Electronic Supplementary Material (ESI) for CrystEngComm

A rhombus channel metal-organic framework comprised of Sr^{2+} and thiophene-2, 5-dicarboxylic acid exhibiting novel dielectric bistability

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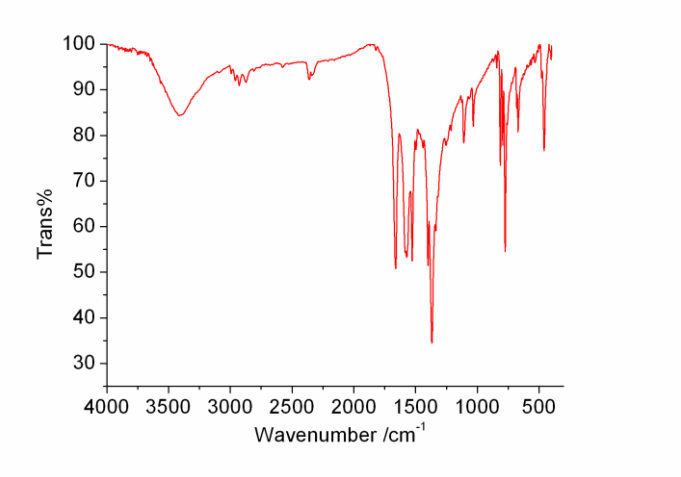


Figure S1 IR spectrum of MOF **1**.

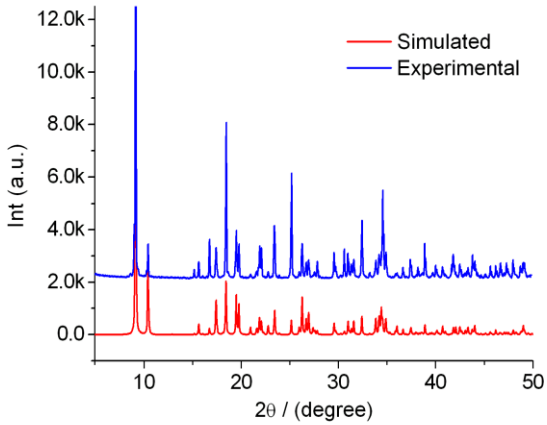


Figure S2 Experimental and simulated PXRD patterns of MOF **1**.

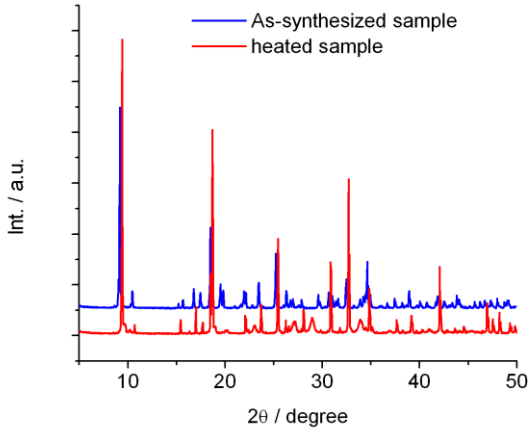


Figure S3 PXRD patterns of MOF **1** (Blue line: as-synthesized sample; red line: heated up to 260 °C and cooling down).

