Two Novel Metal-Organic Coordination Polymer Based on Ligand 1,4-Diazabicyclo[2.2.2]octane N,N'-dioxide with Phase Transition, Ferroelectric and Dielectric Properties

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Supporting Information

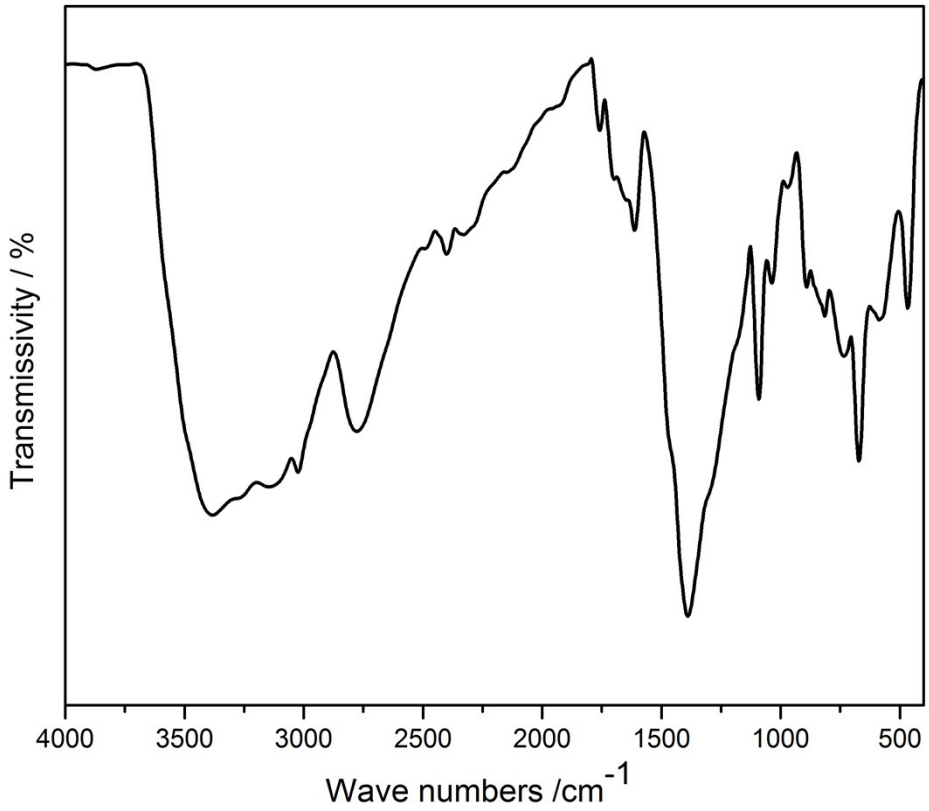

Figure S1. IR spectra of compound **1** in KBr pellet was recorded on a Shimadzu IR prestige-21 FTIR-8400S spectrometer at room temperature.

