

Polymorphism of $(\text{H}_2\text{mela})_2[\text{CuCl}_5]\text{Cl}$ (mela = melamine): Structures, Transformation and Magnetic Properties

Dan-Feng Weng, Bing-Wu Wang, Zhe-Ming Wang* and Song Gao*

Beijing National Laboratory for Molecular Sciences, State Key Laboratory of Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871 (China) Email: gaosong@pku.edu.cn, zmw@pku.edu.cn

Electronic supplementary information

Table S1. IR absorption bands [cm^{-1}] and their assignments for **1** and **2** (s: strong, m: medium, w: weak, sh: shoulder, br: broad).

	1	2
N–H stretching	3334 (sh)	3338(sh)
	3270 (m)	3278 (m)
	3131 (m)	3134 (m)
	3060 (m)	3038 (m)
	2900 (m-w, br)	2888 (m-w, br)
	2748 (m-w)	2739 (m-w)
N–H bending	1696 (vs)	1694 (vs)
		1666 (s)
C=N	1500 (m)	1509 (m)
C–N	1123 (m-w)	1123 (m-w)
Cu–Cl (equatorial)	277 (w)	254 (w)
	235 (w)	
Cu–Cl (axial)	204 (w)	200 (w)

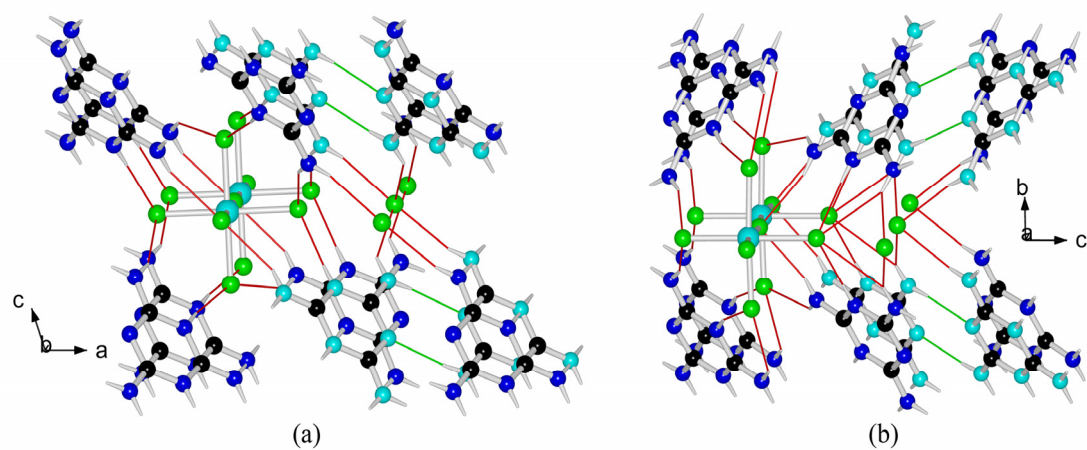


Figure S1. The H-bonding around the $[\text{CuCl}_5^{3-}]_n$ chains in **1** (a) and **2** (b). The intramolecular H-bonds in the H-bonded dimers of $[\text{H}_2\text{mela}^{2+}]_2$ are showed in thin green bonds, other H-bonds are showed in thin red bonds. Atomic color scheme: Cu, cyan; N, blue; C, black; C in $[\text{H}_2\text{mela}^{2+}]_2$ dimers, small cyan ball; H, white.

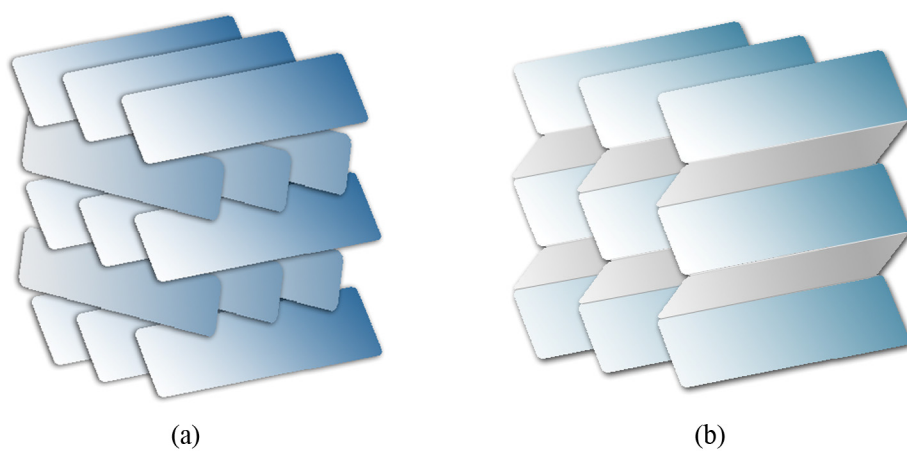


Figure S2. Schematic diagrams of packing of strips of mela dimers in **1** (a) and **2** (b).