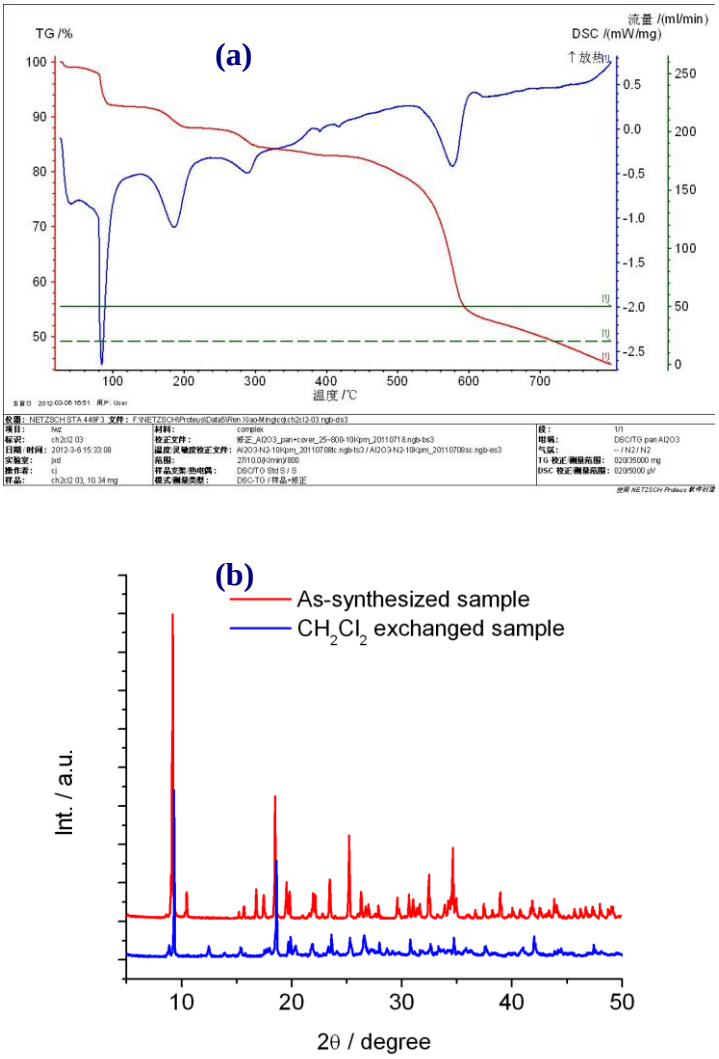
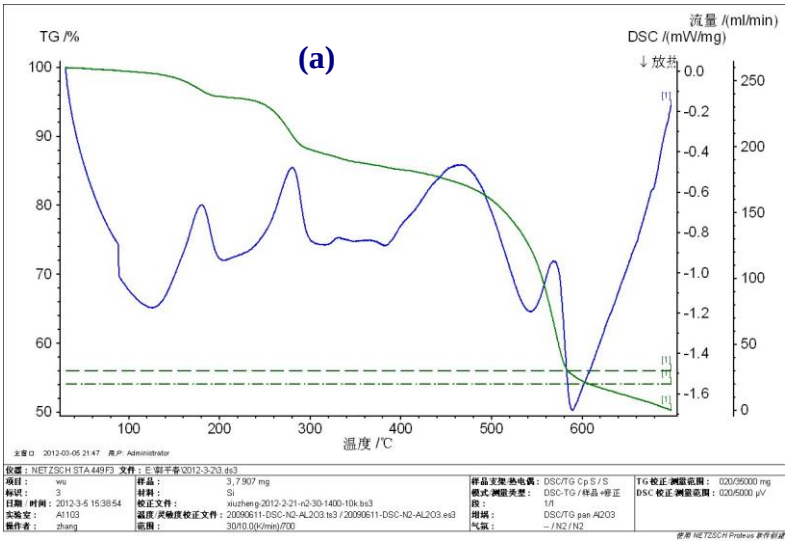


Figure S4 CH_2Cl_2 exchanged sample of MOF **1** (a) TG plot and (b) PXRD profiles for as-synthesized and CH_2Cl_2 exchanged samples.



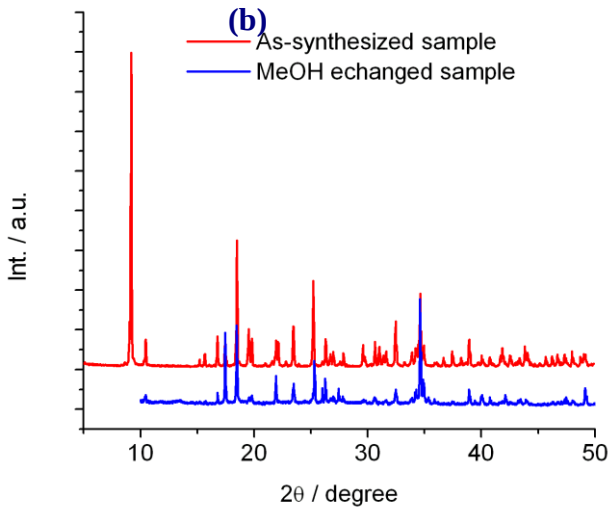


Figure 5 MeOH exchanged sample of MOF **1** (a) TG plot and (b) PXRD profiles for as-synthesized and MeOH exchanged samples.

