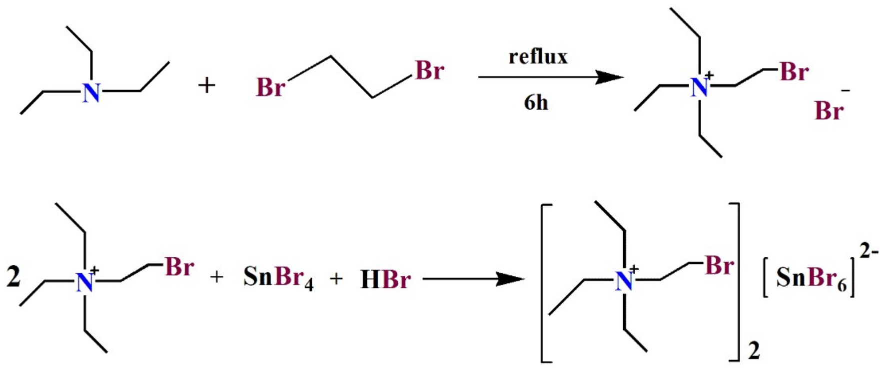
Multisequential reversible phase transition materials with Semiconducting and fluorescence properties：$(C_8H_{18}BrN)_2SnBr_6$

Yao Liu, Yu-Kong Li, Ting-Ting Ying, Ding-Chong Han, Yu-Hui Tan,* Yun-Zhi Tang,* Peng-kang Du, Hao Zhang

(Faculty of Materials Metallurgy and Chemistry, Jiangxi University of Science and Technology, Ganzhou, 341000, Jiangxi Province, P. R. China)



Scheme 1. Schematic diagrams of synthesis of compound **1**

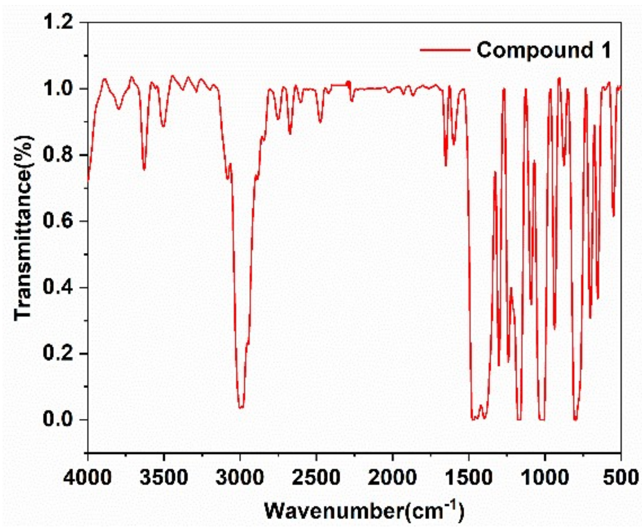


Fig. S1 Infrared spectrum of compound **1**

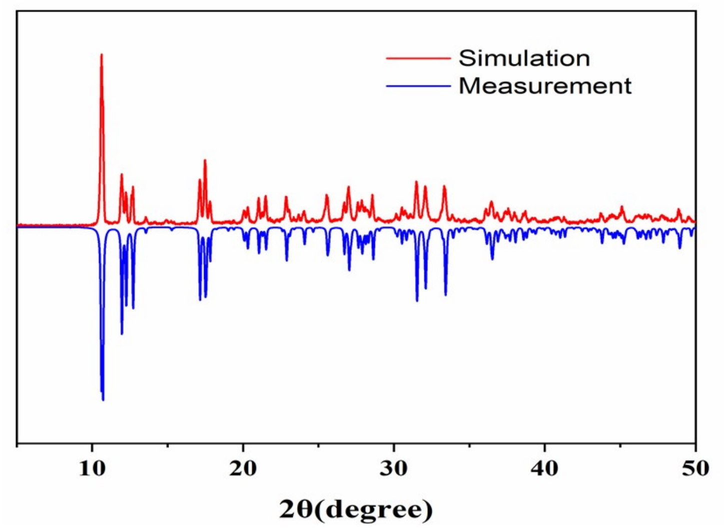


Fig. S2 The powder XRD of **1**.

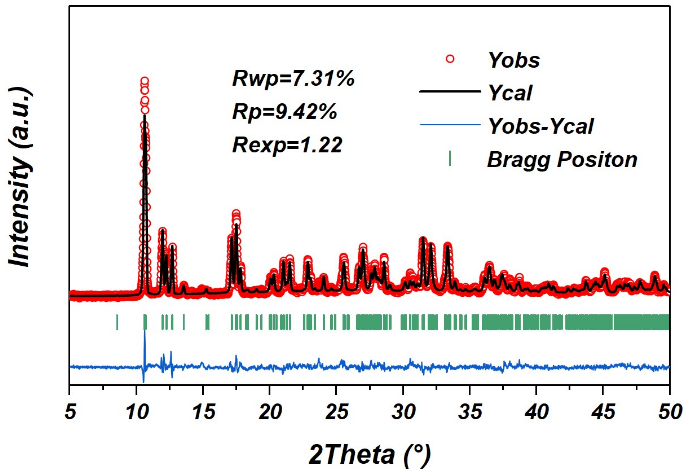


Fig. S3 Powder X-ray diffractograms of **1** collected in 300 K (**LTP**), refined by Le Bail method using the FULLPROF program. The lattice parameters obtained from the fitting: *a*= 14.4563(9), *b*= 14.7985(3), *c*= 13.9563(5) Å (R_p = 7.31%, R_{wp} = 9.42%, R_{exp} = 1.22%).

