Organic-Inorganic Hybrid Multifunctional Materials with High-Tc Reversible Phase Transition and Wide Bandgap Properties

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Experimental Section

Material synthesis and crystal growth

All reagents and solvents used in the synthesis are reagent grade and used without further purification. Weigh 1 mmol n-propyl-N-methylpiperidine and 2 mmol tetra Cadmium bromide hydrate, dissolve them in a mixture of 15 mL methanol and distilled water (1:1), stir for 30 min, and filter to obtain a colorless solution. After standing for volatilization, colorless transparent crystal compound **1** was obtained after one week: $[C_5H_{10}N(CH_3)CH_2CH_2CH_3]_2CdBr_4$ (**1**). Elemental analysis, calculated (%) **1**: C, 30.15; N, 3.910; H, 5.627. Found: C,30.12; N, 3.906; H, 5.629.

Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA)

The thermal properties of compound **1** was measured by differential scanning calorimetry (DSC) at a temperature change rate of 10 K/min during both cooling and heating cycles. The thermogravimetric analysis (TGA) measurement was performed on the TA-Instruments STD2960 system, and its temperature was from room temperature to 1100 K at a rate of 10 K/min.

Single Crystal X-Ray Diffraction Determination

Single crystal X-ray diffraction were carried out with the Bruker Smart Apex II single crystal diffractometer, which used a graphite monochromatic molybdenum sealed tube source (K_α radiation, λ= 0.71073). The single crystal structure data was collected at 300 K in the normal temperature stage, and the temperature of the sample was kept stable with a nitrogen stream, using the Cryostream Plus (Oxford Refrigeration System Company) accessory. The measured data uses the SHELXS and SHELXL programs, the related structural problems have been solved. The crystallographic information of the **1** determined at 300 K has been deposited in the CIF format in the Cambridge Crystallographic Database Center as supporting information (**1-LTP** CCDC 2282715).

Dielectric Measurement

The crystal is ground into powder particles and then pressed into tablets, and silver glue is thinly coated on the surface to make an electrode for dielectric research. In the temperature range (340 K - 400 K) of heating and cooling process, we measured the dielectric constant of the compounds with Agilent or TH2828A impedance analyzer at a frequency of 1 MHz.

UV−Vis Absorption

A Shimadzu UV-2550 spectrophotometer was used to measure UV−vis absorption spectra of crystal powder **1** in the range of 300-700 nm. The band gap is determined by the change of *Tauc*'s equation:

$$\left[hv \cdot F(R_\infty)\right]^{1/n} = A(hv - E_g)$$

Where h is the Planck constant, v is the vibration frequency, A is the proportional constant, E_g is the band gap, and $F(R_\infty)$ comes from the *Kubelka−Munk* equation: $F(R_\infty) = (1 - R_\infty)^2/2R_\infty$.