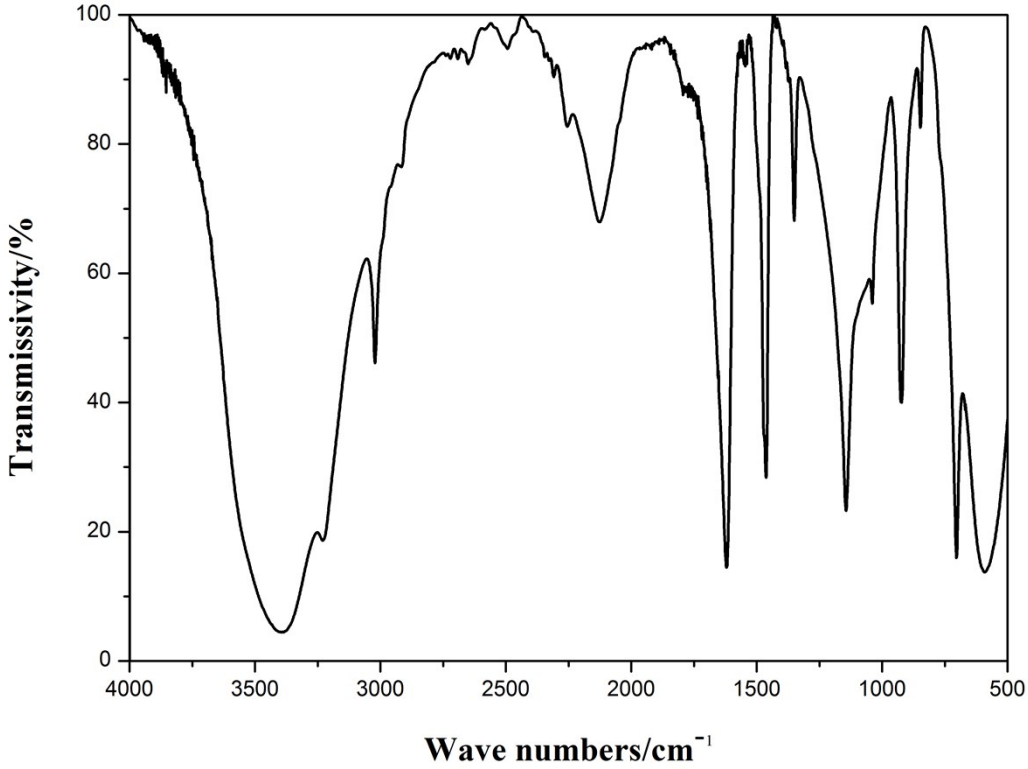

Figure S2. IR spectra of compound **2** in KBr pellet was recorded on a Shimadzu IR prestige-21 FTIR-8400S spectrometer at room temperature.

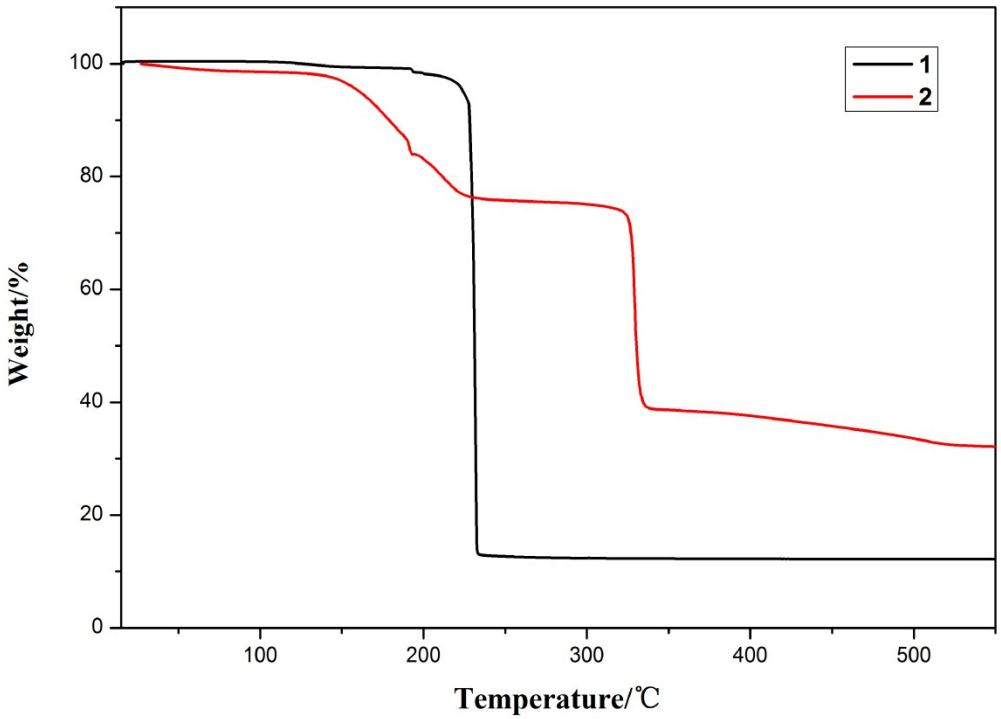

Figure S3. TG curves of compound **1** and **2** in the heating mode.

