Electronic Supplementary Information (ESI)

High-T_p-Triggered Phase Transition Exhibiting Switchable Dielectric-Thermal Responses and Long Photoluminescence Lifetime in a Novel Inclusion Luminophor

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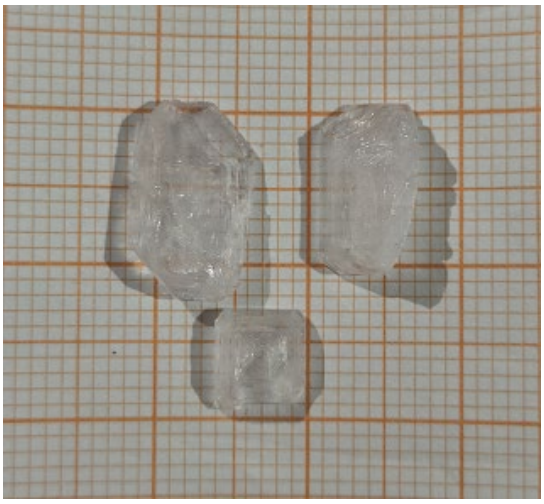

Fig. S1. The single crystals of **1**.

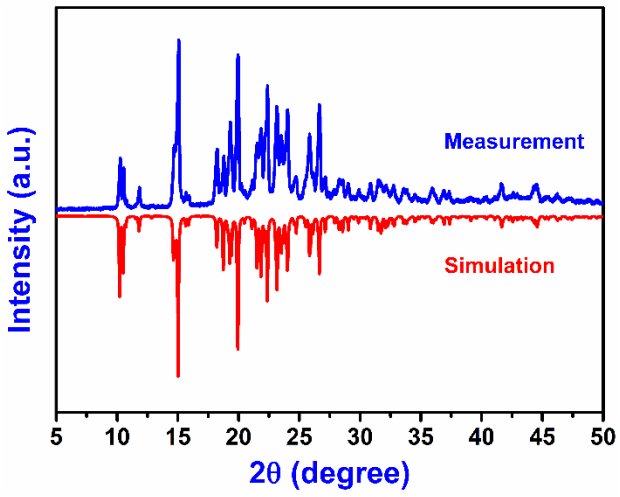

Fig. S2. PXRD (powder X-ray diffraction) measurement comparison with single crystal simulation of **1** at room temperature.

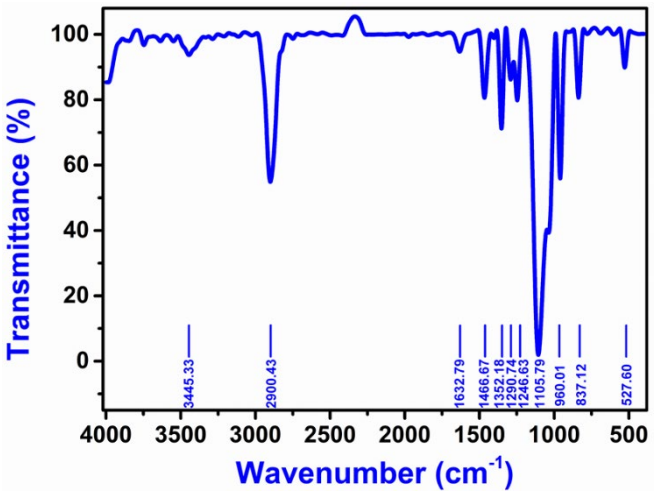

Fig. S3. The infrared (IR) spectra of **1** at room temperature.

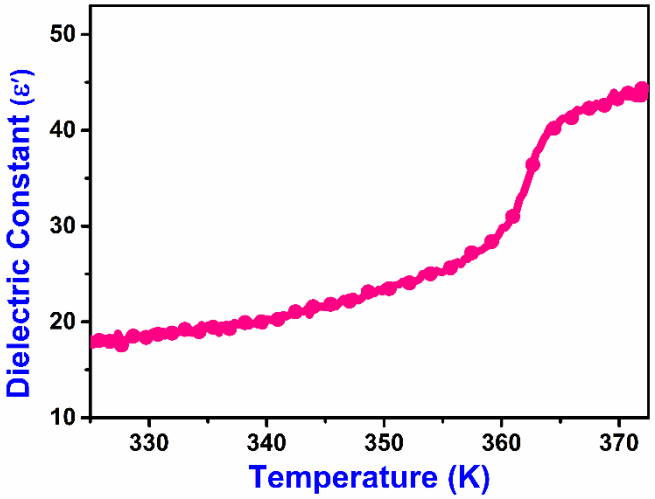

Fig. S4. The temperature-dependence of dielectric constant (ε′) at the frequency of 100 kHz of **1**.

