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

Supporting Information

Ferroelectric Properties in Metal Coordinated Complex Tris(2-Hydroxyethyl) ammonium Trichloro Cadmium(II)

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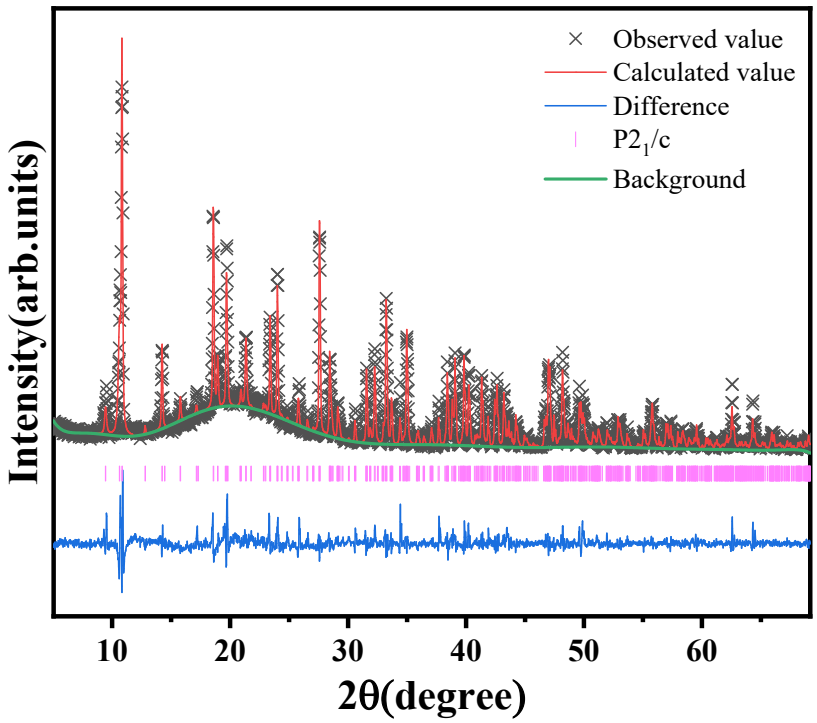

Figure S1. The experimental PXRD patterns and the simulated PXRD patterns of the synthesized sample.

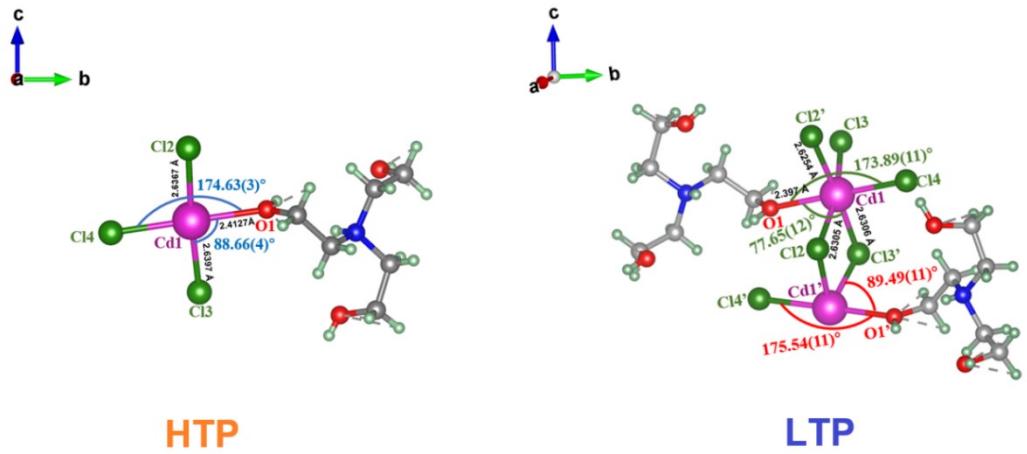

Figure S2. The crystal figures in the asymmetric unit at HTP and LTP.

