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

Supporting Information

Supra-Molecular Switchable Dielectric Material with Non-Linear Optical Property

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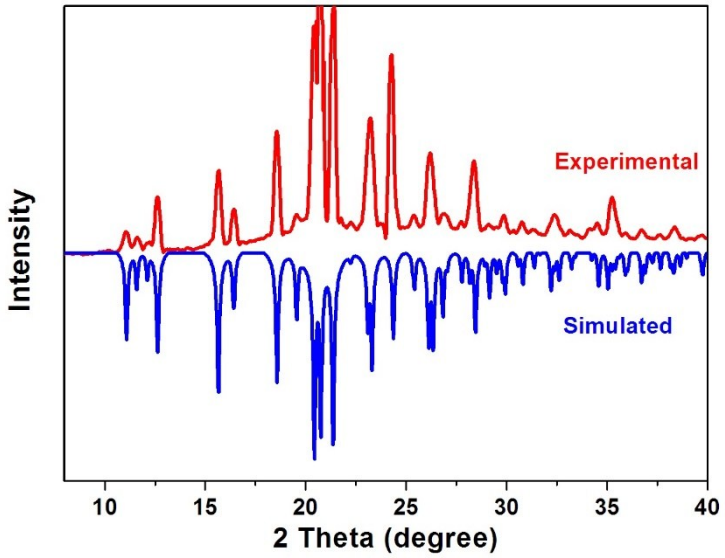

Fig. S1. Experimental and simulated X-ray powder diffraction patterns of **1** at room temperature.

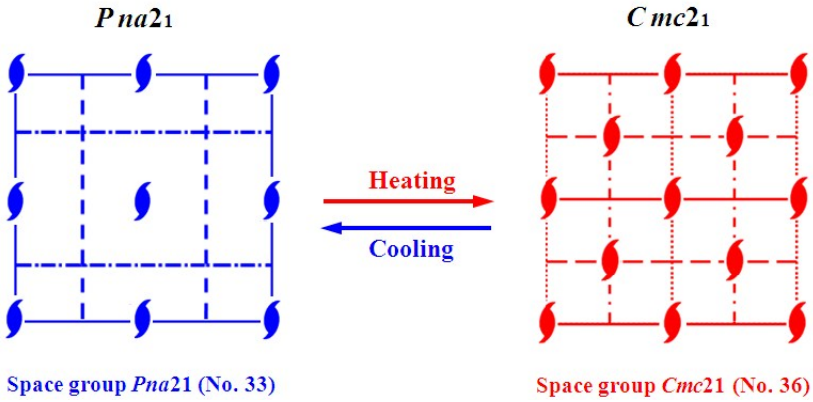

Fig. S2. Symmetry transformation of space group from $Cmc2_1$ (HTP) to $Pna2_1$ (LTP, equivalent to $Pn2_1a$) in **1**.

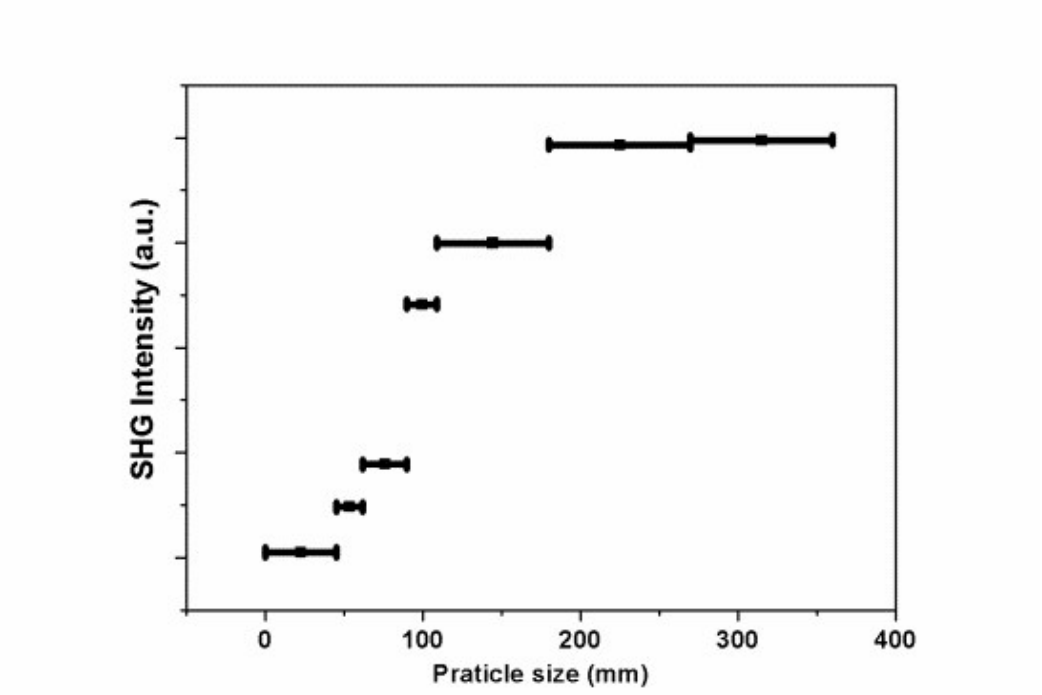

Fig. S3. SHG intensity versus particle size curves measured at 1064 nm.