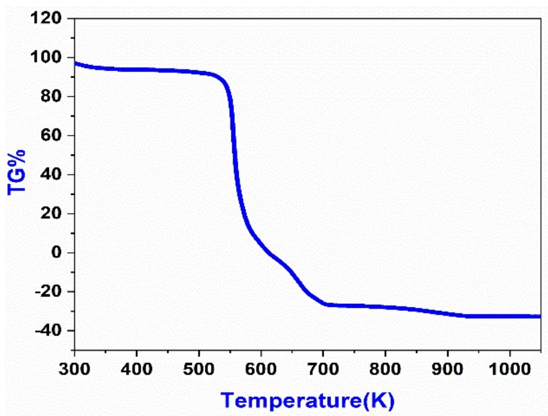


Fig. S4 TG-DTA curves for **1.**

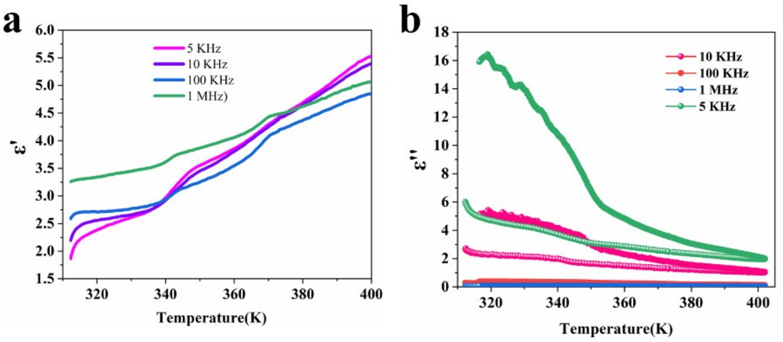


Fig. S5 (a) The frequency dependence of the dielectric of compound **1** during heating. (b) Temperature-dependent imaginary part (ε'') of the permittivity of **1** measured at selected frequencies in heating and cooling modes

Table.S1 Crystal data and refinement parameters for **1**

Compound	**1**
Empirical formula formula	$C_{16}H_{36}Br_8N_2Sn$
Temperature (K)	300 K
Crystal system	monoclinic
Space group	*C*2/*c*
a (Å)	14.4401(14)
b (Å)	14.7764(13)
c (Å)	13.9147(12)
α/°	90
β/°	90.855(3)
γ/°	90
V (Å^3)	2968.7(5)
Z	4
ρ calcg/cm^3	2.270
μ/mm^{-1}	11.636
F(000)	1904.0
R_1, wR_2[I> 2σ(I)]	R_1 = 0.0655, wR_2 = 0.1322
R_1, wR_2(all data)	R_1 = 0.1151, wR_2 = 0.1596

Calculation of ΔS and N

The first stage：

In the cycle heating mode

$\Delta S_H = R\ln N$

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

$$\approx \frac{\Delta H}{Tc}$$

$$= \frac{4.300J^{-1}mol \times 1014.44g^{-1}mol}{353K}$$

$=12.36J\cdot mol^{-1}\cdot K^{-1}$

$$N_1 = \exp\left(\frac{\Delta S_H}{R}\right) = \exp\left(\frac{12.36J \cdot mol^{-1} \cdot K^{-1}}{8.314J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$=4.410$

In the cooling cycle mode

$\Delta S_C = R\ln N$

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

$$\approx \frac{\Delta H}{Tc}$$

$$= \frac{4.104J^{-1}mol \times 1014.44g^{-1}mol}{345K}$$

$=12.07J\cdot mol^{--1}\cdot K^{--1}$

$$N_2 = \exp\left(\frac{\Delta S_C}{R}\right) = \exp\left(\frac{12.07J \cdot mol^{-1} \cdot K^{-1}}{8.314J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$=4.263$

$\Delta S_H = R\ln N1$

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

$$\approx \frac{\Delta H}{Tc}$$

$$= \frac{4.300J^{-1}mol \times 1014.44g^{-1}mol}{353K}$$

$=12.36J\cdot mol^{-1}\cdot K^{-1}$

$$N_1 = \exp\left(\frac{\Delta S_H}{R}\right) = \exp\left(\frac{12.36J \cdot mol^{-1} \cdot K^{-1}}{8.314J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$=4.410$

In the heating cycle mode

$\Delta S_{H} = R\ln N1$

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

$$\approx \frac{\Delta H}{Tc}$$

$$= \frac{0.854 J^{-1} mol \times 1014.44 g^{-1} mol}{384 K}$$

$=2.25 J\cdot mol^{-1}\cdot K^{-1}$

$$N_1 = \exp\left(\frac{\Delta S_H}{R}\right) = \exp\left(\frac{2.25 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$=1.310$

In the cooling cycle mode

$\Delta S_{C} = R\ln N$

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

$$\approx \frac{\Delta H}{Tc}$$

$$= \frac{0.975 J^{-1} mol \times 1014.44 g^{-1} mol}{374 K}$$

$=2.645 J\cdot mol^{--1}\cdot K^{--1}$

$$N_2 = \exp\left(\frac{\Delta S_C}{R}\right) = \exp\left(\frac{2.645 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$=1.374$