Table S1. Crystal data and geometry details of compound 1.

	The LTP	The HTP
Chemical formula	$C_{12}H_{32}Cd_2Cl_6N_2O_6$	$C_6H_{16}CdCl_3NO_3$
M_r	737.92	368.96
Space group	$P2_1$	$P2/c$
Temperature/K	213 K	293 K
a(Å)	9.4760(2)	9.5109(3)
b(Å)	16.5098(4)	16.5687(6)
c(Å)	7.7069(2)	7.7219(3)
β	101.6235(10)	101.6989(13)
Volume($Å^3$)	1180.99(5)	1191.56(7)
Z	2	4
R,*wR2*,*S*	0.0249, 0.0992, 0.856	0.0230, 0.0795, 0.886
Bond length (Å)	LTP	HTP
Cd1-O1	2.397(6)	2.4127(14)
Cd1-Cl4	2.558(2)	2.5617(5)
Cd1-Cl2’	2.6253(13)	2.6308(6)
Cd1-Cl2	2.6305(16)	2.6367(6)
Cd1-Cl3’	2.6306(15)	2.6397(6)
Cd1-Cl3	2.6385(16)	2.6397(6)
Cd1’-O1’	2.408(6)	2.4127(14)
Cd1’-Cl4’	2.563(2)	2.5617(5)
Cd1’-Cl3’	2.6372(15)	2.6397(6)
Cd1’-Cl3	2.6422(16)	2.6397(6)
Cd1’-Cl2	2.6280(17)	2.6307(5)
Cd1’-Cl2’	2.6360(13)	2.6367(6)
N1-C1	1.516(9)	1.504(2)
N1-C5	1.513(8)	1.508(2)
N1-C3	1.501(10)	1.507(2)
O1-C2	1.474(8)	1.427(2)
O2-C6	1.396(6)	1.407(3)
O3-C4	1.399(7)	1.421(3)
C1-C2	1.490(10)	1.505(3)
C3-C4	1.555(8)	1.510(3)
C5-C6	1.479(10)	1.513(3)
N1’-C1’	1.491(8)	1.504(2)
N1’-C5’	1.508(8)	1.508(2)
N1’-C3’	1.517(9)	1.507(2)
O1’-C2’	1.384(9)	1.427(2)
O2’-C6’	1.451(7)	1.407(3)
O3’-C4’	1.353(7)	1.421(3)