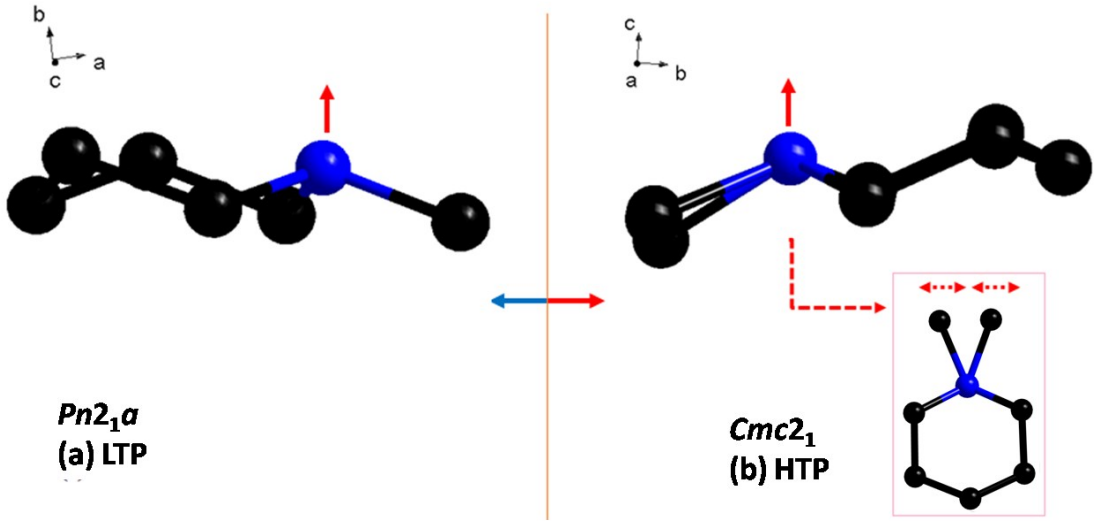

Fig. S4. The picortial repersentaion of cation at (a) LTP (b) HTP.

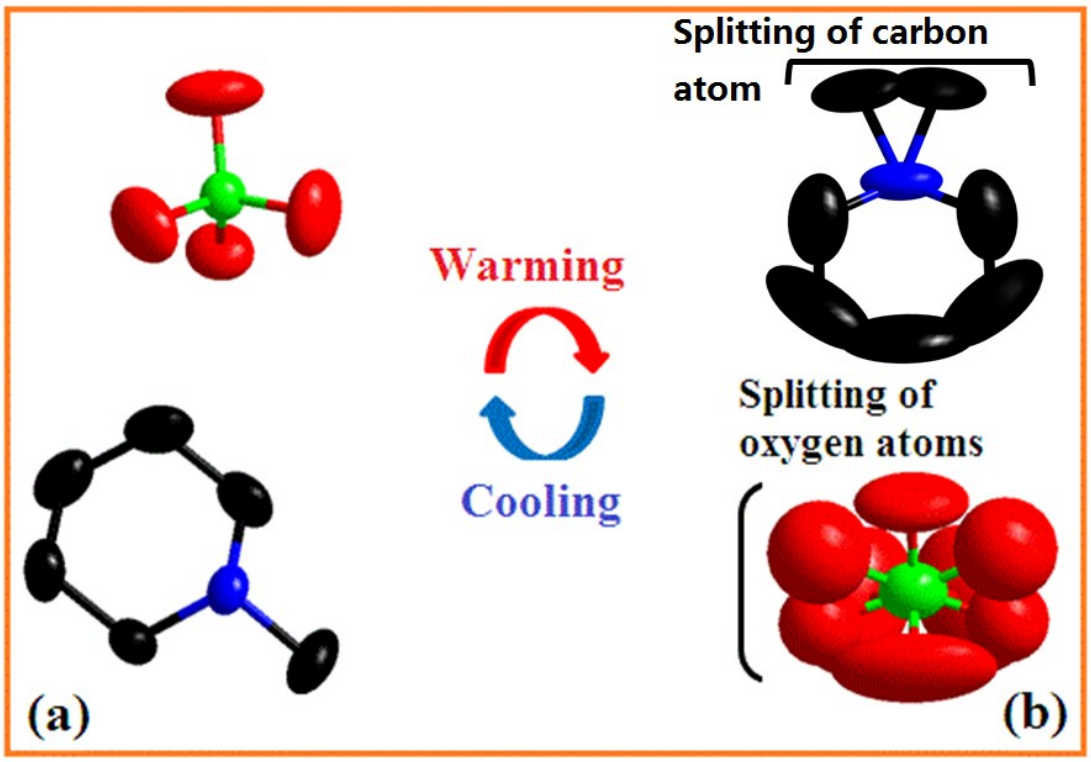

Fig. S5. Thermal ellipsoid of selected moieties of **1** at LTP (a) and (b) HTP. Hydrogen atoms are omitted for clarity.

