Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Exceptional Dielectric Performance Induced by the Stepwise Reversible Phase Transitions of an Organic Crystal: Betainium Chlorodifluoroacetate

Zhihua Sun, Shuquan Zhang, Chengmin Ji,Tianliang Chen, and Junhua Luo *

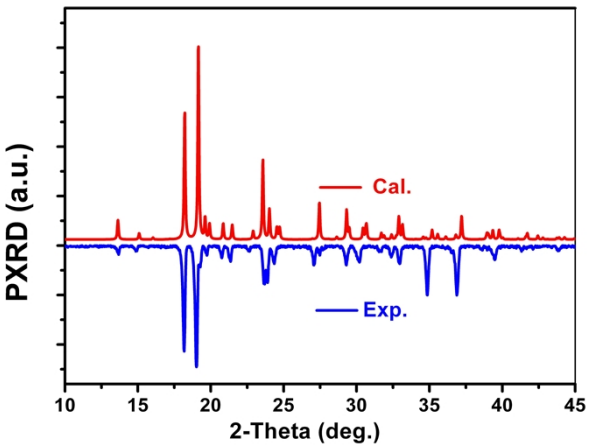


Figure S1. Experimental and calculated XRPD patterns of **1** at room temperature.

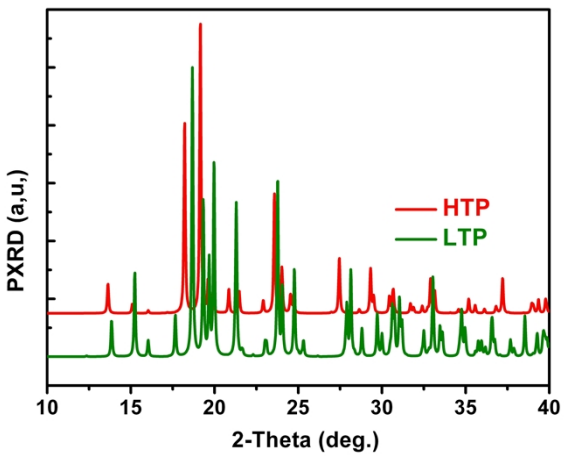


Figure S2. XRPD patterns obtained from the single-crystal structure determination of **1** in HTP and LTP, respectively. The obvious discrimination confirms its phase transition process.

