Electronic Supplementary Materials (ESI)

Rare earth molecular ferroelectrics with piezoelectric response

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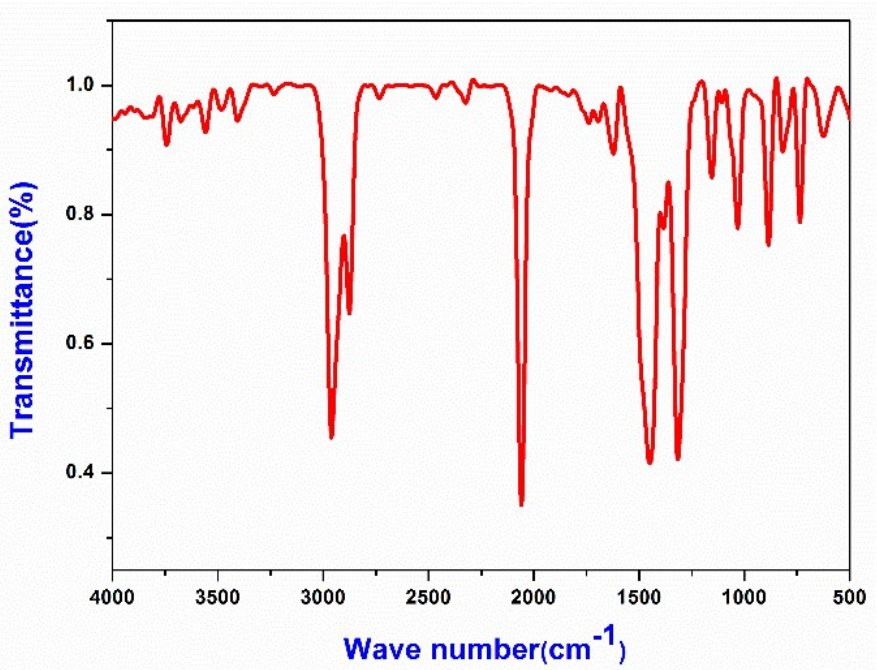

Fig. S1 Infrared spectrum of compound **1.**

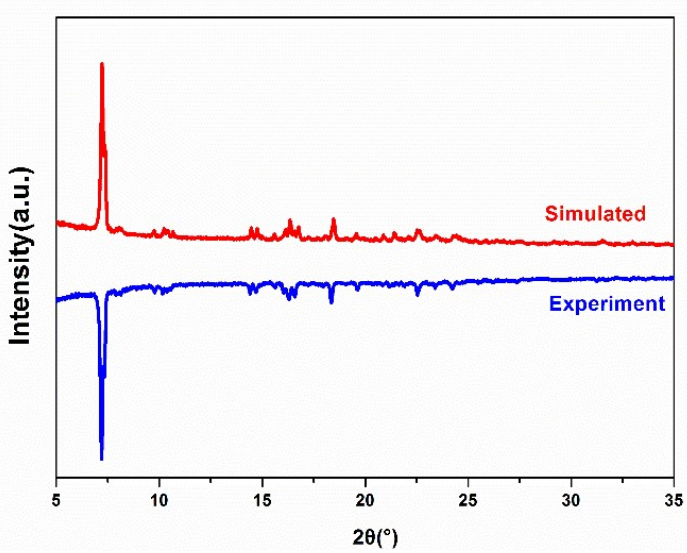

Fig. S2 The powder XRD of **1** with the simulated one in red and the measurement in blue.