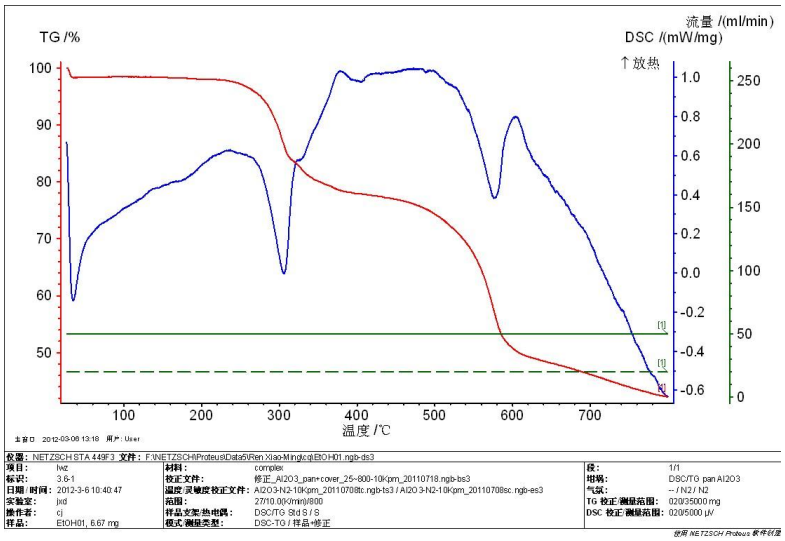


Figure S6 TG plot for the sample of MOF **1** using MeOH exchange.

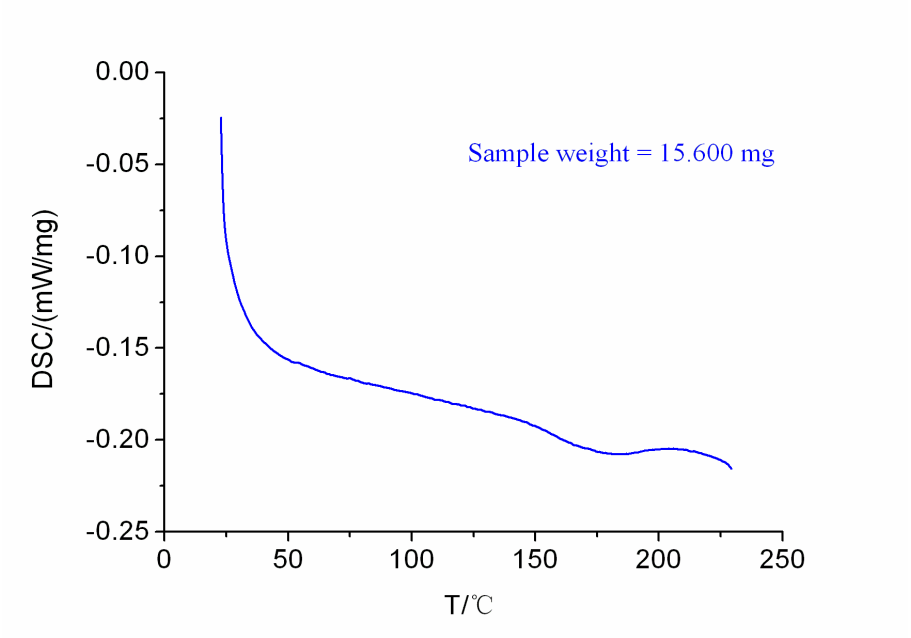


Figure S7 DSC curve of **1** in the region from 20 to 230°C.

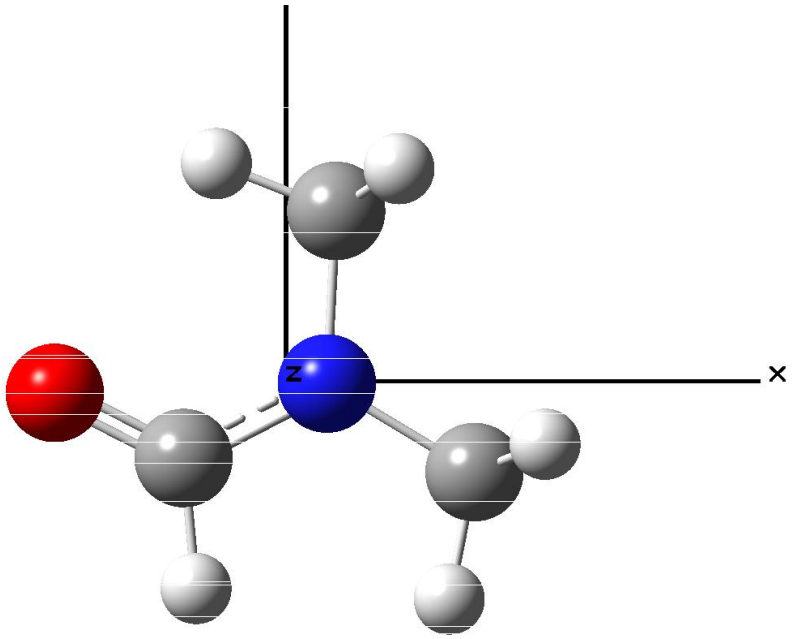


Figure S8 Optimized molecule structure of DMF and the Cartesian axes with dipole moments of X = 4.2073, Y = -0.4061, Z = 0.0001 and Tot = 4.2268 Debye.