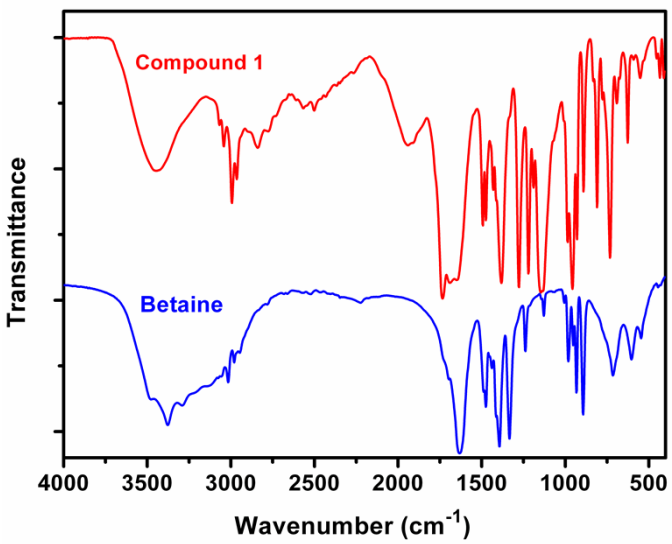
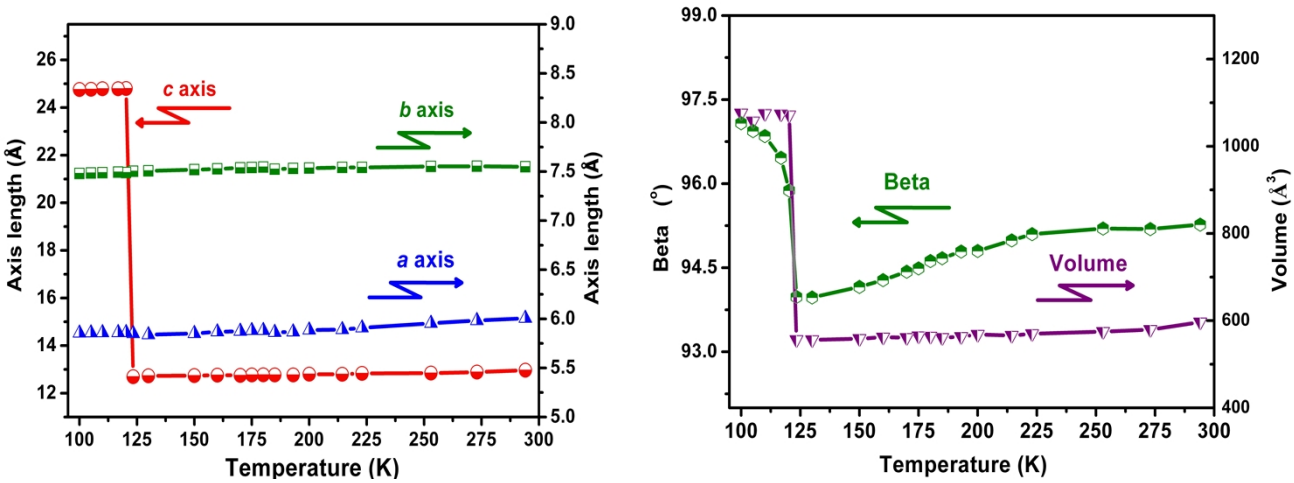
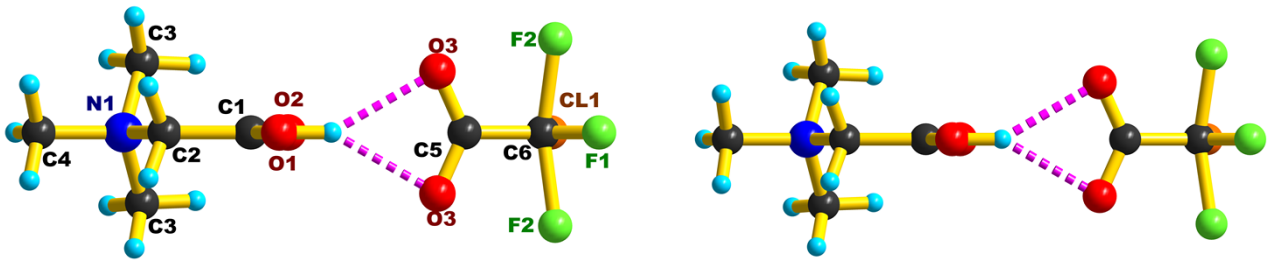


Figure S3. IR spectra of betaine and **1**.



