Supporting Information for

Temperature-induced reversible structural phase transition of 1-(Chloromethyl)-1,4- diazoniabicyclo[2.2.2] octane bis(perchlorate)

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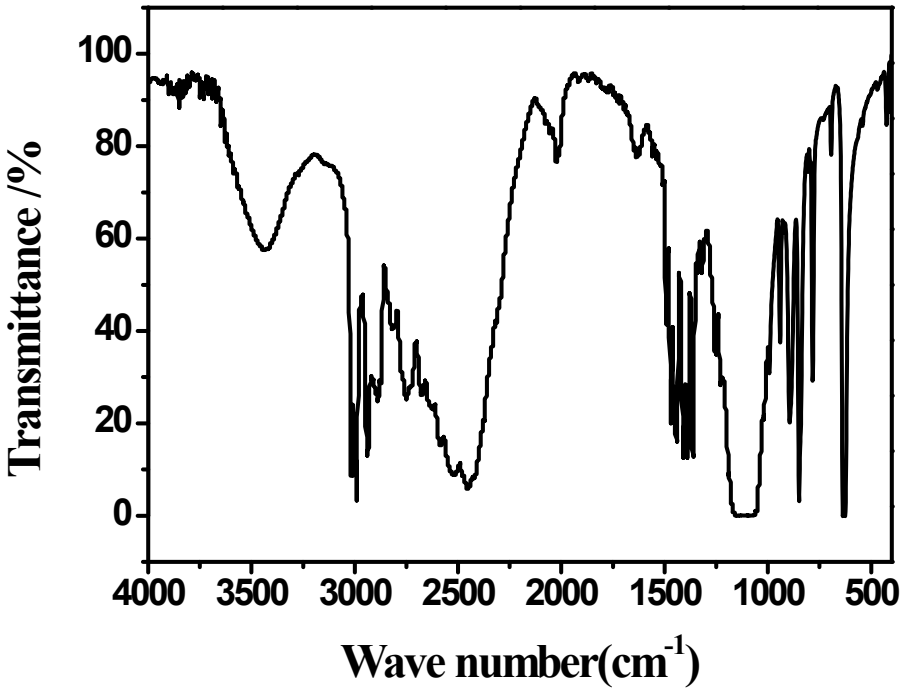

Figure S1 IR of compound **1**

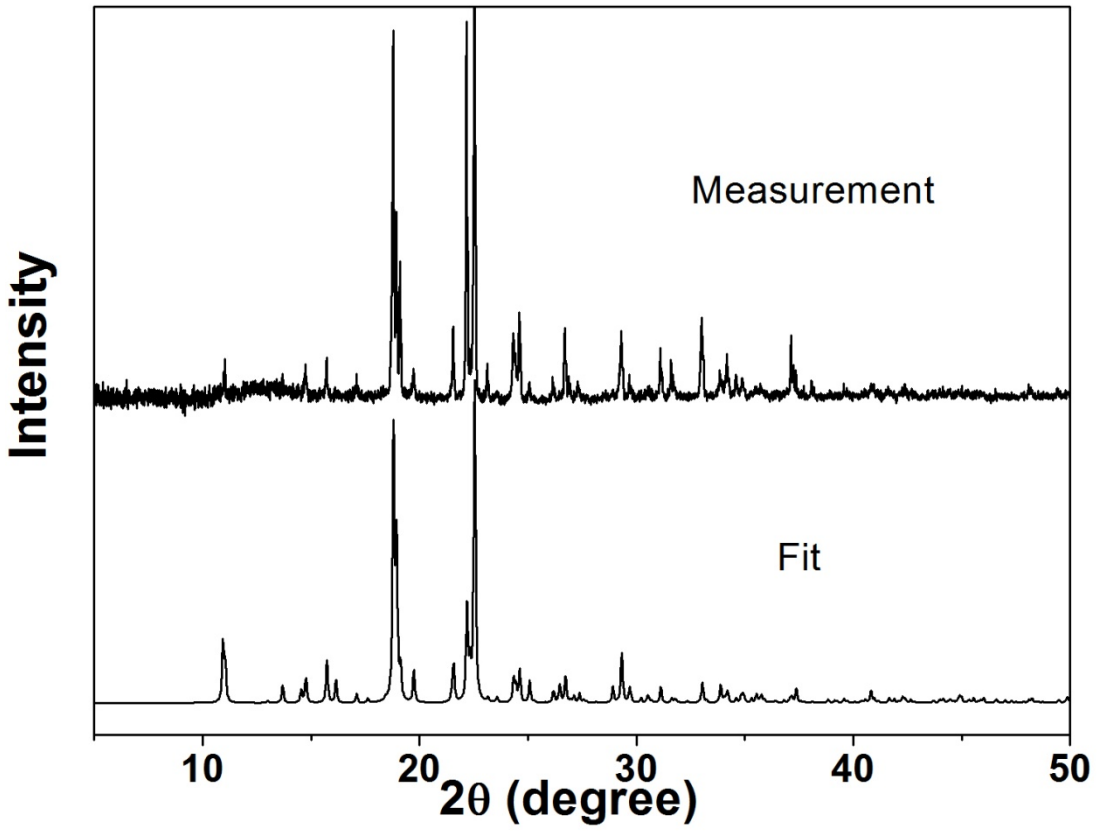

Figure S2 XRPD pattern of compound **1**, where the lower line is the simulated pattern.