New x-ray single crystal data

Table S1 Crystal data and structure refinements at 298 and 123 K for **1**

Chemical formula	$C_9H_9NO_5SSr$	
Formula weight	330.85	
Temperature (K)	298(2)	123(2)
Wavelength(Å)	0.71073	
Crystal system	Monoclinic	
Space group	$P\ 2_1/n$	
a (Å)	6.0028(12)	5.9896(5)
b (Å)	16.916(3)	17.0674(16)
c (Å)	11.649(2)	11.3975(10)
α (°)	90.00	90.00
β (°)	91.350(3)	91.2390(10)
γ (°)	90.00	90.00
V ($Å^3$) / Z	1182.5(4)/ 4	1164.86(18)/ 4
Density(g/cm^3)	1.858	1.887
Absorption coefficient (mm^{-1})	4.744	4.815
F(000)	656	656
Data collection θ range	2.12-27.56	2.15-27.55
Index range	$-7 \le h \le 5$	$-5 \le h \le 7$
	$-22 \le k \le 22$	$-22 \le k \le 22$
	$-15 \le l \le 15$	$-14 \le l \le 14$
Reflections collected	10549	10394
Independent reflections	2722	2686
R(int)	0.0494	0.0372
Absorption correction	Semi-empirical from equivalents	
Refinement method on F^2	Full-matrix least-squares	
Data/restraints/parameters	2722/0/182	2686/0/154
Goodness-of-fit on F^2	1.066	1.144
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0297, wR2 = 0.0822	R1 = 0.0327, wR2 = 0.0989
R indices (all data)	R1 = 0.0431, wR2 = 0.0885	R1 = 0.0398, wR2 = 0.1039

$R_1 = \Sigma(||F_0|-|F_c||)/\Sigma|F_0|$, $wR_2 = \Sigma w(|F_0|^2-|F_c|^2)^2/\Sigma w\ (|F_0|^2)^2]^{1/2}$

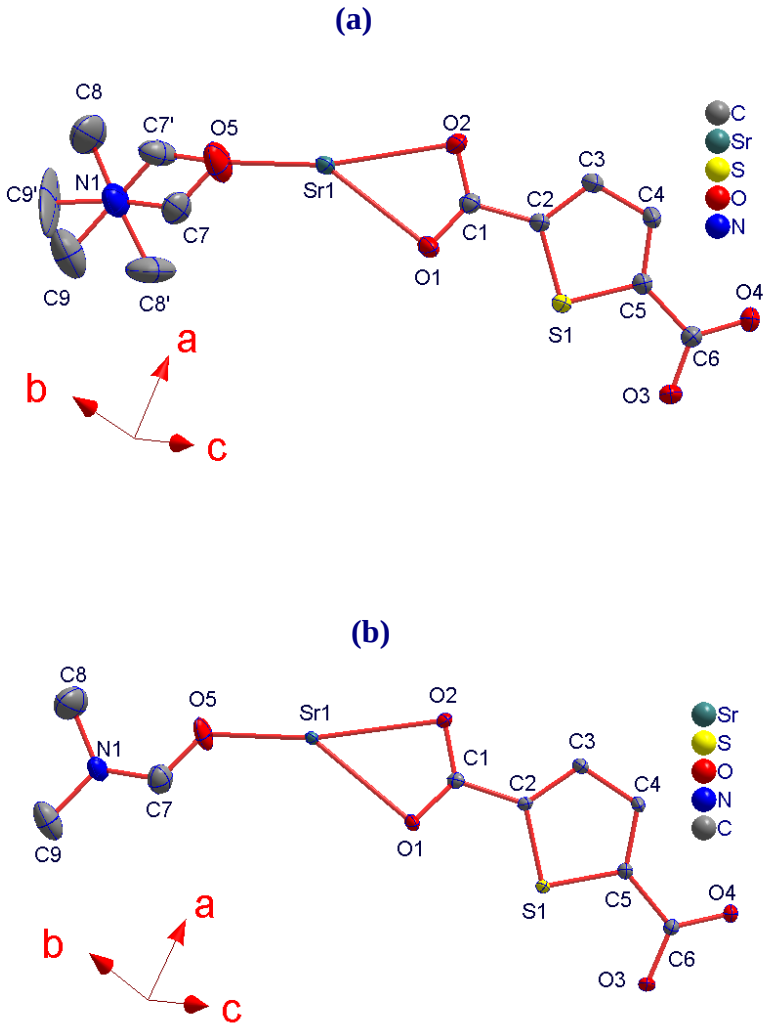


Figure S9 Asymmetric unit with thermal ellipsoids at 50% probability level (a) at 298 K and (b) 123 K, which show the disordered DMF molecule at 298 K froze at 123 K.