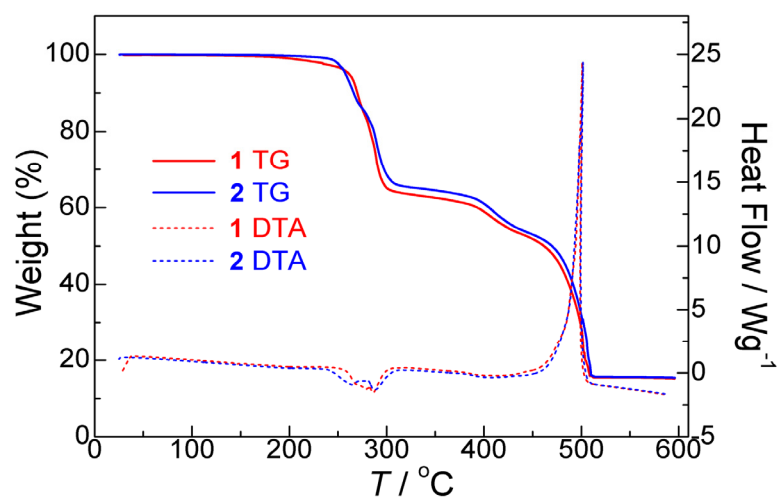


Figure S3. Combined TGA/DSC runs for **1** (red) and **2** (blue) at a rate of $5^\circ\text{C}/\text{min}$ under air atmosphere.

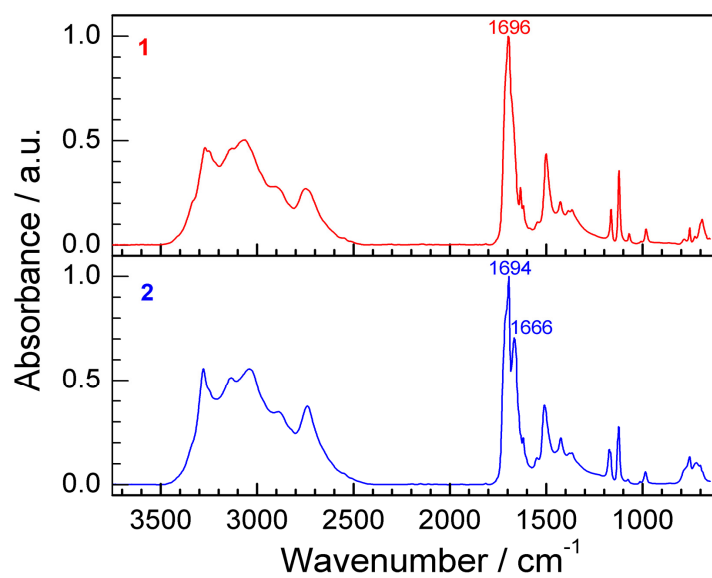


Figure S4. IR spectra of **1** (red) and **2** (blue).

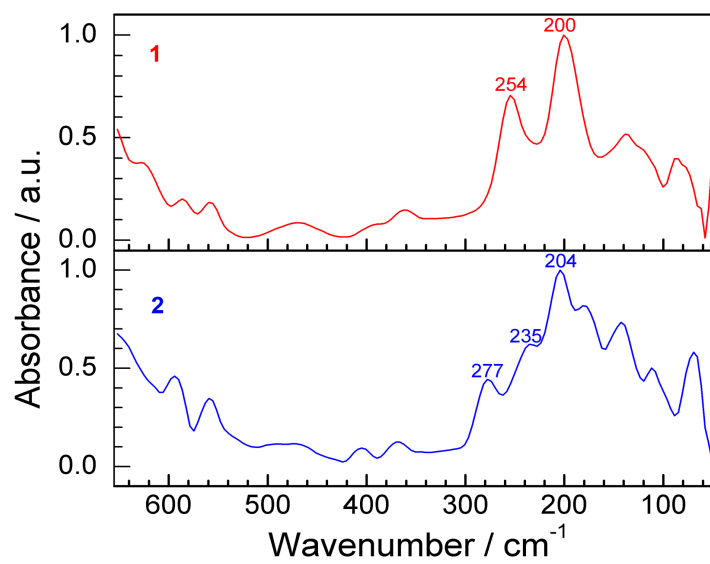


Figure S5. FIR spectra of **1** (red) and **2** (blue).

