Supporting Information

for

Thermal hysteresis induced by external pressure in a 3D Hofmann-type SCO-MOF

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Table S1. Crystal structure and refinement details for compounds **1** and **2** at different temperature.

	Compound **1**		Compound **2**	
Temp (K)	293	95	250	100
formula	$FePtC_{16}N_6O_4H_{18}Br_2$		$FePdC_{16}N_6O_4H_{18}Br_2$	
M	769.12		680.43	
cryst syst	tetragonal		tetragonal	
space group	*P*4/*m*		*P*4/*m*	
a, Å	7.4386(2)	7.3121(5)	7.4285(7)	7.2533(5)
b, Å	7.4386(2)	7.3121(5)	7.4285(7)	7.2533(5)
c, Å	13.733(2)	13.3878(18)	13.648(3)	13.346(2)
α, deg	90	90	90	90
β, deg	90	90	90	90
γ, deg	90	90	90	90
V, Å^3	759.88(13)	715.80(14)	753.1(2)	702.16(14)
Z	1	1	1	1
D_c, g cm^{-3}	1.681	1.784	1.500	1.609
μ, mm^{-1}	7.729	8.205	3.757	4.029
F(000)	362.0	362.0	330.0	330.0
goodness-of-fit on F^2	1.201	1.077	1.136	1.112
R1 (I ≥ 2σ(I))[a]	0.0757	0.0561	0.0672	0.0806
wR2 (all data)[a]	0.1936	0.1554	0.2215	0.2422

a: $I \geq 2\sigma(I)$: $R1 = \sum||F_o| - |F_c||/\sum|F_o|$, $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$.
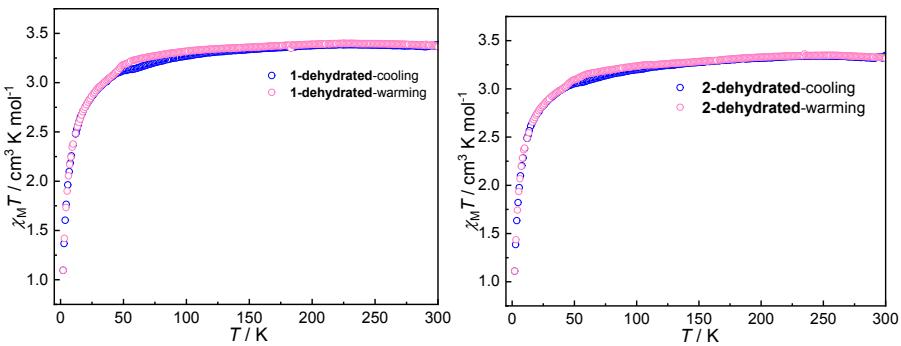
Fig. S1 The $\chi_M T$ versus T plots for compounds **1-dehydrated** and **2-dehydrated**.


Fig. S2 The asymmetric unit of compound **1**.
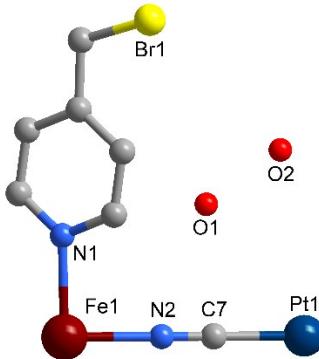
Table S2. The Fe^{II}–N bond distances in compounds **1** and **2** at different temperature.

	Compound **1**		Compound **2**	
T / K	293	95	250	100
Fe^{II}–N_{dbdpe} (Å)	2.20(2)	2.022(12)	2.129(11)	2.023(14)
Fe^{II}–N_{NC} (Å)	2.132(12)	2.032(11)	2.132(7)	2.002(9)
Fe^{II}–N_{ave} (Å)	2.167(6)	2.027(12)	2.130(9)	2.013(12)

Table S3. The Fe···Fe distances and Σ_{Fe} of {FeN$_6$} at different temperature for compounds **1** and **2**.

	Compound **1**		Compound **2**	
T / K	293	95	250	100
d_1(Fe···Fe) (Å)	7.439	7.312	7.428	7.253
d_2(Fe···Fe) (Å)	13.733	13.388	13.648	13.346
Σ_{Fe} of {FeN$_6$} (°)	12.0	4.8	9.6	6.8

$$\sum_{(i=1}^{12} |\varphi_i - 90°|_{)}$$

Table S4. The host-host, host-guest and guest-guest interactions in compounds **1** and **2**.

