Electronic Supplementary Material (ESI) for RSC Advances.

Reversible structural phase transition, ferroelectric and switchable dielectric properties in an adduct molecule of hexamethylenetetramine ferrocene carboxylic acid

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Supporting Materials

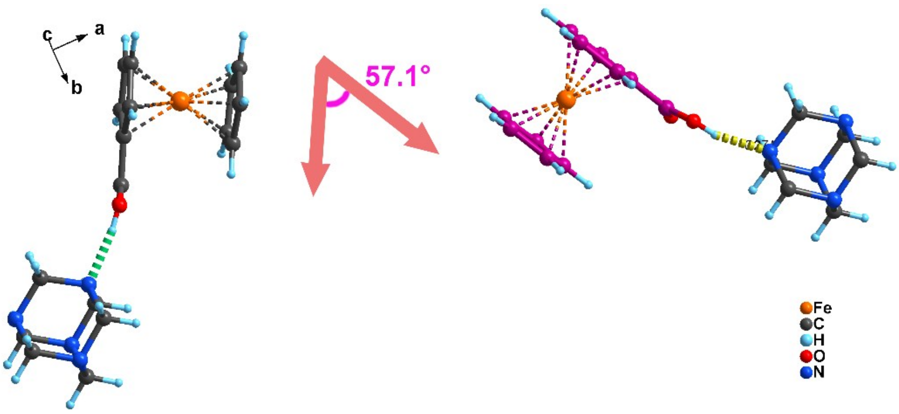

Figure S1the torsionangle between the two cyclopentadienyl carboxylic acid planes of **1-LTP**.

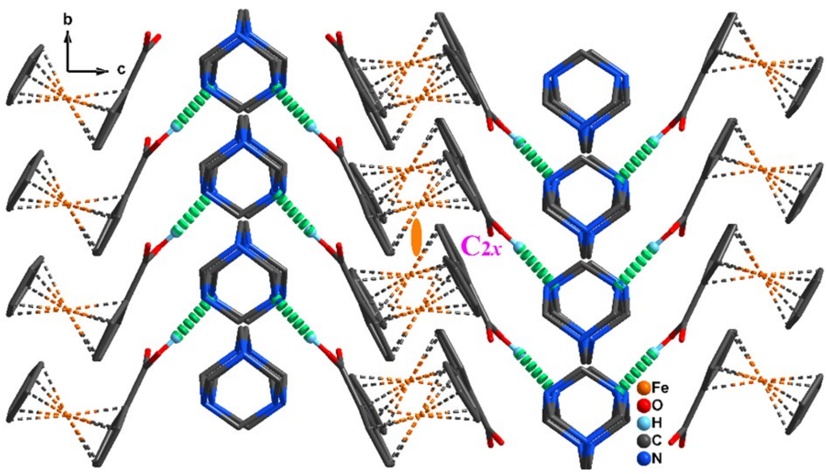

Fig. S2 the packing structure of **1-RTP** shows the symmetrical operations along the *a*-axis direction

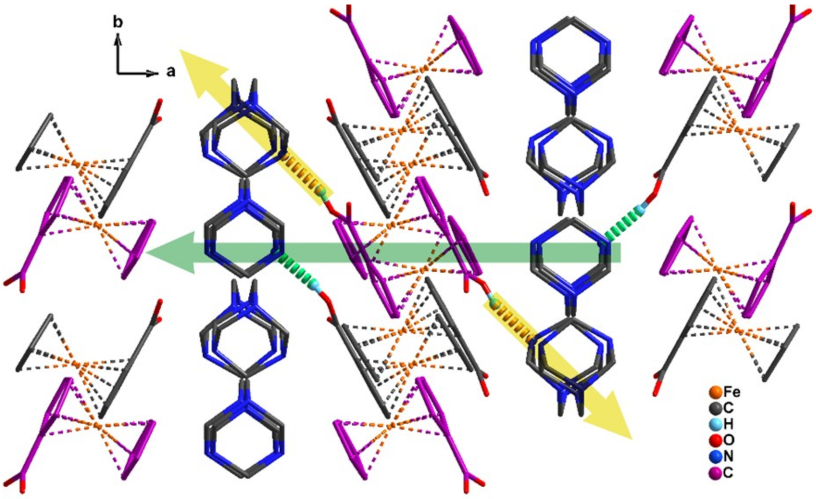

Fig. S3 the packing structure of **1-LTP** shows the symmetrical operations along the *c* axis direction