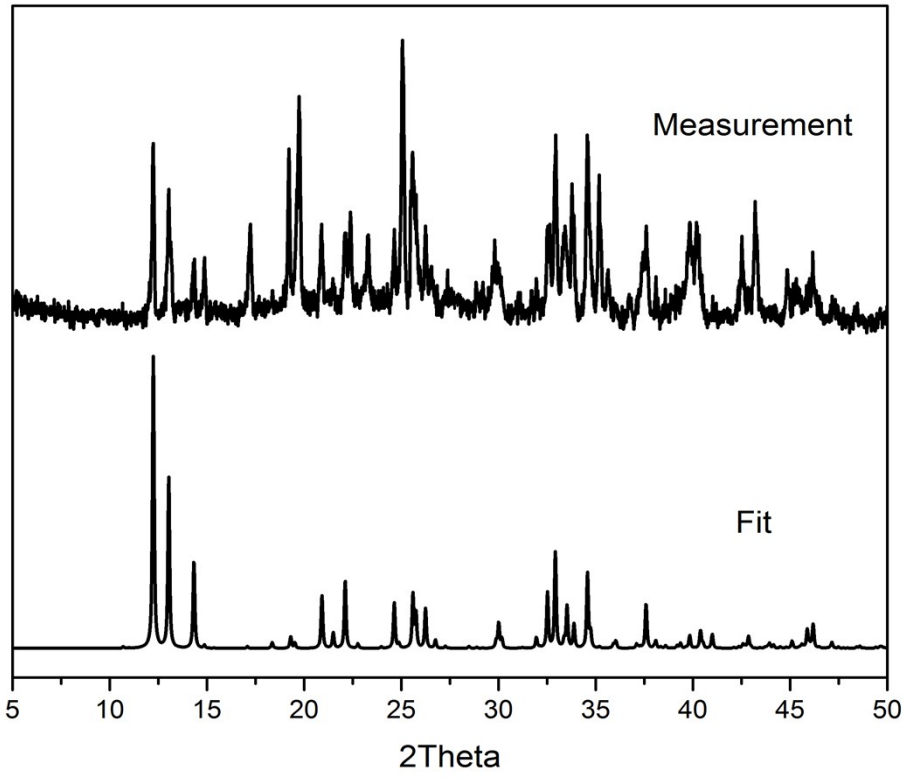

Figure S4. PXRD pattern of compound **1** measured at room temperature, compared with the simulated data based on the single crystal structure.

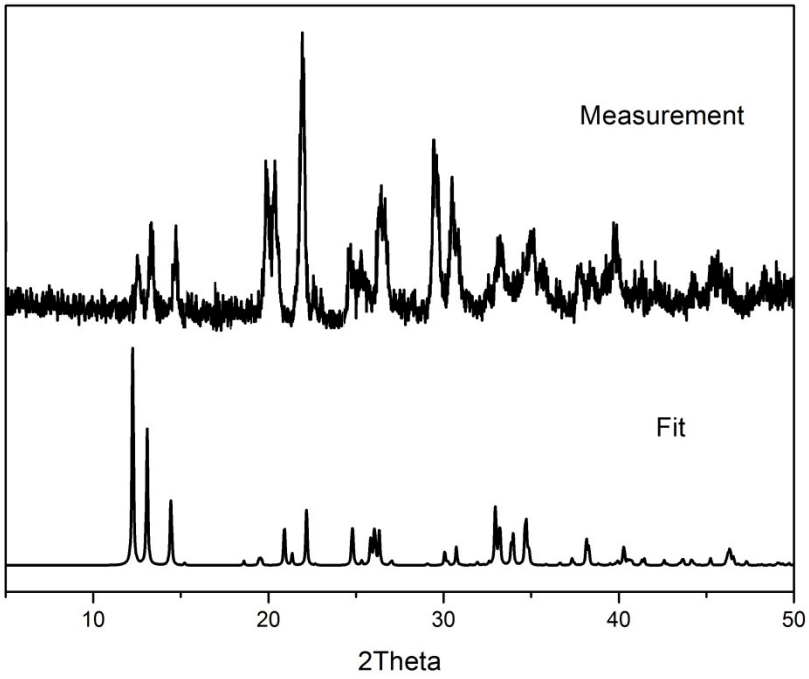

Figure S5. PXRD pattern of compound **1** measured at low temperature, compared with the simulated data based on the single crystal structure.