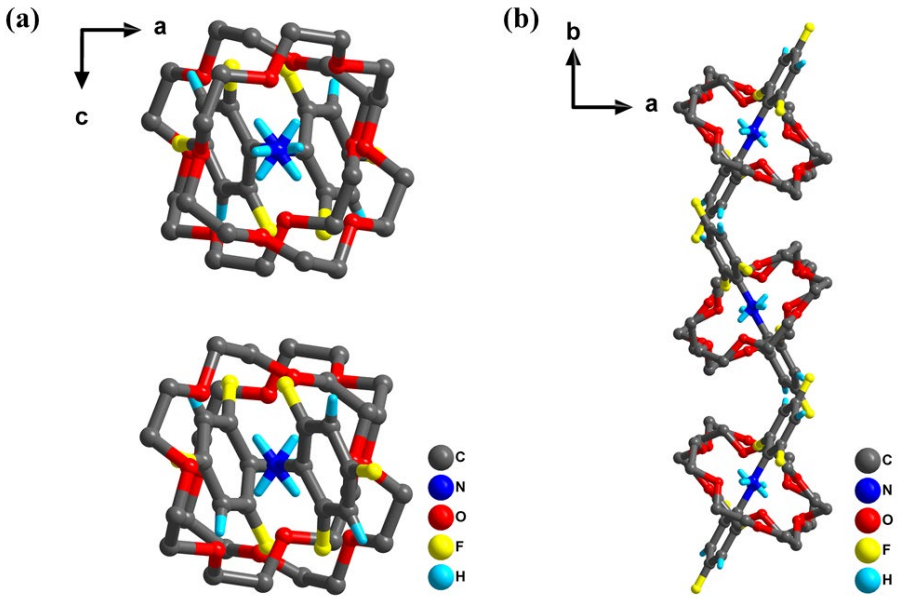

Fig. S5. The packing of supramolecular cations viewed along *b*-axis (a) and *c*-axis (b) of **1**, respectively.

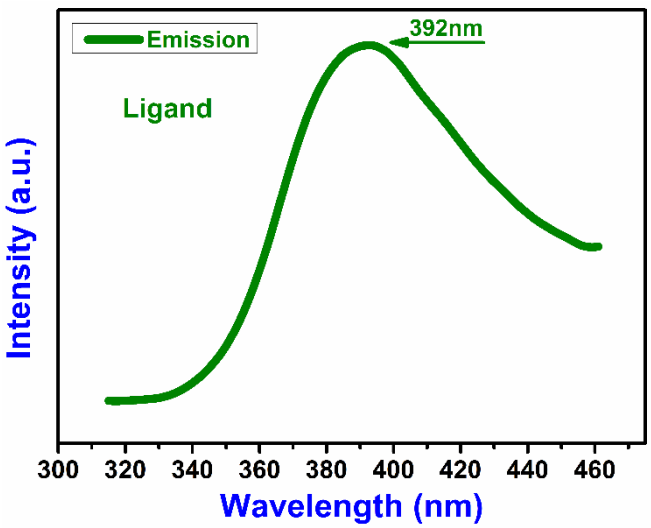

Fig. S6. The room-temperature photoluminescence (PL) spectrum of the ligand (2,4,6-trifluoroaniline).

Model	ExpDec2		
Equation	y = A1*exp(-x/t1) + A2*exp(-x/t2) + y0		
Reduced Chi-Sqr	6.09488E8		
Adj. R-Square	0.93762		
		Value	Standard Error
S1	y0	75815.95284	2762.30836
	A1	336143.23106	18045.72693
	t1	0.28378	0.01984
	A2	6.36353E7	2.90989E7
	t2	0.01084	0.00107
	k1	3.52384	0.2464
	k2	92.25289	9.06822
	tau1	0.1967	0.01375
	tau2	0.00751	7.38563E-4

Fig. S7. The related parameters of fluorescence lifetime of **1**.

Table S1. The crystallographic data and structure refinements for **1** at room temperature.

[(2,4,6-trifluoroanilinium)-(18-crown-6)][BF_4]			
294 K			
Formula weight	499.23	*Z*	4
Crystal system	Monoclinic	Density (g/cm^3)	1.377
Space group	$P2_1/c$	m (mm^{-1})	0.134
a (Å)	8.4188(4)	F (000)	1040.0
b (Å)	16.5033(8)	Data/restraints/parameters	5488/58/336
c (Å)	17.3275(8)	GOF	1.019
α (°)	90	R_1, $wR_2[I >= 2\sigma(I)]$	R_1 = 0.0730, wR_2 = 0.1699
β (°)	90.263(2)	R_1, wR_2 (all data)	R_1 = 0.1244, wR_2 = 0.2053
γ (°)	90	$\triangle\rho_{max}/\triangle\rho_{min}$ (eÅ^{-3})	0.50/-0.36
V (Å^3)	2407.4(2)	CCDC	2130929

Table S2. Intermolecular hydrogen bond lengths (Å) and angles (degrees) for **1**.

D−H···A	D−H	H···A	D···A	∠D−H···A
N1−H1C···O3	0.89	1.97	2.861(3)	174
N1−H1D···O1	0.89	2.02	2.884(3)	164
N1−H1E···O5	0.89	1.94	2.815(3)	169

Calculation of Δ*S* and *N*

In the heating cycle mode

$\Delta S_1 = R\ln N_1$

$$\Delta S_1 = \int_{T_2}^{T_1} \frac{Q}{T} dT$$

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

$$= \frac{11.82 g^{-1} J \times 499.23 mol^{-1} g}{364 K}$$

$$= 16.21 J \cdot mol^{-1} \cdot K^{-1}$$

$$N_1 = \exp\left(\frac{\Delta S_1}{R}\right) = \exp\left(\frac{16.21 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$$= 7.03$$

In the cooling cycle mode

$\Delta S_2 = R\ln N_2$

$$\Delta S_2 = \int_{T_2}^{T_1} \frac{Q}{T} dT$$

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

$$= \frac{9.30 g^{-1} J \times 499.23 mol^{-1} g}{361 K}$$

$$= 12.86 J \cdot mol^{-1} \cdot K^{-1}$$

$$N_2 = \exp\left(\frac{\Delta S_1}{R}\right) = \exp\left(\frac{12.86 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}\right)$$

$$= 4.70$$