

Temperature identification on two 3D Mn(II) metal-organic frameworks : syntheses, adsorption and magnetism

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Supporting Information

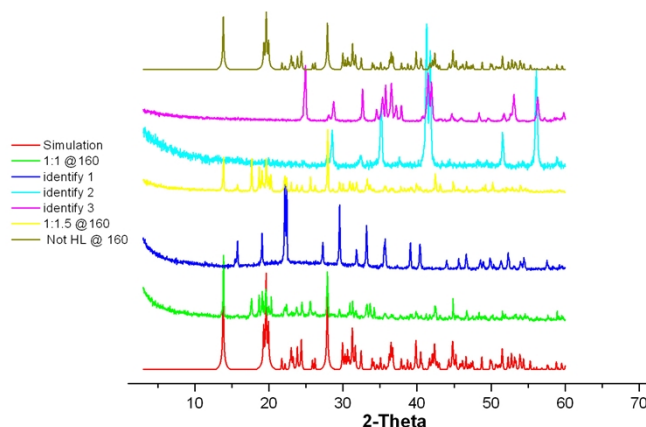


Fig. S1 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination, the as-synthesized product and different condition products in compound **1**.

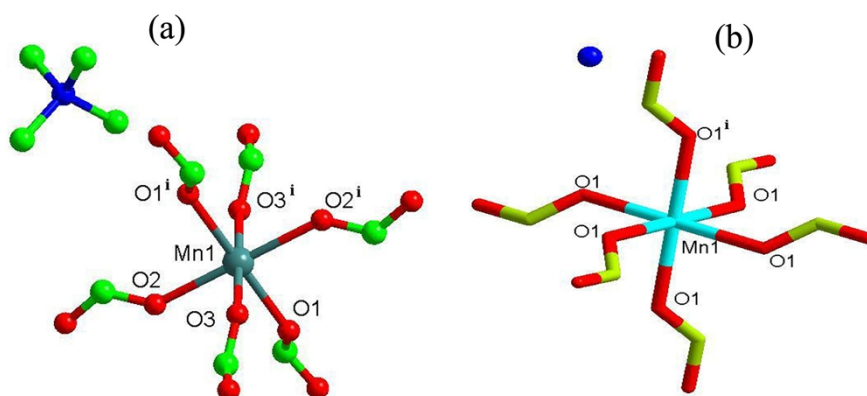


Fig. S2 View of the coordination modes of Mn(II) in **1** (symmetric code: (i) $-x+1, -y, -z+1$) and **2** (symmetric code: (i) $-x+1/2, -y+1/2, -z+1/2$).

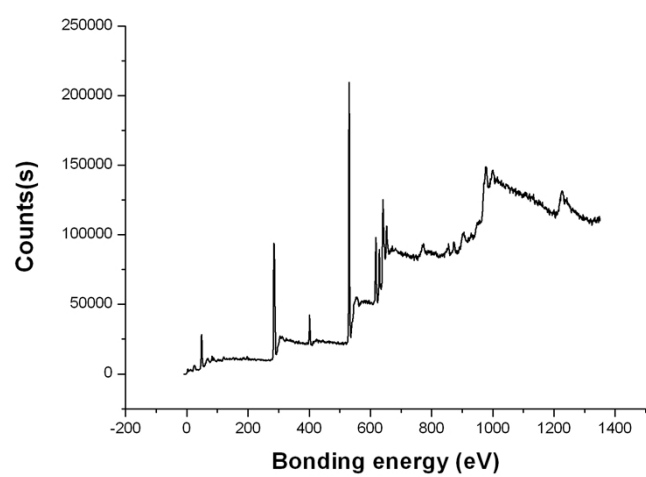


Fig. S3 the XPS pattern in **1**.

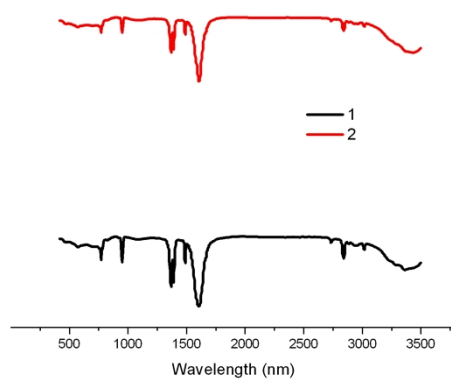


Fig. S4 View of the IR in **1** and **2**.

