

Above-room-temperature dielectric and nonlinear optical switching materials based on the $[(\text{CH}_3)_3\text{S}]_2[\text{MBr}_4]$ ($\text{M} = \text{Cd}$, Mn and Zn)

Xiao-Gang Chen,^a Yao-Zu Zhang,^a Dong-Sheng Sun,^a Ji-Xing Gao,^a Xiu-Ni Hua,^a Wei-Qiang Liao^{*ab}

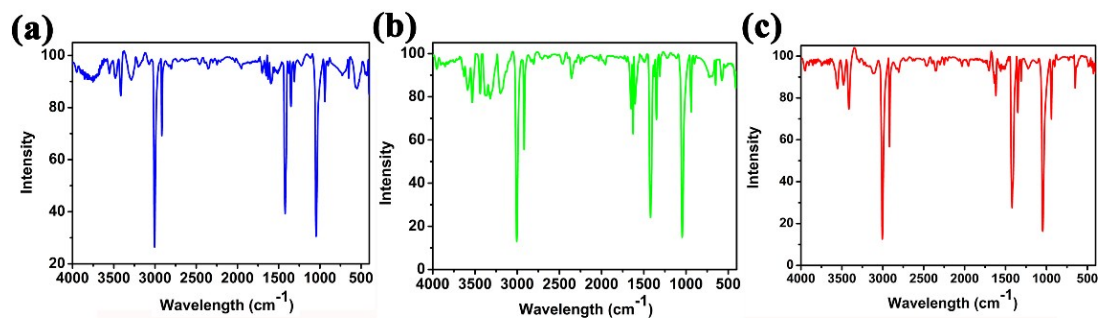


Figure S1. Infrared (IR) spectra of solids **1** (a), **2** (b) and **3** (c) in KBr pellet recorded on a Shimadzu model IR-60 spectrometer at room temperature.

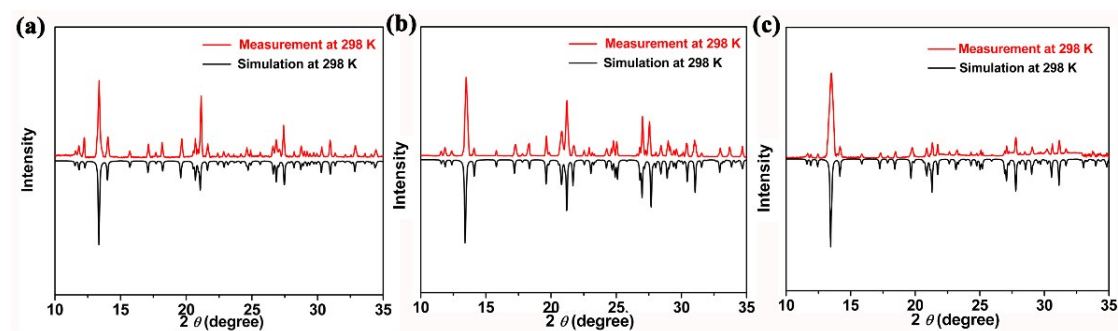


Figure S2. PXRD patterns of **1** (a) and **2** (b) and **3** (c) at room temperature.