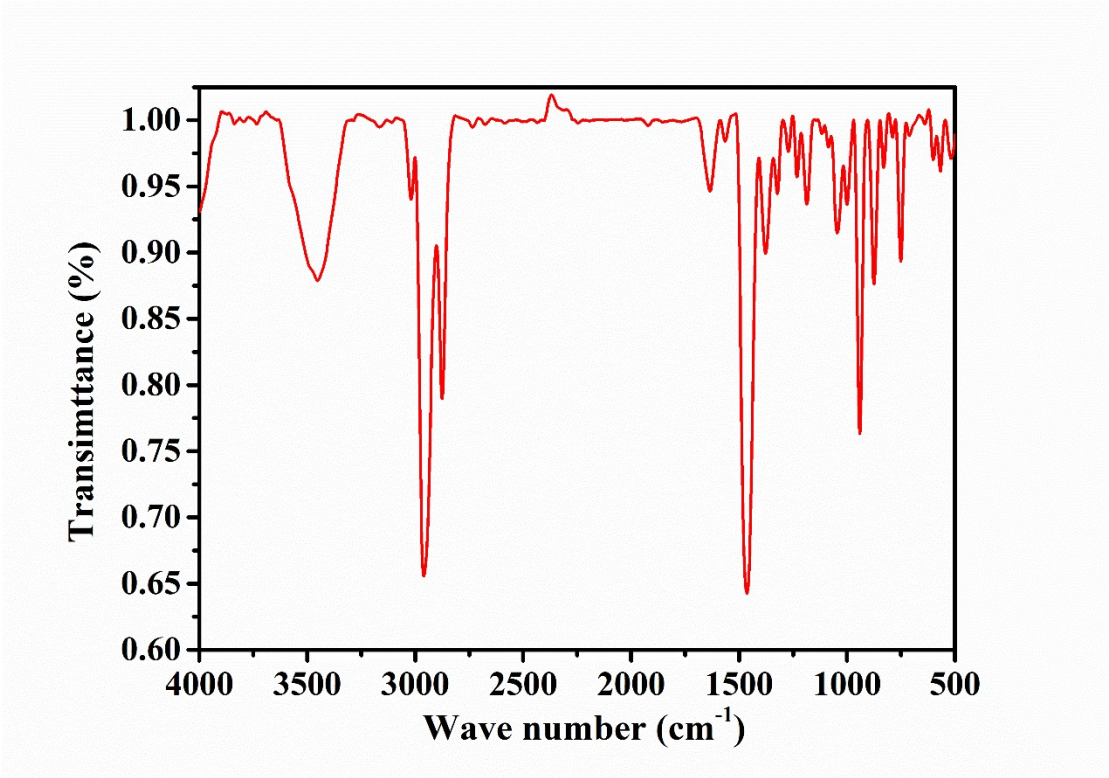

Fig. S1 Infrared spectrum of **1**.

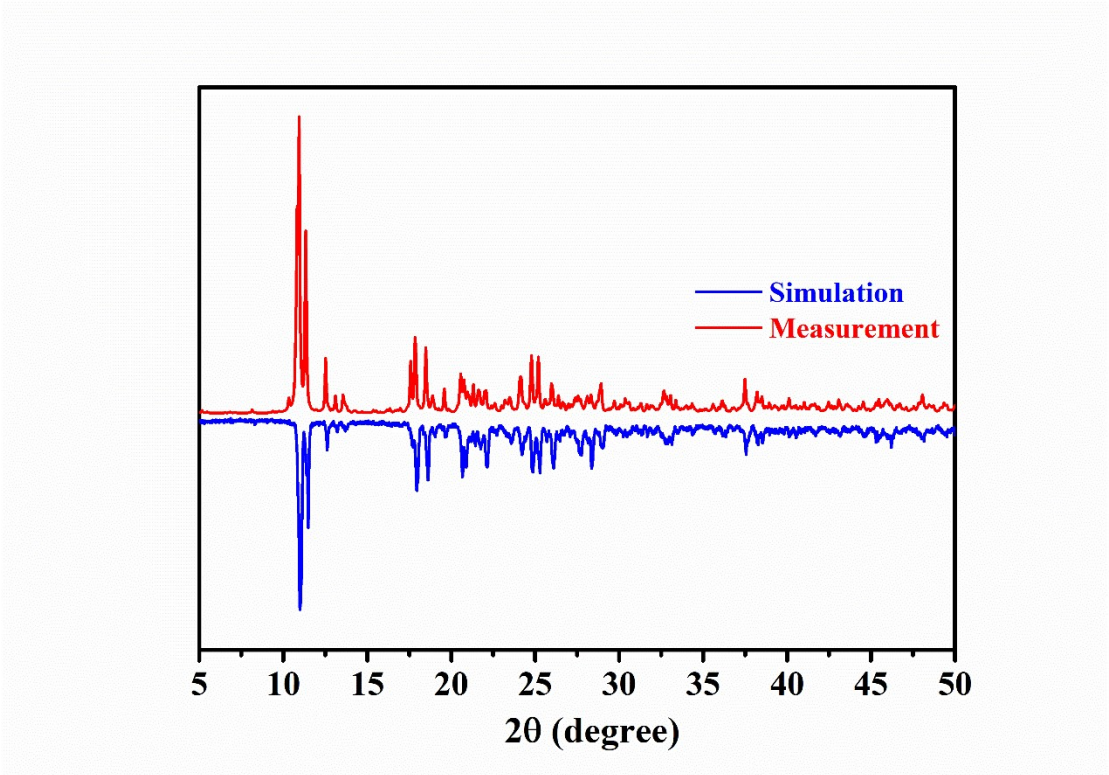

Fig. S2. The powder XRD of **1** with the simulated one in red and the measurement in blue.