	Compound **1**		Compound **2**	
Temperature	293 K	95 K	250 K	100 K
C1–H1···O1 (Å)	2.62(7)	2.49(13)	2.57(9)	2.44(8)
Br1···Br1 (Å)	3.02(1)	2.75(9)	2.85(3)	2.66(7)
O1···O2 (Å)	2.95(1)	2.86(17)	3.13(2)	2.99(12)
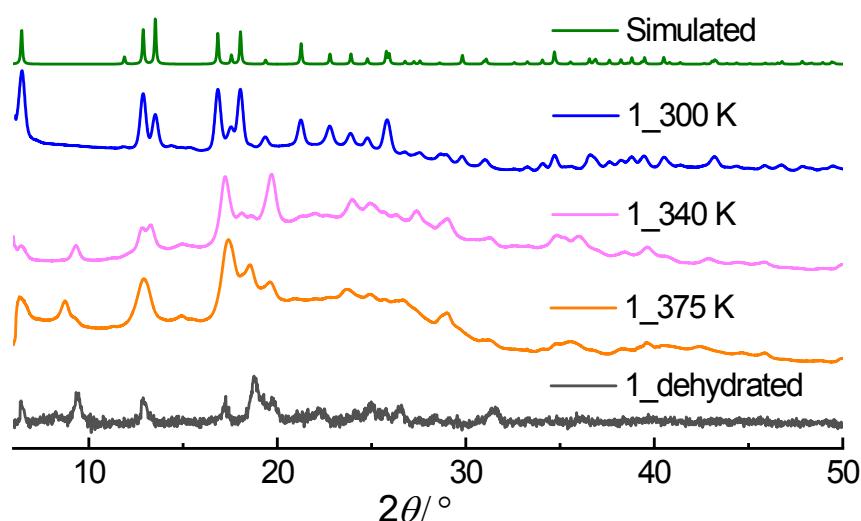
Fig. S3 The PXRD patterns of compound **1** at different temperature.
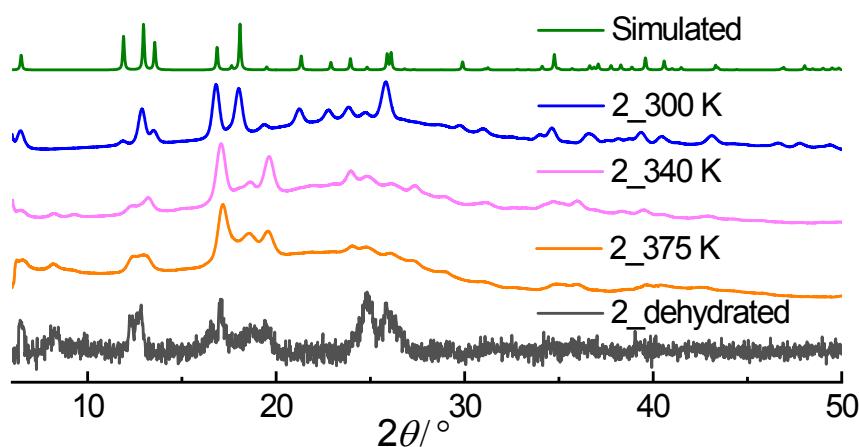
**Fig. S4** The PXRD patterns of compound **2** at different temperature.
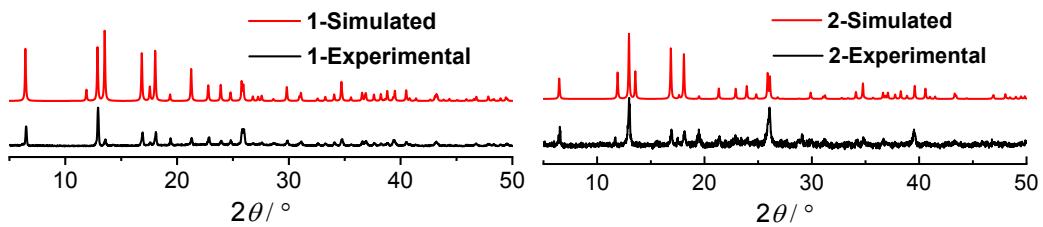
Fig. S5 The PXRD data of compounds **1** and **2** at room temperature collected for each batch.
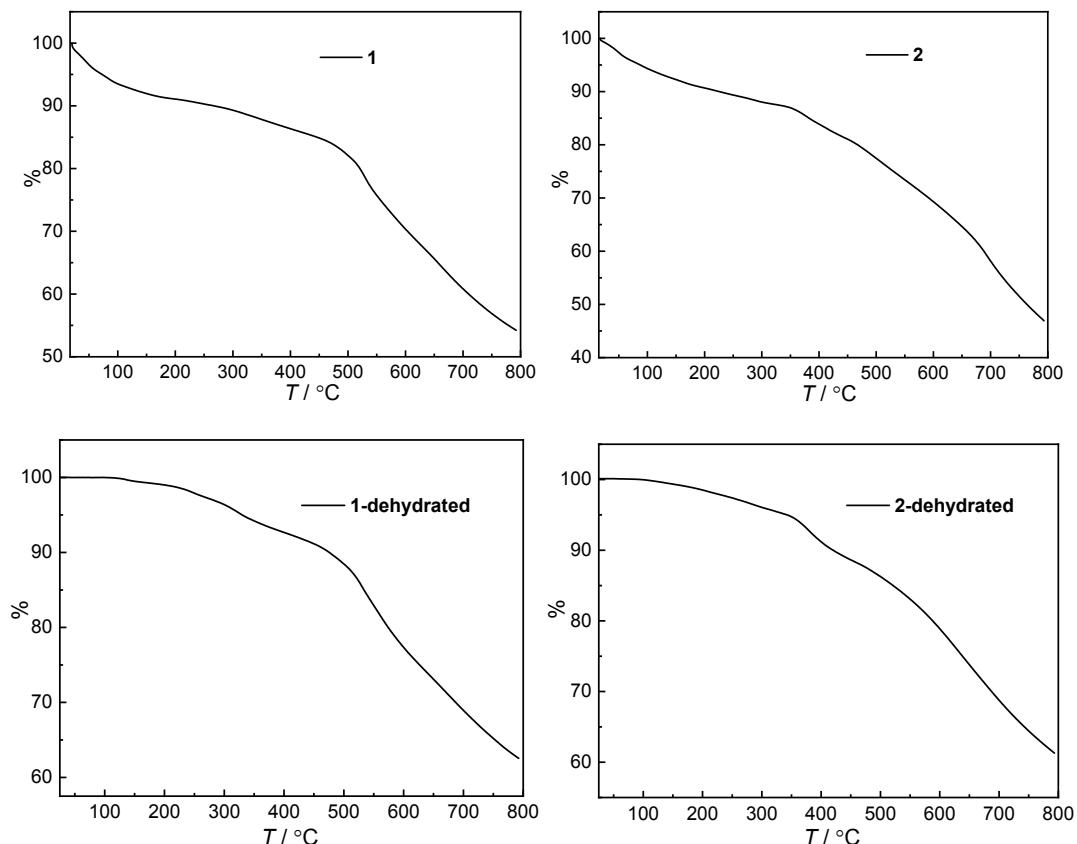