C1’-C2’	1.526(10)	1.505(3)
C3’-C4’	1.485(8)	1.510(3)
C5’-C6’	1.543(9)	1.513(3)
Bond angle (˚)	LTP	HTP
O1-Cd1-Cl4	173.89(11)	174.63(3)
O1-Cd1-Cl2’	90.04(11)	89.72(4)
O1-Cd1-Cl2	88.21(11)	87.69(4)
O1-Cd1-Cl3’	77.65(12)	78.17(3)
O1-Cd1-Cl3	88.28(11)	88.66(4)
Cl4-Cd1-Cl2	95.14(7)	95.182(16)
Cl4-Cd1-Cl2’	94.72(7)	94.516(16)
Cl4-Cd1-Cl3	88.32(7)	88.431(17)
Cl4-Cd1-Cl3’	97.52(7)	97.539(16)
Cl2-Cd1-Cl2’	95.35(4)	95.500(17)
Cl2-Cd1-Cl3’	84.95(5)	84.765(18)
Cl2’-Cd1-Cl3’	167.68(8)	167.871(18)
Cl2’-Cd1-Cl3	85.11(5)	84.883(18)
Cl2-Cd1-Cl3	176.46(8)	176.322(16)
Cl3-Cd1-Cl3’	93.85(5)	94.091(18)
Cd1-Cl2’-Cd1’	94.70(5)	94.809(17)
Cd1-Cl3-Cd1’	94.24(5)	94.527(18)
O1’-Cd1’-Cl4’	175.54(11)	174.63(3)
O1’-Cd1’-Cl2’	87.53(11)	87.69(4)
O1’-Cd1’-Cl2	89.47(12)	89.72(4)
O1’-Cd1’-Cl3’	89.49(11)	88.66(4)
O1’-Cd1’-Cl3	78.78(12)	78.17(3)
Cl4’-Cd1’-Cl2	93.99(7)	94.516(16)
Cl4’-Cd1’-Cl2’	94.92(7)	95.182(16)
Cl4’-Cd1’-Cl3	97.70(7)	97.539(16)
Cl4’-Cd1’-Cl3’	88.02(7)	88.431(17)
Cl2-Cd1’-Cl2’	95.61(4)	95.500(17)
Cl2-Cd1’-Cl3’	84.87(5)	84.883(18)
Cl2’-Cd1’-Cl3’	176.97(7)	176.322(16)
Cl2’-Cd1’-Cl3	84.83(5)	84.765(18)
Cl2-Cd1’-Cl3	168.22(8)	167.871(18)
Cl3-Cd1’-Cl3’	94.09(5)	94.091(18)
Cd1’-Cl2-Cd1	94.72(5)	94.809(17)
Cd1’-Cl3’-Cd1	94.51(5)	94.527(18)
C1-N1-C5	110.3(5)	110.45(13)
C1-N1-C3	112.1(5)	112.31(13)
C5-N1-C3	109.4(6)	110.66(14)
C1’-N1’-C5’	111.1(4)	110.45(13)
C1’-N1’-C3’	112.5(4)	112.31(13)

C5’-N1’-C3’	111.6(6)	110.66(14)
N1-C1-C2	113.9(5)	114.34(14)
O1-C2-C1	109.7(5)	110.79(14)
N1-C3-C4	110.9(6)	114.84(16)
N1-C5-C6	116.3(5)	115.07(14)
O2-C6-C5	108.5(6)	108.45(18)
O3-C4-C3	110.7(5)	109.32(16)
N1’-C1’-C2’	113.6(5)	114.34(14)
O1’-C2’-C1’	111.3(5)	110.79(14)
N1’-C3’-C4’	117.0(6)	114.84(16)
N1’-C5’-C6’	114.7(5)	115.07(14)
O2’-C6’-C5’	107.3(6)	108.45(18)
O3’-C4’-C3’	109.5(5)	109.32(16)
C2-O1-Cd1	123.2(4)	124.52(10)
C2’-O1’-Cd1’	125.3(4)	124.52(10)

Table S2. Point charge model analysis of **TATC**. According to the crystal structure data collected at 213 K (LTP). We assume positive charge center influenced by the Cd^{II} and protonated N while negative charge center influenced by Cl^- from their equilibrium position within the unit cell.

Atoms	Equivalent Crystal Coordination			Center Coordination
N^+	(0.7219(6)	0.9160(4)	0.9162(8))	(0.5, 0.4674(4), 0.5)
	(0.2781(6)	0.4160(4)	0.0838(8))	
	(0.7236(5)	0.5188(4)	0.4138(6))	
	(0.2764(5)	0.0188(4)	0.5862(6))	
Cd^{2+}	(0.81868(5)	0.22802(2)	0.96564(6))	(0.5, 0.46751(2), 0.5)
	(0.18132(5)	0.72802(2)	0.03436(6))	
	(0.81858(5)	0.20700(2)	0.46551(5))	
	(0.18142(5)	0.70700(2)	0.53449(5))	
Cl^-	(0.00840(15)	0.23347(16)	0.26595(19))	(0.5, 0.46725(15), 0.5)
	(0.99160(15)	0.73347(16)	0.73405(19))	
	(0.00806(15)	0.19993(15)	0.766789(17))	
	(0.99194(15)	0.69993(15)	0.23322(17))	
	(0.62620(16)	0.22205(15)	0.1681(2))	
	(0.37380(16)	0.72205(15)	0.8319(2))	
	(0.62522(17)	0.21316(15)	0.6689(2))	
	(0.37478(17)	0.71316(15)	0.3311(2))	
	(0.81294(18)	0.38125(13)	0.9153(2))	
	(0.18706(18)	0.88125(13)	0.0847(2))	
	(0.81203(19)	0.05361(13)	0.4130(2))	
	(0.18797(19)	0.55361(13)	0.5870(2))	