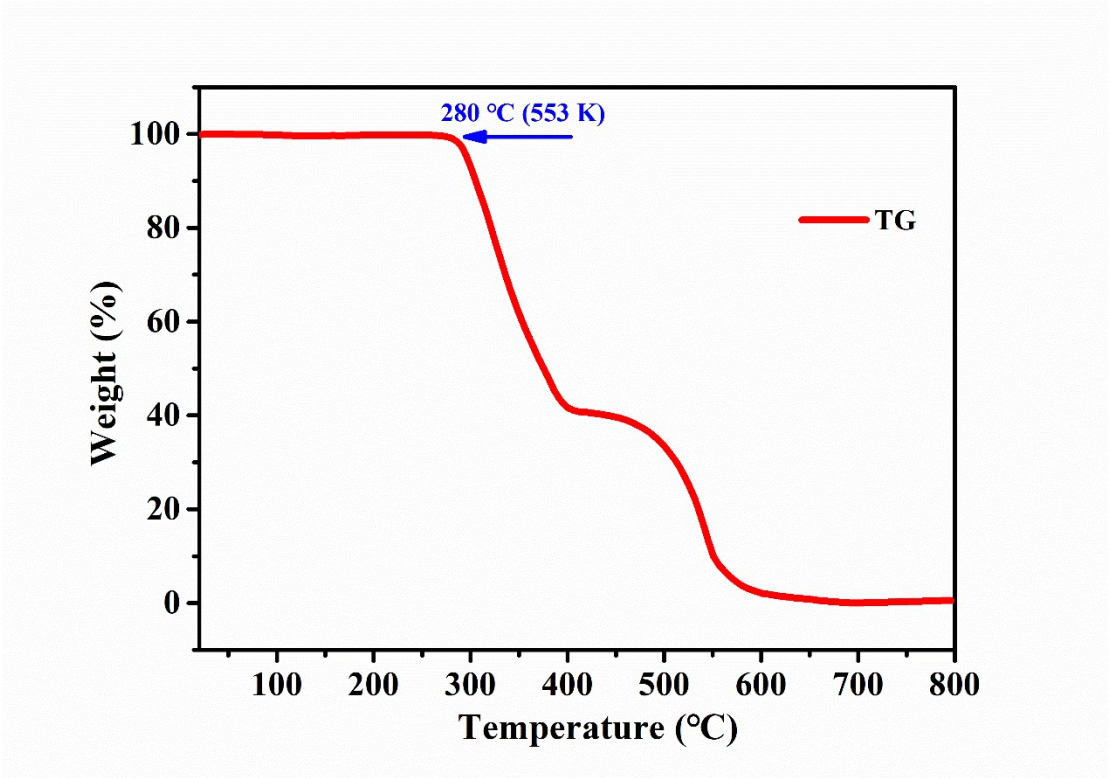

Fig. S3 TGA diagram for **1**

Table S1 Crystal data and structure refinement for 1

Compound	**1**
Empirical formula	$C_{18}H_{40}Br_4CdN_2$
Formula weight	716.53
Temperature/K	293.0
Crystal system	triclinic
Space group	*P*-1
a/Å	16.8749(14)
b/Å	19.2139(15)
c/Å	19.8184(15)
α/°	118.783(2)
β/°	92.300(2)
γ/°	103.276(2)
Volume/Å^3	5395.1(7)
Z	4
ρ_{calc}g/cm^3	1.764
μ/mm^{-1}	6.740
F(000)	2800.0
Final R indexes [I>=2σ (I)]	R_1 = 0.1389, wR_2 = 0.2239
Final R indexes [all data]	R_1 = 0.2067, wR_2 = 0.2510

Calculation of ΔS and N

1:

In the heating cycle mode

$$\Delta S_{\text{н}} = RlnN_1$$

$$= \int_{T_2}^{T_1} \frac{Q}{T} dT$$

$$= \frac{11.14\, J \cdot g^{-1} \times 716.6\, g \cdot mol^{-1}}{333.0K}$$

$$= 23.97\, J \cdot mol^{-1} \cdot K^{-1}$$

$$N_1 = \exp\left(\frac{\Delta S_2}{R}\right)$$

$$= \exp \frac{23.97\, J \cdot mol^{-1} \cdot K^{-1}}{8.314\, J \cdot mol^{-1} \cdot K^{-1}}$$

$$= 17.87$$

In the cooling cycle mode

$$\Delta S_{\text{с}} = RlnN_2$$

$$= \int_{T_1}^{T_2} \frac{Q}{T} dT$$

$$= \frac{10.92\, J \cdot g^{-1} \times 716.6\, g \cdot mol^{-1}}{325.0\, K}$$

$$= 24.08\, J \cdot mol^{-1} \cdot K^{-1}$$

$$N_2 = \exp\left(\frac{\Delta S_2}{R}\right)$$

$$= \exp \frac{24.08\, J \cdot mol^{-1} \cdot K^{-1}}{8.314\, J \cdot mol^{-1} \cdot K^{-1}}$$

$= 18.11$