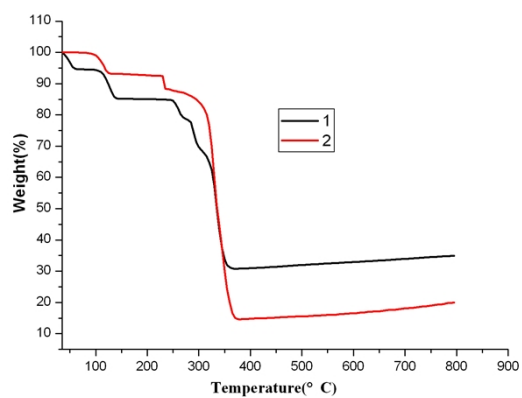


Fig. S5 View of the TGA in **1** and **2**.

Table S1 The Magnetism behavior of cationic @metal ion(formate)₃

Formula	Starting material	Magnetism feature	Refs
$[(CH_3)_2NH_2Co(HCOO)_3]$	PD-DMF (CD_3) ₂ NCDO] in D ₂ O (2 mL) and CoCl ₂	order-disorder- type ferroelectrics	1
$[(HONH_3)Mn^{II}(HCOO)_3]$	Mn(ClO ₄) ₂ ·6H ₂ O, formic acid, triethylamine, hydroxylamine, hydrochloride	antiferromagnetic long-range ordering of spin canting	2
$[(dmenNH_2)Mn^{II}(HCOO)_6]$	Mn(ClO ₄) ₂ ·HCOOH, ammonia	spin-canted antiferromagnetism	3
$[AmineH][Mn^{II}(HCOO)_3]$ AmineH = Methylamine, Ethylamine, Dimethylamine, Cyclotrimethyleneamine	AmineH ₂ ,HCOOH and MnCl ₂	long-range antiferromagnetism below 9 K with a slight non-collinear arrangement of the moments.	4
$K[Co(HCOO)_3]$	CoCl ₂ ·6H ₂ O HCOOH, KCOOH	spin-canted antiferromagnet ($T_N = 8.3$ K) displaying two steps	5
$[Mn_3(HCOO)_6](CH_3OH)(H_2O)$	CoCl ₂ ·6H ₂ O triethylamine HCOOH CH ₃ OH	antiferromagnetic with a spin canting arrangement below 2 K	6
$[(Fmd)Ln(III)(HCOO)_4]$ Fmd ⁺ =NH ₂ -CH-NH ₂	Ln(III) salt cyclobutane-1,1- dicarboxylic acid, formamide	antiferromagnetic interaction	7
$[NH_4][Zn(HCOO)_3]$	Zn(ClO ₄) ₂ ·6H ₂ O, HCO ₂ H, ammonium formate	paraelectric- ferroelectric phase transition	8
$[NH_4][Mn(HCOO)_3]$	MnCl ₂ HCO ₂ H, ammonium formate	paraelectric to ferroelectric phase transitions between 191 and 254 K	9
$[NH_4][M^{II}(HCOO)_3]$ (M= Mn, Co, Ni)	Mn(ClO ₄) ₂ ·HCOOH, ammonia	weak spontaneous magnetization	10
$[CH_3NH_2(CH_2)_2NH_2CH_3][M_2(HCOO)_6]$ (M = Mn ^{II} and Co ^{II})	[dmenH ₂][HCOO] ₂ , M(ClO ₄) ₂	3D long-range antiferromagnetic	11

		ordering with small spin canting	
$[(\text{CH}_3)_2\text{NH}_2][\text{Mn}(\text{HCOO})_3]$	$\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ DMF under 140°C	order-disorder type of ferroelectricity below 185 K.	12
$[(\text{CH}_3)_2\text{NH}_2][\text{Mn}(\text{HCOO})_3]$	$\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$, DMF, ethanol, 1 mL of water, formic acid under 140°C	a dielectric transition around 190 K	13
$[(\text{CH}_3)_2\text{NH}_2][\text{Mn}(\text{HCOO})_3]$	$\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ DMF under 140°C for 6 days	multiferroics with well separated magnetic and antiferroelectric transitions	14

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The fitting equation for compounds **1** and **2**

$$\hat{H} = \sum_{nn} J.S_i.S_j$$

$$\frac{Ng^2\mu_B^2}{\chi J} = 3\theta + \sum_{n=1}^{\infty} \frac{C_n}{\theta^{N-1}}$$

$$\theta = \frac{kT}{JS(S+1)}$$