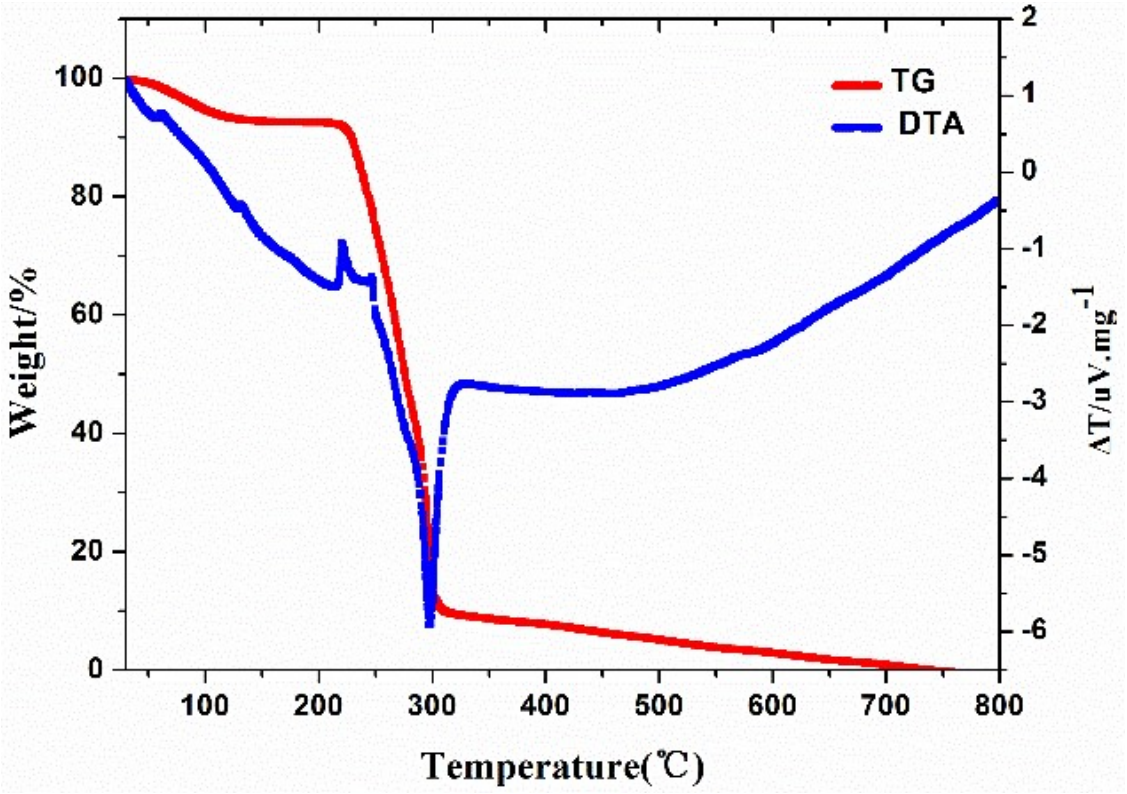

Fig. S3 TG-DTA curves for **1**

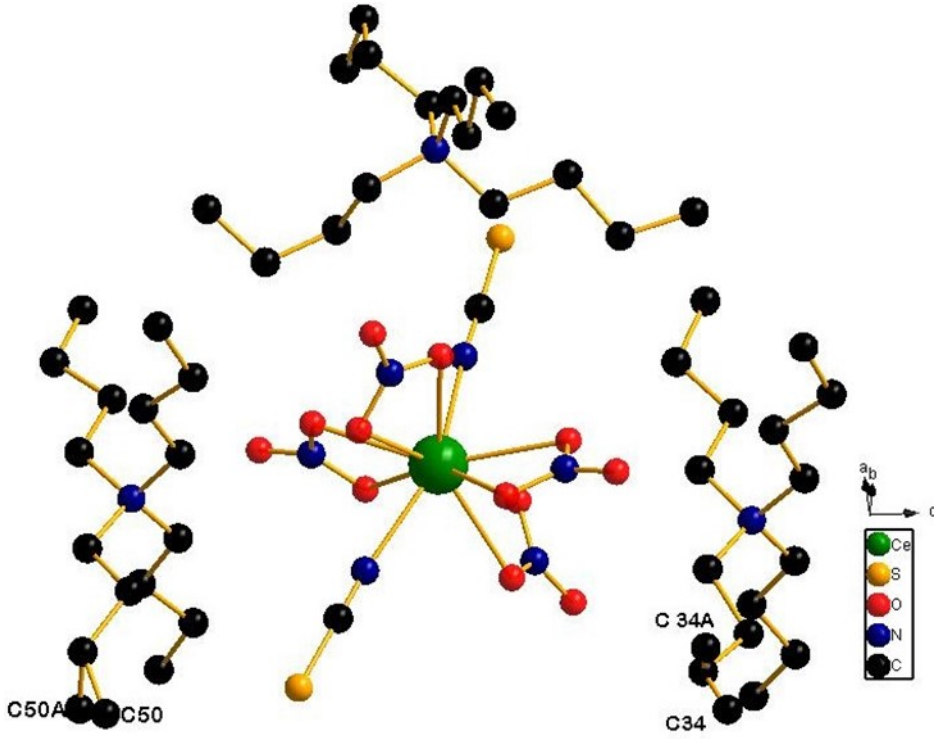

Fig. S4. The asymmetric structure of **1**-LTP

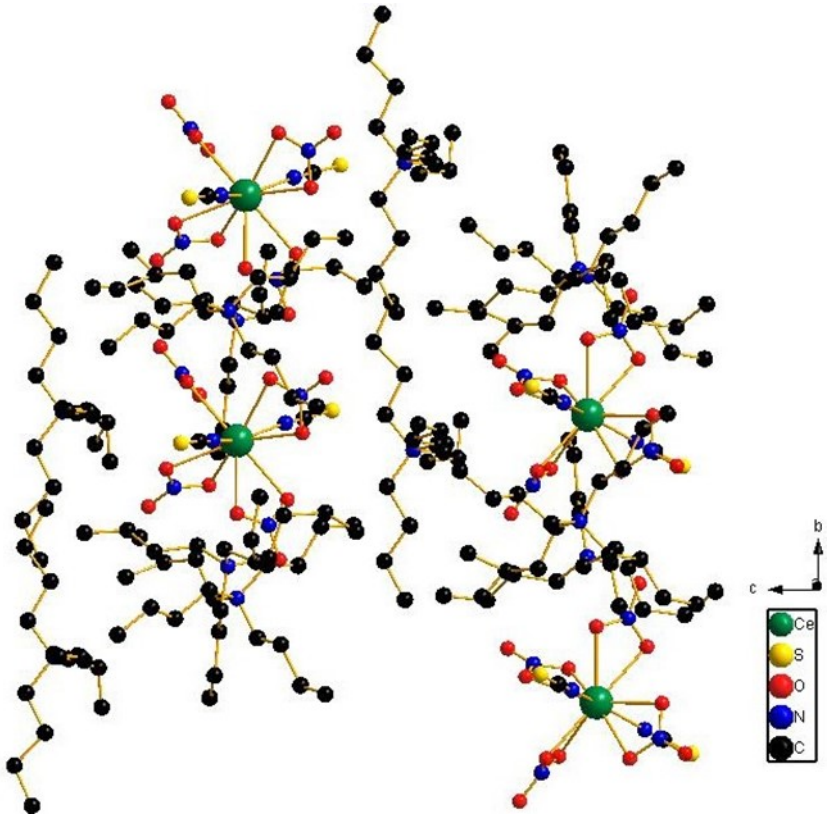

Fig. S5. The unit cell structure of **1-LTP**

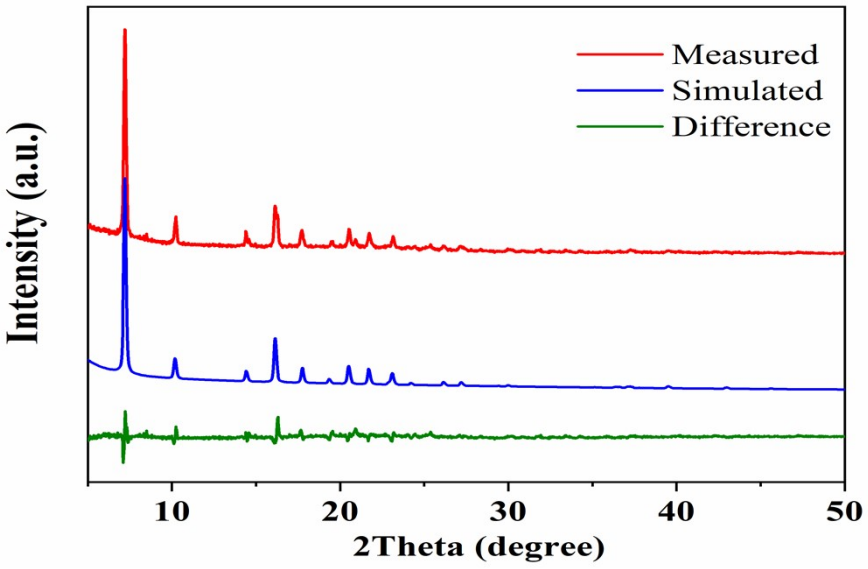

Fig. S6. The structural refinement results of PXRD data for **1** in 350 K.

Table S1 Crystal data and structure refinement for 1

Compound	**1**
Empirical formula	$C_{50}H_{108}CeN_9O_{12}S_2$
Formula weight	1231.69
Temperature/K	293
Crystal system	monoclinic
Space group	Cc
a/Å	16.1541(2)

b/Å	18.0486(2)
c/Å	23.7037(3)
α/°	90
β/°	91.1550(10)
γ/°	90
Volume/Å^3	6909.62(14)
Z	4
ρ_{calc}g/cm^3	1.184
μ/mm^{-1}	0.774
F(000)	2628.0
Final R indexes [I>=2σ (I)]	R_1 = 0.0363, wR_2 = 0.0981
Final R indexes [all data]	R_1 = 0.0390, wR_2 = 0.0994

Calculation of ΔS and N

Compound 1:

In the heating cycle mode

$$\Delta S_H = R\ln N_1$$

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

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

$$= \frac{11.62 J^{-1} mol \times 1231.7 g^{-1} mol}{408 K}$$

$$= 35.32\ J \cdot mol^{-1} \cdot K^{-1}$$

$$N_1 = \exp\left(\frac{\Delta S_H}{R}\right) = \exp\left(\frac{35.32 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$$= 54.00$$

In the cooling cycle mode

$$\Delta S_C = R\ln N_2$$

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

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

$$= \frac{7.9 J^{-1} mol \times 1231.7 g^{-1} mol}{376 K}$$

$$=25.97 J \cdot mol^{-1} \cdot K^{-1}$$

$$N_2 = \exp\left(\frac{\Delta S_c}{R}\right) = \exp\left(\frac{25.97 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$$=24.00$$