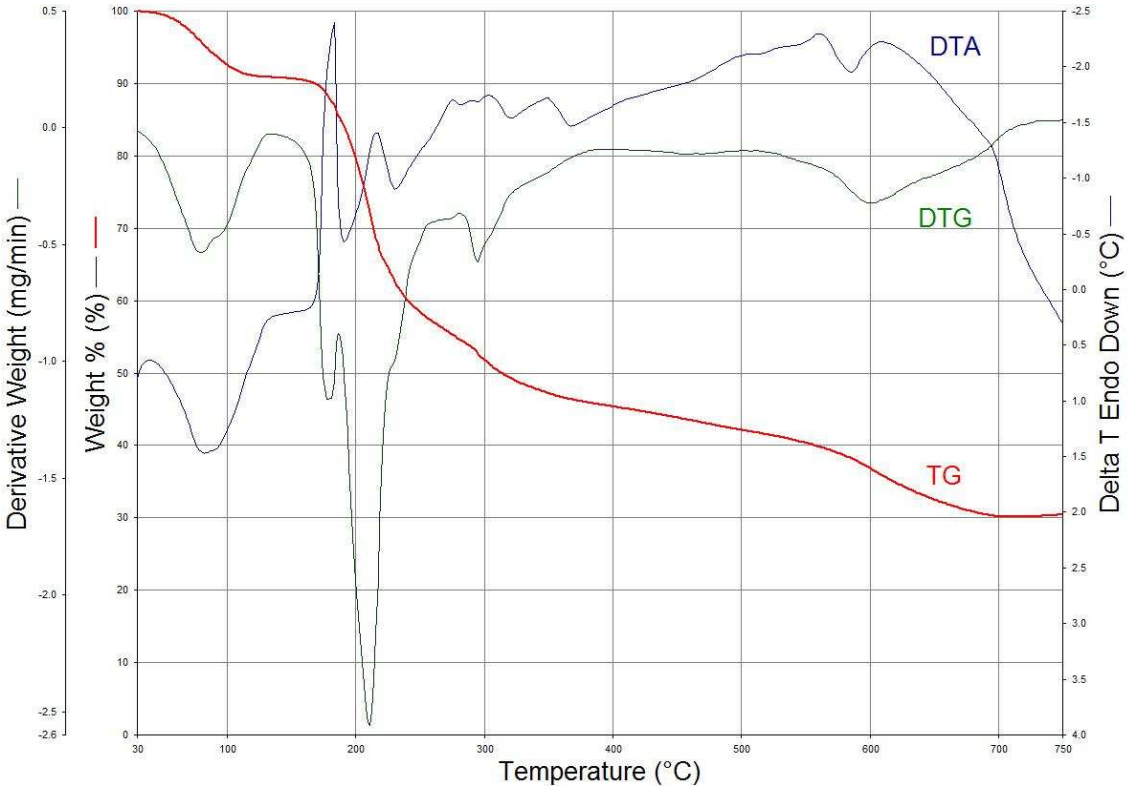


Figure S3. Differential thermal analysis plots of **1** (a) and **2** (b).

Table S1. Summary of Differential Thermal Analysis for **1** and **2**[a]

Thermal effect	Compound **1**			Compound **2**		
	Temperature, °C		∑ Mass loss, %	Temperature, °C		∑ Mass loss, %
	interval	maximum		interval	maximum	
I	30–120	88	6.2 (6.3)[b]	30–130	75	8.4 (8.1)[d]
II	120–177	173	9.3 (9.9)[c]	130–188	180	15.8 (16.1)[e]
III[f]	177–230	211	25.5	188–227	216	37.8
IV	230–279	–	34.5	227–320	294	50.5
V	279–400	331	52.5	320–360	345	53.2
VI	400–585	500	57.9	360–560	500	60.0
VII	585–750	608	70.0	560–700	582	70.0

[a] Allocation of thermal effects is based on the DTA curve. [b–e] Calculated value (in parentheses) for elimination of: [b] $6H_2O$, [c] NO_3^-, [d] $7H_2O$, [e] $2NO_3^-$. [f] Beginning of the multi-step complex decomposition of organic moieties.