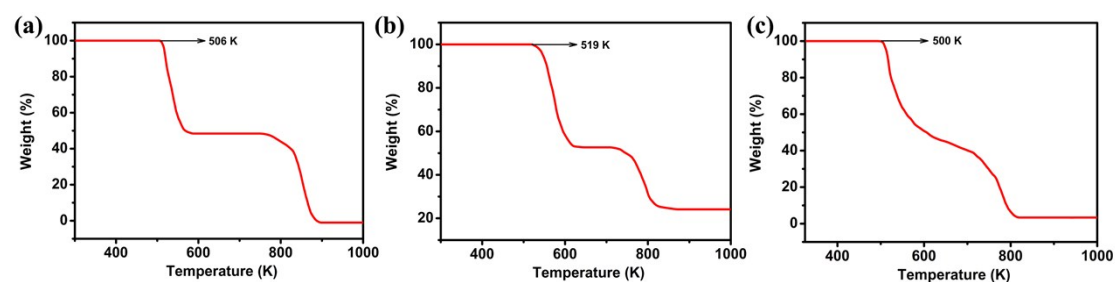


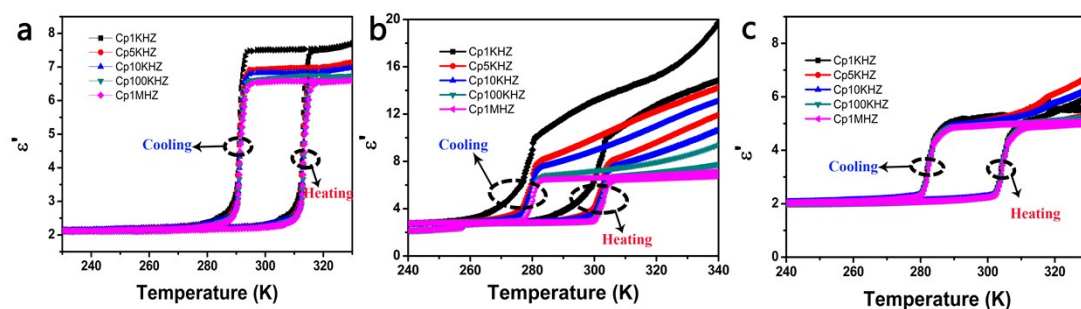
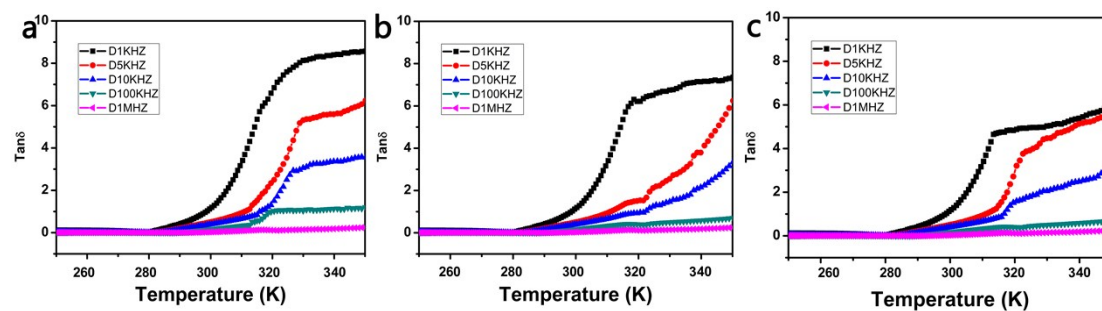
Figure S3. The TG curves of **1** (a), **2** (b) and **3** (c).

Table S1. Thermal analysis of **1**, **2** and **3** in the third circle.

Compound	T_c/K		$\Delta H/\text{KJ mol}^{-1}$	$\Delta S/\text{J K}^{-1}\text{mol}^{-1}$	N
1	heating	315 K	20.7	38.5	103
	cooling	283 K	19.8	41.0	139
2	heating	315 K	23.9	40.1	124
	cooling	283 K	22.9	42.8	172
3	heating	315 K	20.4	35.0	67
	cooling	278 K	19.4	37.6	92

Table S2. Crystal data of **1**, **2** and **3**.

Compound	1	2	3
Temperature	273 K	343 K	273 K
Formula	$[\text{Me}_3\text{S}]_2[\text{CdBr}_4]$	$[\text{Me}_3\text{S}]_2[\text{CdBr}_4]$	$[\text{Me}_3\text{S}]_2[\text{MnBr}_4]$
Formula weight	586.33	586.33	528.86
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$Pnma$	$Pnma$
a, b, c (Å)	9.0610(5) 13.2205(9) 14.3990(7)	12.547(3) 8.969(2) 16.063(4)	9.0416(3) 13.1334(6) 14.2839(6)
α, β, γ (°)	90 90 90	90 90 90	90 90 90
Volume /Å ³	1724.87(17)	1807.6(7)	1696.17(12)
Z	4	2	4

**Figure S4.** Temperature-dependent dielectric constants of **1** (a), **2** (b) and **3** (c) measured at selected frequencies (1 kHz -1 MHz)**Figure S5.** The temperature-dependence of dielectric loss ($\tan\delta$) of **1**, **2** and **3** measured at selected frequencies (1000 Hz-1 MHz) in the heating process.