$P_s = [(e \times 0.4674) \times 4 + (e \times 0.46751) \times 8 - (e \times 0.467245) \times 12] \times b / V$
$=0.06\ \mu C/cm^2$

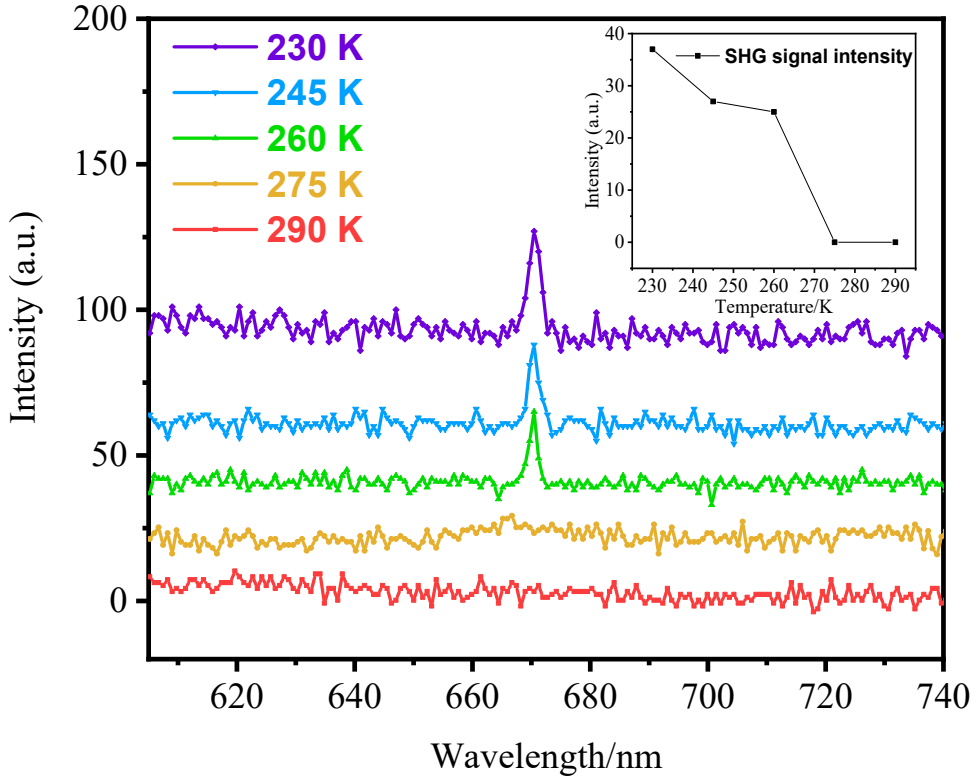

Figure S3. The second harmonic generation (SHG) measurements at several temperatures. The inset picture shows the variation of signal intensity with increasing of the temperature.