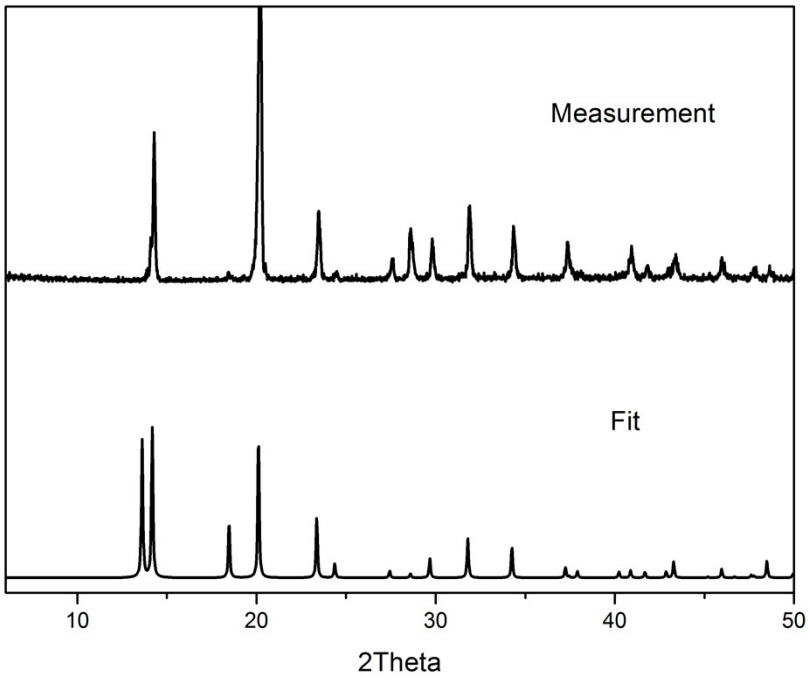

Figure S6. PXRD pattern of compound **2** measured at room temperature, compared with the simulated data based on the single crystal structure.

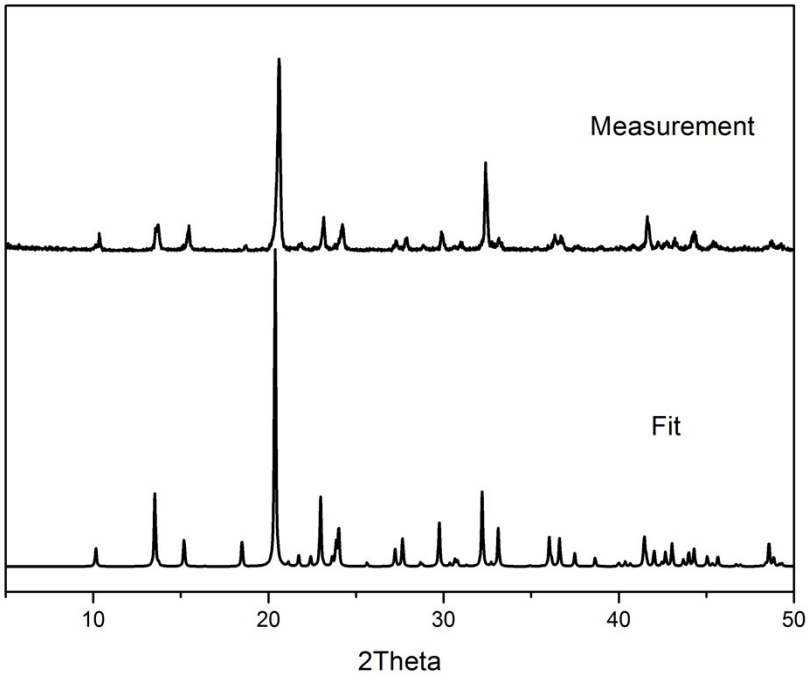

Figure S7. PXRD pattern of compound **2** measured at low temperature, compared with the simulated data based on the single crystal structure.

Table S1. Selected Bond Lengths (Å) and Bond Angles (°) of **1** at 293 K and 123K

293K					
Ag(1)-O(1)	2.456(5)	Ag(1)-O(2)	2.353(5)	Ag(1)-O(3)	2.395(7)
Ag(1)-O(9)	2.534(8)	Ag(1′)-O(1)	2.483(5)	Ag(1′)-O(2)	2.384(5)
Ag(1′)-O(11)	2.484(9)	Ag(2)-O(1)	2.403(4)	Ag(2)-O(2)	2.413(5)
Ag(2)-O(3)	2.414(6)	Ag(2)-O(8)	2.480(9)	Ag(3)-O(1)	2.396(4)
Ag(3)-O(2)	2.442(5)	Ag(3)-O(5)	2.484(6)	Ag(3)-O(6)	2.412(9)
123K					
Ag(1)-O(1)	2.515(13)	Ag(1)-O(2)	2.387(15)	Ag(1)-O(5)	2.446(16)
Ag(1)-O(7)	2.591(14)	Ag(1′)-O(2)	2.358(15)	Ag(1′)-O(1)	2.482(14)
Ag(1′)-O(3)	2.512(13)	Ag(1′)-O(7)	2.370(15)	Ag(2)-O(1)	2.392(11)
Ag(2)-O(2)	2.392(11)	Ag(2)-O(7)	2.402(12)	Ag(2)-O(10)	2.470(14)
Ag(2)-O(3)	2.557(11)	Ag(3)-O(2)	2.355(12)	Ag(3)-O(9)	2.371(11)
Ag(3)-O(1)	2.492(13)	Ag(3)-O(8)	2.524(11)	Ag(3)-O(4)	2.525(13)
293K					
O(2)-Ag(1)-O(1)	68.58(18)	O(3)-Ag(1)-O(1)	177.20(2)	O(2)-Ag(1)-O(9)	167.00(2)
O(3)-Ag(1)-O(9)	84.10(3)	O(1)-Ag(1)-O(9)	98.70(2)	O(2)-Ag(1)-O(3)	108.6 (2)
O(2)-Ag(1′)-O(11)	169.40(3)	O(1)-Ag(1′)-O(11)	109.60(2)	O(2)-Ag(1′)-O(1)	67.66(17)
O(1)-Ag(2)-O(3)	164.25(18)	O(2)-Ag(2)-O(3)	107.32(19)	O(1)-Ag(2)-O(8)	95.10(3)
O(2)-Ag(2)-O(8)	120.30(2)	O(3)-Ag(2)-O(8)	99.90(3)	O(1)-Ag(2)-O(2)	68.49(17)
O(1)-Ag(3)-O(5)	165.30(2)	O(1)-Ag(3)-O(6)	98.80(3)	O(2)-Ag(3)-O(5)	97.50(2)