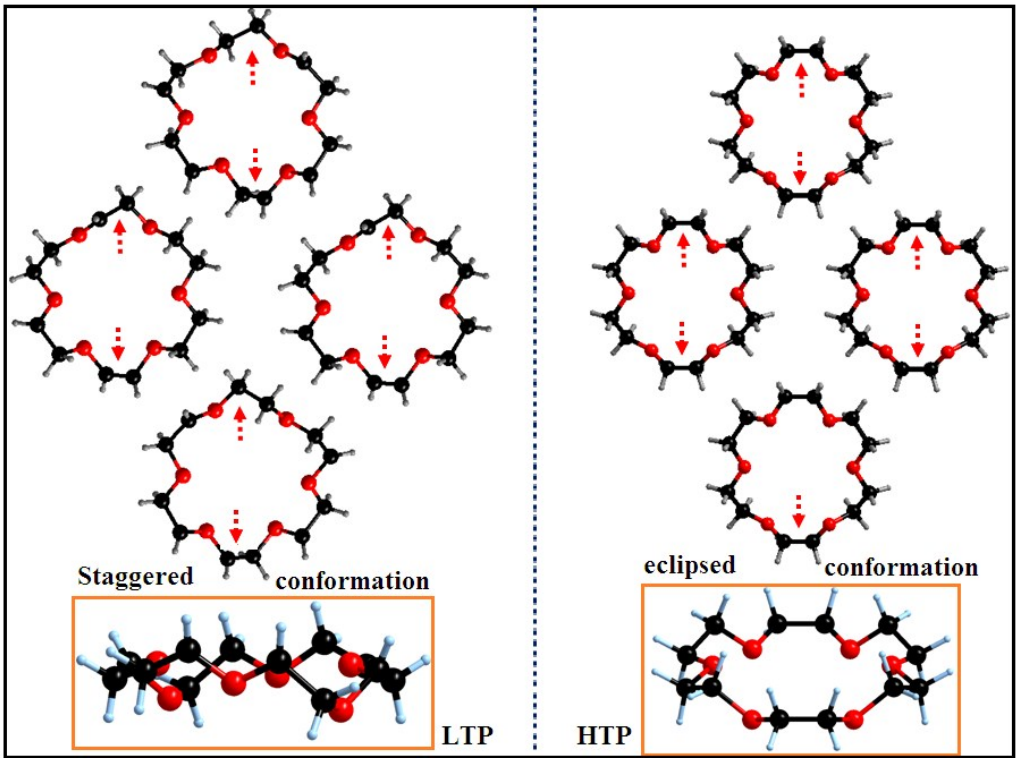

Fig. S6. Structure diagram of crown-ether in **1**. The pictorial representations show the staggered and eclipsed conformer at LTP and HTP, respectively.