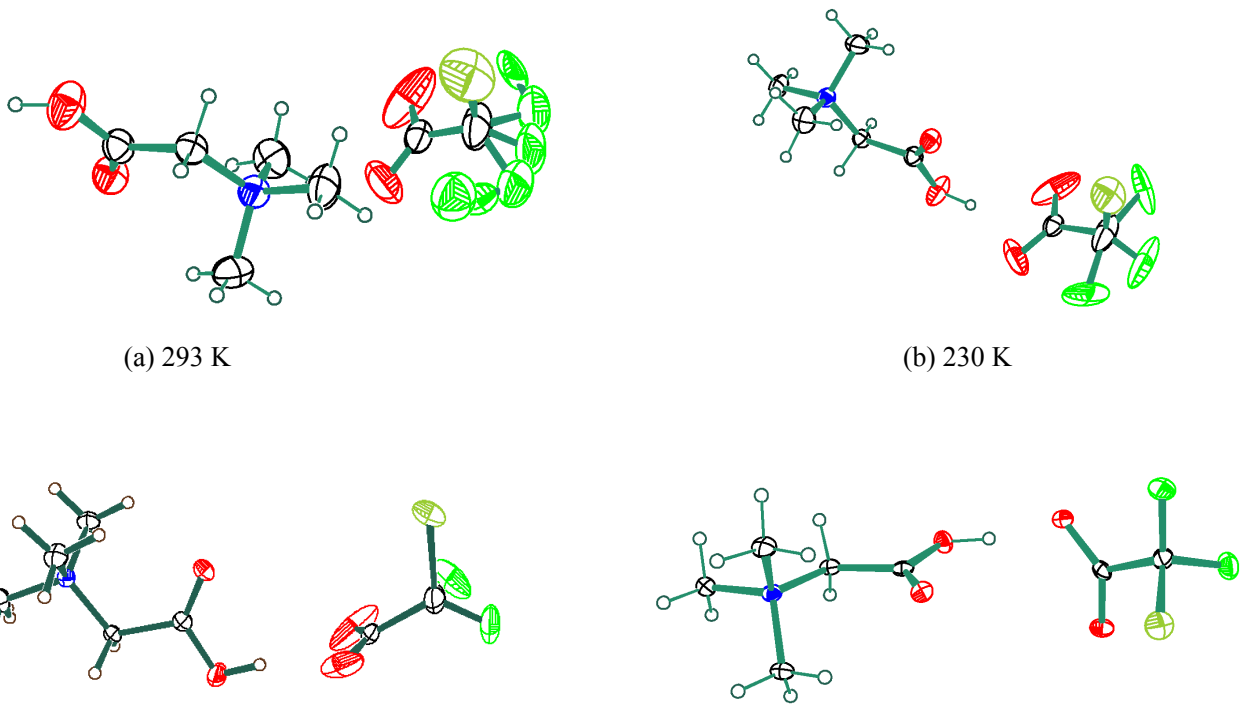
(a) (b)

Figure S4. Temperature dependence of (a) cell parameter changes of three axis lengths, and (b) cell volume and β in the range from 100 to 300 K for **1**.



(a) 150 K (b) 200 K

Figure S5. Molecular structures of **1** collected at 150 K (a) and 200 K (b), respectively. Chlorodifluoroacetate moieties are slightly disordered and both models are comparable to its structure determined at 230 K, which is labeled as the representative state in its HTP.



(a) 293 K (b) 230 K

(c) 200 K (d) 100 K

Figure S6. Schematic diagram of the thermal ellipsoids (30%) of **1** at different temperatures. The ratio changes of U_{eq} (average of F atoms)/U_{eq} (N atom in cation) confirm its order-disorder phase transition.

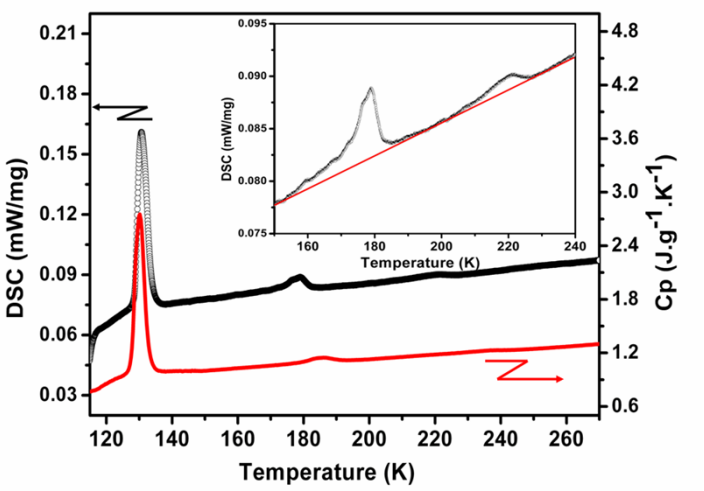


Figure S7. DSC and specific heat results measured on the deuterated analogue of **1**. There is no obvious isotope effect on T_c, which supports the phase transition is mainly induced by the order-disorder transformation.