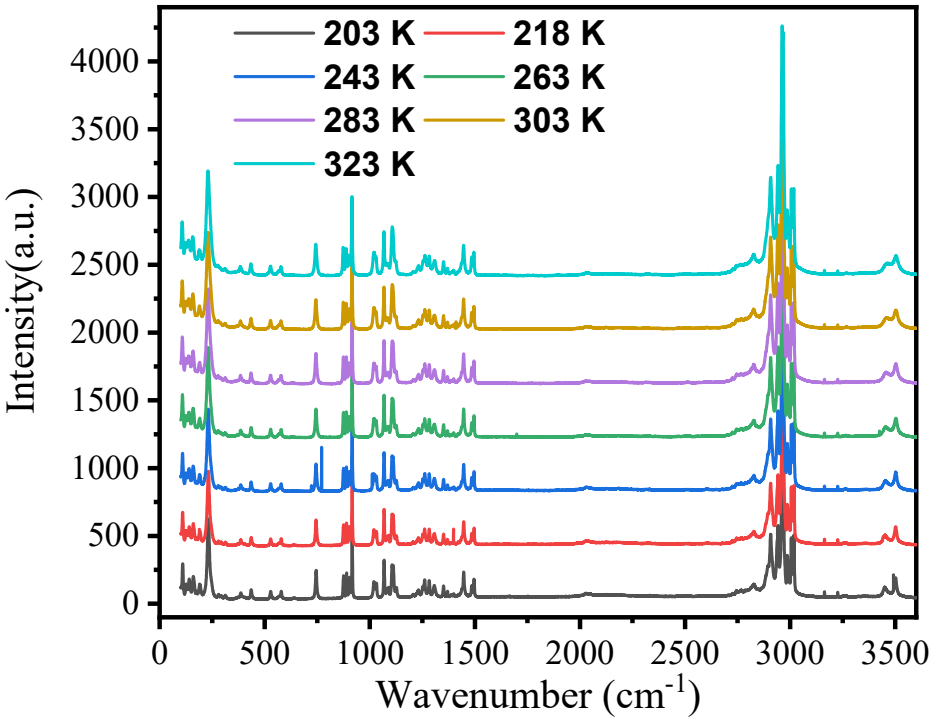

Figure S4. Raman spectra of **TATC**.

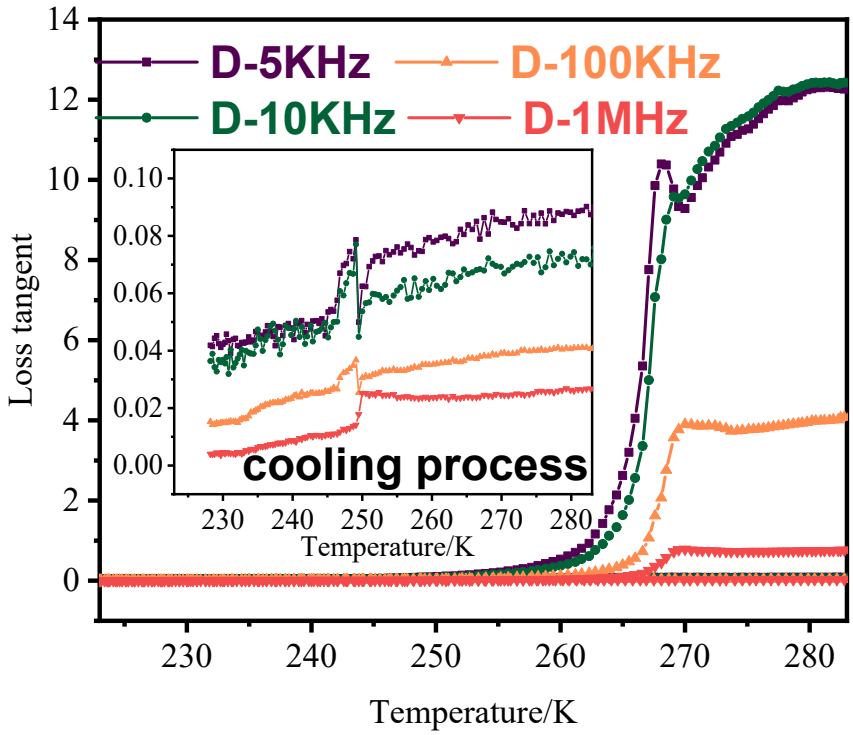

Figure S5. Temperature-dependence of the loss tangent of **TATC** measured in a heating and cooling cycle.