2 Calculation ofΔS and N for Compound 1

According to the Boltzmann equation, $\Delta S = nR\ \ln(N)$, where ΔS is the entropy change extracted from the C_p data, n is the number of guest molecules per mole (n = 1, here), R is the gas constant, and N is the number of possible orientations for the disordered system. The calculations of ΔS and N values on the heating and cooling processes of **1** are as follows:

2.1 In the cooling cycle mode

$$\Delta S_1 = \int_{T1}^{T2} \frac{Q}{T} dT$$

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

$$= \frac{0.9171\ J{\cdot}g\ -1 \times\ 370.24\ g{\cdot}mol - 1}{182.0\ K}$$

$$= 1.866\ J{\cdot}mol^{-1}{\cdot}K^{-1}$$

$$\Delta S_1 = R \ln N_1$$

$$N_1 = \exp\left(\frac{\Delta S1}{R}\right) = \exp\left(\frac{1.866\ J\cdot mol^{-1}\cdot K^{-1}}{8.314\ J\cdot mol^{-1}\cdot K^{-1}}\right)$$

$$=1.252$$

2.2 In the heating cycle mode

$$\Delta S_2 = \int_{T1}^{T2} \frac{Q}{T} dT$$

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

$$= \frac{0.9038\ J\cdot g^{-1} \times 370.24\ g\cdot mol^{-1}}{186.9\ K}$$

$$= 1.790\ J\cdot mol^{-1}\cdot K^{-1}$$

$$\Delta S_2 = R \ln N_2$$

$$N2 = \exp\left(\frac{\Delta S2}{R}\right) = \exp\left(\frac{1.790\ J\cdot mol^{-1}\cdot K^{-1}}{8.314\ J\cdot mol^{-1}\cdot K^{-1}}\right)$$

$$=1.240$$

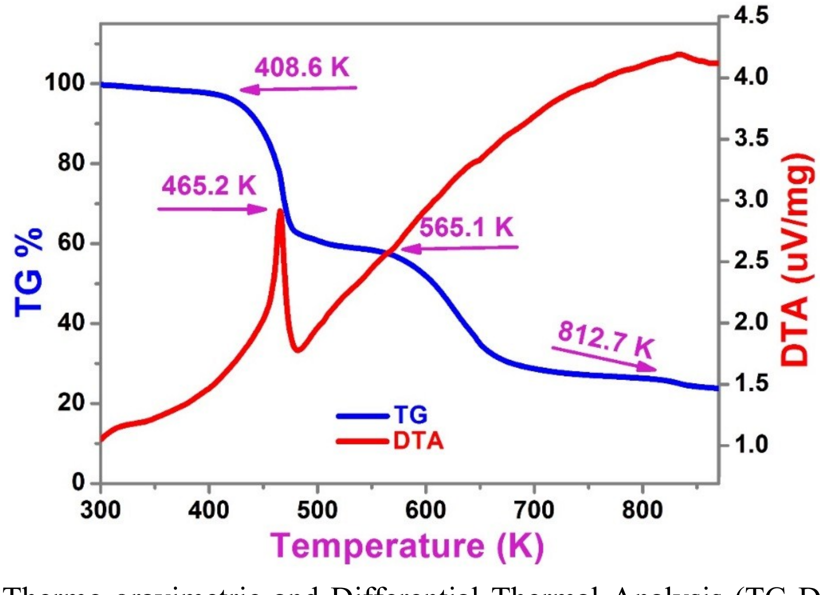

Figure S4 Thermo-gravimetric and Differential Thermal Analysis (TG-DTA) curves for **1**