**Fig. S6** The TGA plots of compounds **1**, **2** and the dehydrated samples.
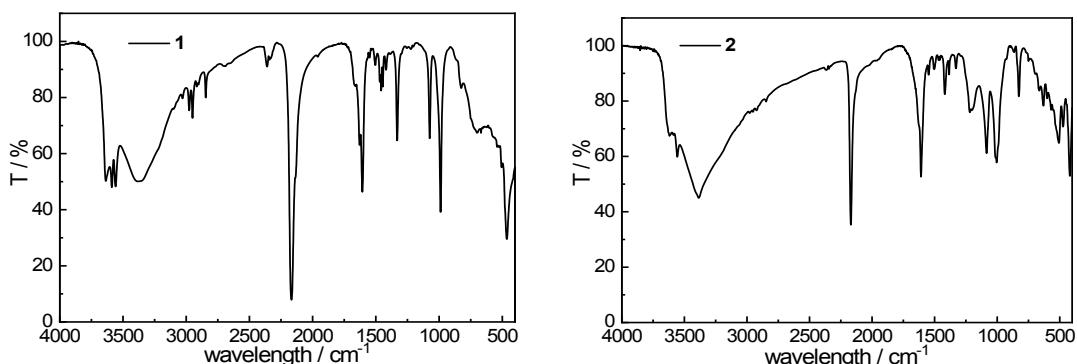
Fig. S7 The FIT-IR plots of compounds **1** and **2**.