O(6)-Ag(3)-O(2)	119.30(2)	O(6)-Ag(3)-O(5)	91.00(3)	O(1)-Ag(3)-O(2)	68.14(17)
			123K		
O(2)-Ag(1)-O(5)	166.6(5)	O(2)-Ag(1)-O(1)	67.1(3)	O(5)-Ag(1)-O(1)	102.9(5)
O(2)-Ag(1)-O(7)	103.7(4)	O(5)-Ag(1)-O(7)	89.6(4)	O(1)-Ag(1)-O(7)	143.3(5)
O(2)-Ag(1′)-O(7)	111.9(5)	O(2)-Ag(1′)-O(1)	68.1(3)	O(7)-Ag(1′)-O(1)	174.5(10)
O(2)-Ag(1′)-O(3)	160.9(6)	O(7)-Ag(1′)-O(3)	83.1(5)	O(1)-Ag(1′)-O(3)	95.8(5)
O(1)-Ag(2)-O(2)	69.1(3)	O(1)-Ag(2)-O(7)	164.6(4)	O(2)-Ag(2)-O(7)	103.8(4)
O(1)-Ag(2)-O(10)	97.9(5)	O(2)-Ag(2)-O(10)	123.9(5)	O(7)-Ag(2)-O(10)	97.3(4)
O(1)-Ag(2)-O(3)	99.9(4)	O(2)-Ag(2)-O(3)	157.1(4)	O(7)-Ag(2)-O(3)	81.6(4)
O(10)-Ag(2)-O(3)	76.5(4)	O(2)-Ag(3)-O(9)	112.6(4)	O(2)-Ag(3)-O(1)	68.0(3)
O(9)-Ag(3)-O(1)	98.5(4)	O(2)-Ag(3)-O(8)	160.1(4)	O(9)-Ag(3)-O(8)	73.6(4)
O(1)-Ag(3)-O(8)	92.6(4)	O(2)-Ag(3)-O(4)	121.9(4)	O(9)-Ag(3)-O(4)	108.0(4)
O(1)-Ag(3)-O(4)	142.4(4)	O(8)-Ag(3)-O(4)	70.6(4)		

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) of **2** at 296 K and 173K

		296 K	
Ca(1)-O(2)	2.177(7)	Ca(1)-O(2)	2.177(7)
Ca(1)-O(1)	2.366(6)	Ca(1)-O(1)	2.366(6)
Ca(1)-O(1)	2.366(6)	Ca(1)-O(1)	2.366(6)
O(2)- Ca (1)-O(2)	180.0	O(2)- Ca (1)-O(1)	90.0
O(2)- Ca (1)-O(1)	90.0	O(2)- Ca(1)-O(1)	90.0
O(1)- Ca (1)-O(1)	90.0	O(1)- Ca (1)-O(1)	180.0
		173 K	
Ca(1)-O(1)	2.169(6)	Ca(1)-O(2W)	2.342(6)
Ca(1)-O(1W)	2.347(7)	Ca(1)-O(1)	2.169(6)
Ca(1)-O(2W)	2.342(6)	Ca(1)-O(1W)	2.347(7)
O(1)-Ca(1)-O(1)	173.4(4)	O(1)-Ca(1)-O(2W)	87.68(14)
O(2W)-Ca(1)-O(2W)	91.2(3)	O(1)-Ca(1)-O(1W)	92.39(14)
O(2W)-Ca(1)-O(1W)	90.6(3)	O(2W)-Ca(1)-O(1W)	178.2(3)