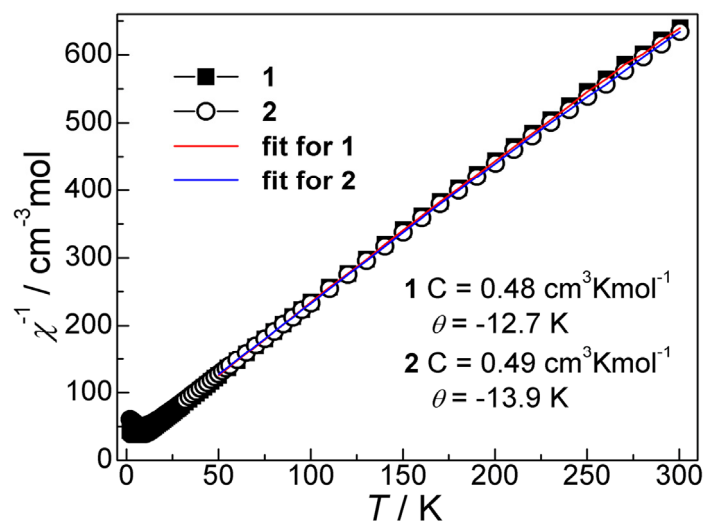


Figure S6. The $1/\chi$ vs T plots (under 1000 Oe field) for complexes **1** and **2**, red (**1**) and blue (**2**) lines are Curie-Weiss fitting.

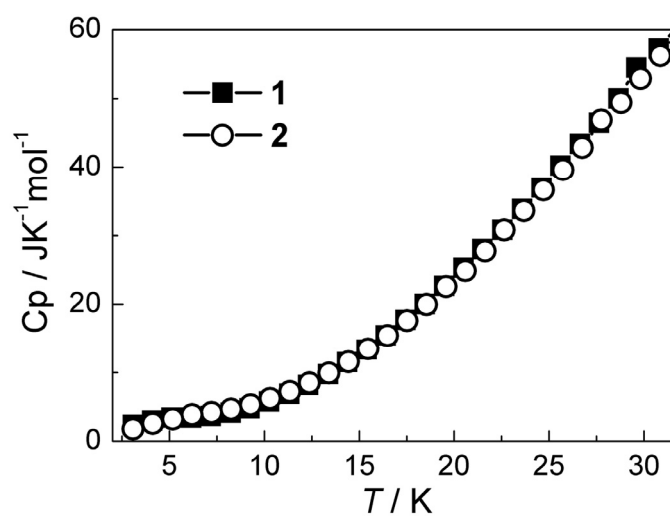
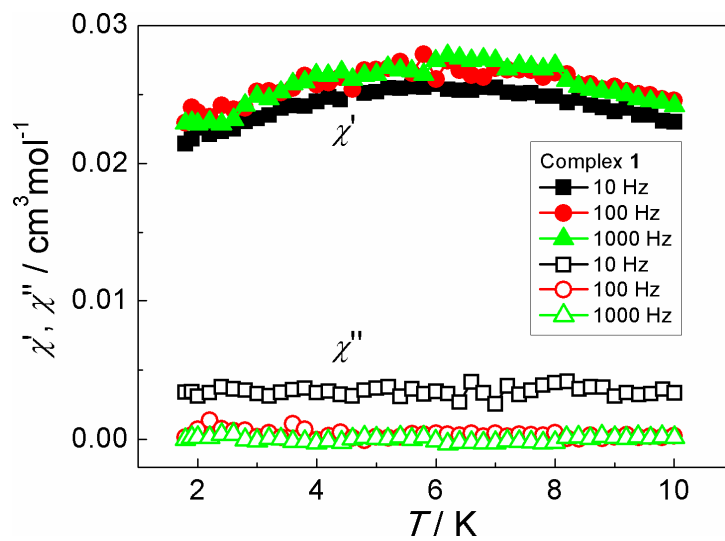
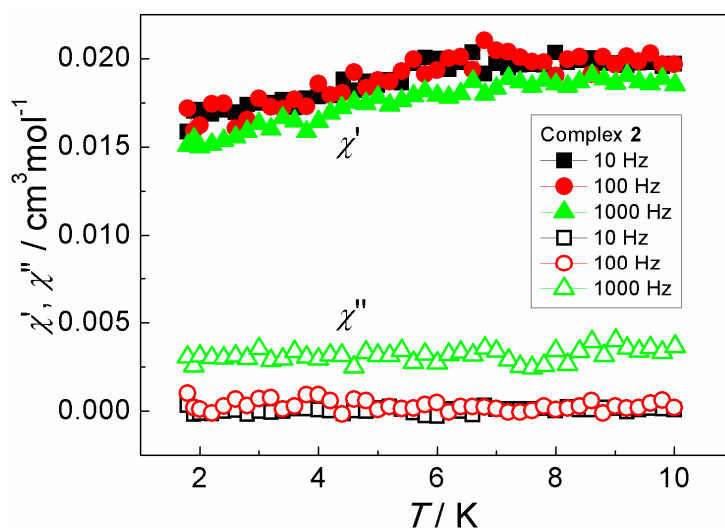