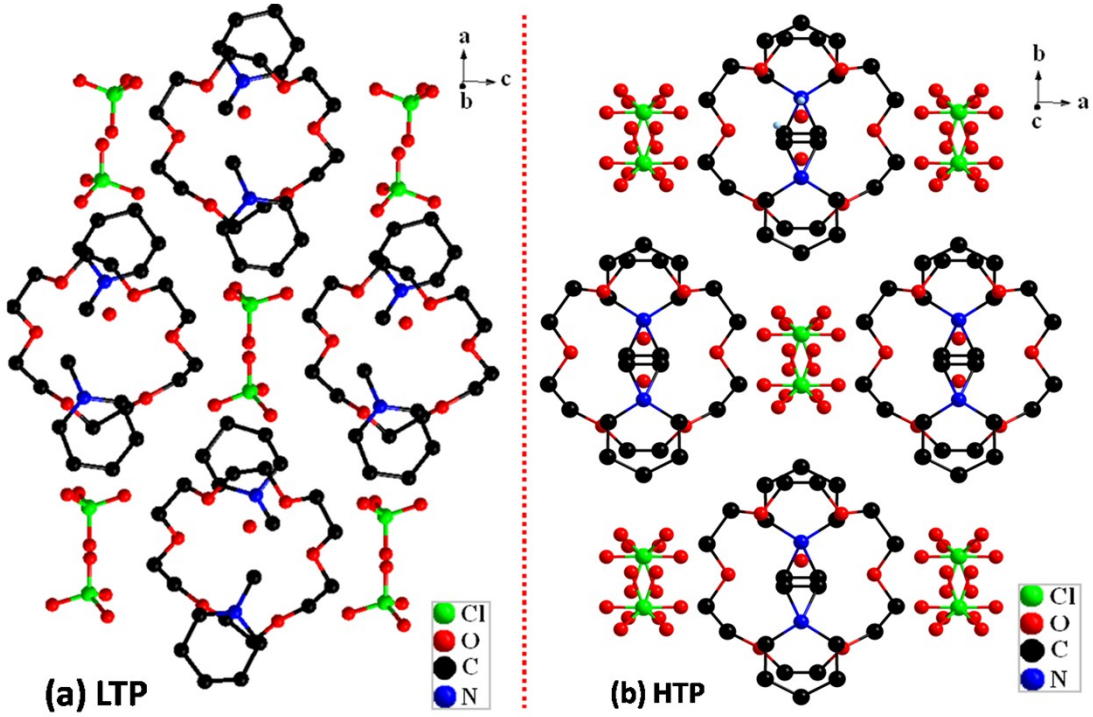

Fig. S7. Packing diagram of **1** at (a) LTP and (b) HTP. Hydrogen atoms are omitted for clarity.

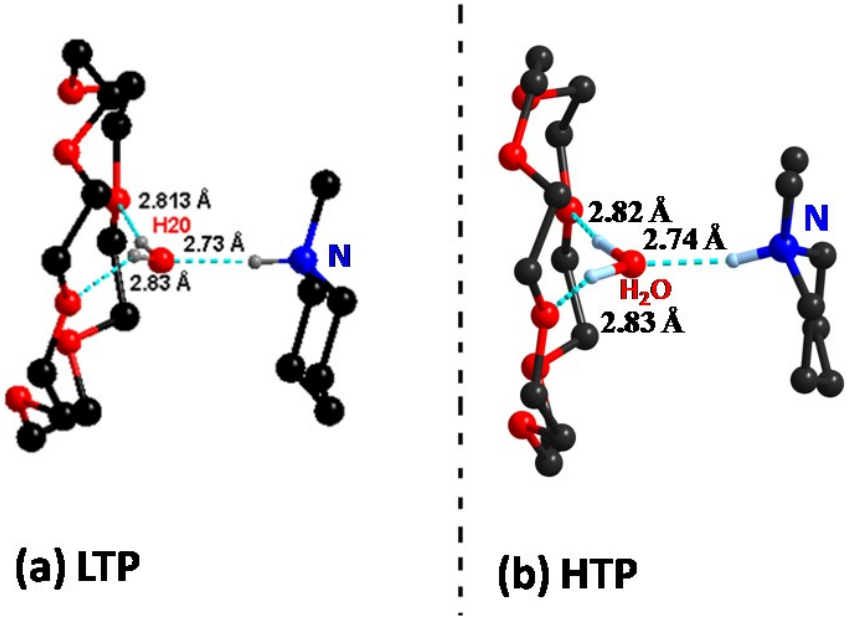

Fig. S8. Hydrogen bonding interactions in the complex cation of **1** at (a) LTP and (b) HTP.

Table S1. Crystal data and structure refinement details of **1** at 285 and 220 K.

Sum formula	$C_{18}H_{40}ClNO_{11}$	$C_{18}H_{40}ClNO_{11}$
Formula weight	481.96	481.96
Temperature (K)	285	220
Crystal system	Orthorhombic	Orthorhombic
Space group	$Cmc2_1$	$Pn2_1a$
a/Å	10.8029(4)	31.3826(3)
b/Å	15.9579(5)	14.50650(10)
c/Å	14.6015(3)	10.79330(10)
α/ deg	90.0	90.0
β/ deg	90.0	90.0
γ/ deg	90.0	90.0
Volume (Å^3)	2517.18(13)	4913.67(7)
Z	4	4
D_{calcd}, g cm^{-3}	1.272	1.303
F(000)	1040	2080
wR_2 (on F_o^2,I>2σ(I))	0.1813(1799)	0.1532 (7264)
Goodness-of-fit on F^2	S = 1.070	1.049
Completeness (%)	99.4	98.1
T_{min}/T_{max}	0.543,0.517	0.555/0.529
R indices[I>2σ(I)]	R_1=0.0674;wR_2=0.1813	R_1=0.0543;wR_2=0.1532
R indices (all data)	R_1=0.0731;wR_2=0.1900	R_1=0.0573;wR_2=0.1567

α$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma(|F_o|^2 - |F_c|^2) / \Sigma|F_o|^2]^{1/2}$