Figure S7. Specific heat capacity plots of complexes 1 and 2.

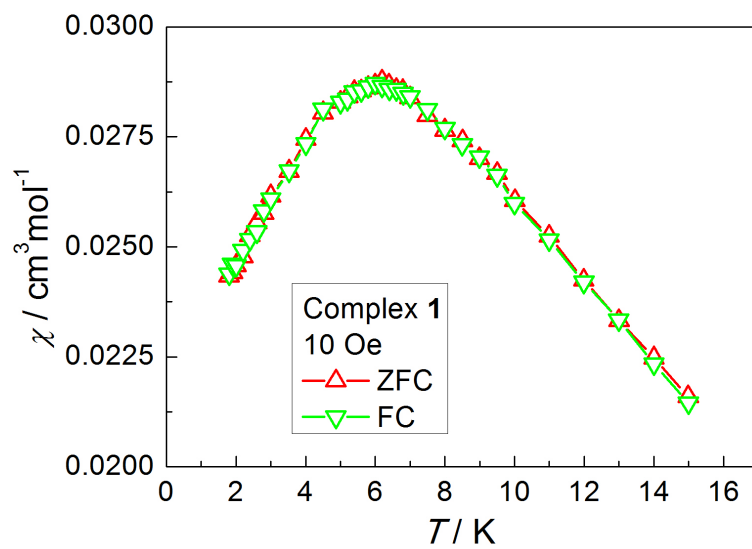


(a)

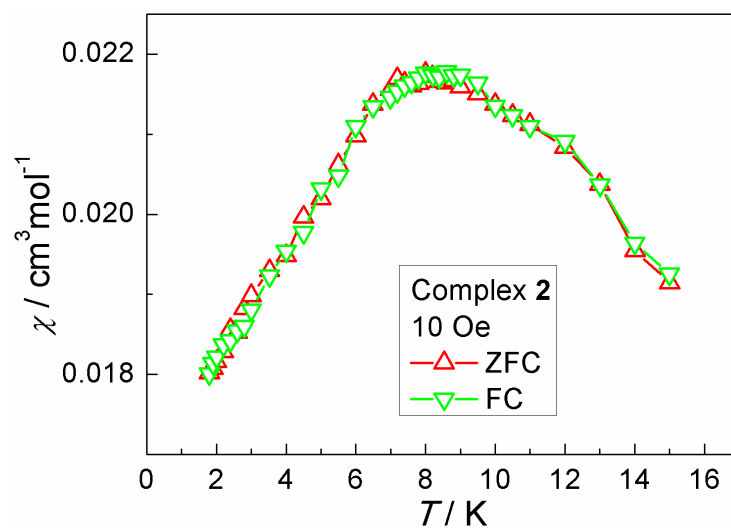


(b)

Figure S8. AC plots of complexes 1 (a) and 2 (b).



(a)



(b)

Figure S9. ZFC-FC plots of complexes **1** (a) and **2** (b).