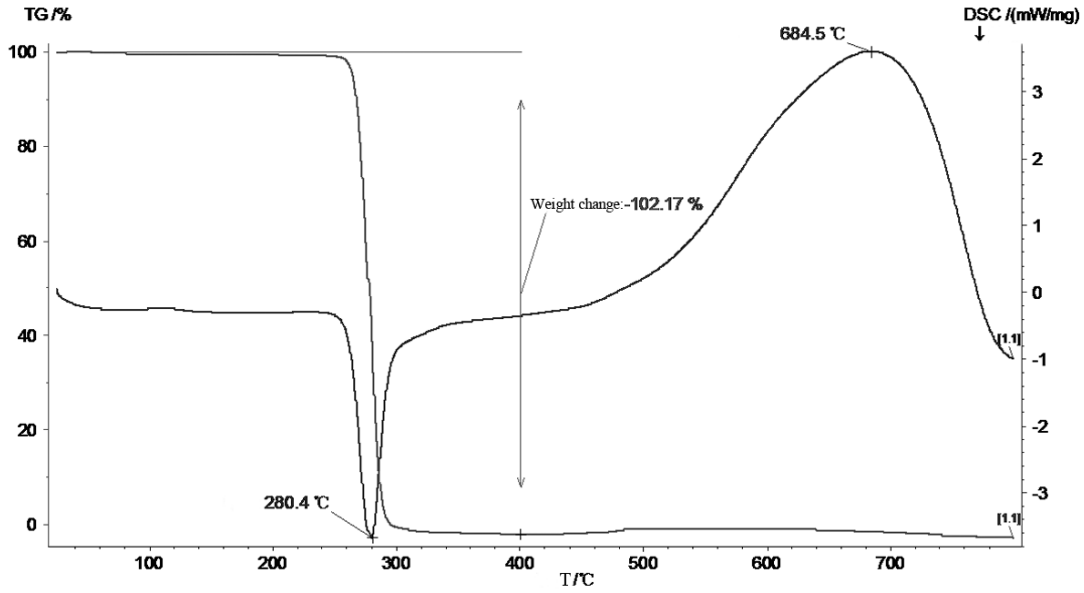

Figure S3 TG and DSC curve of compound **1**

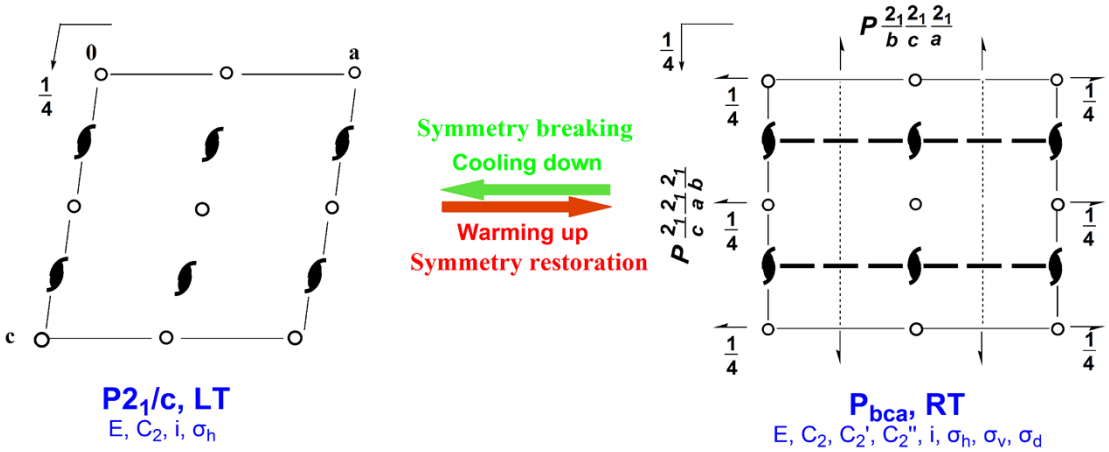

Figure S4 Changes of symmetry operations of 1 from Pbca at HTP to $P2_1/c$ at LTP.

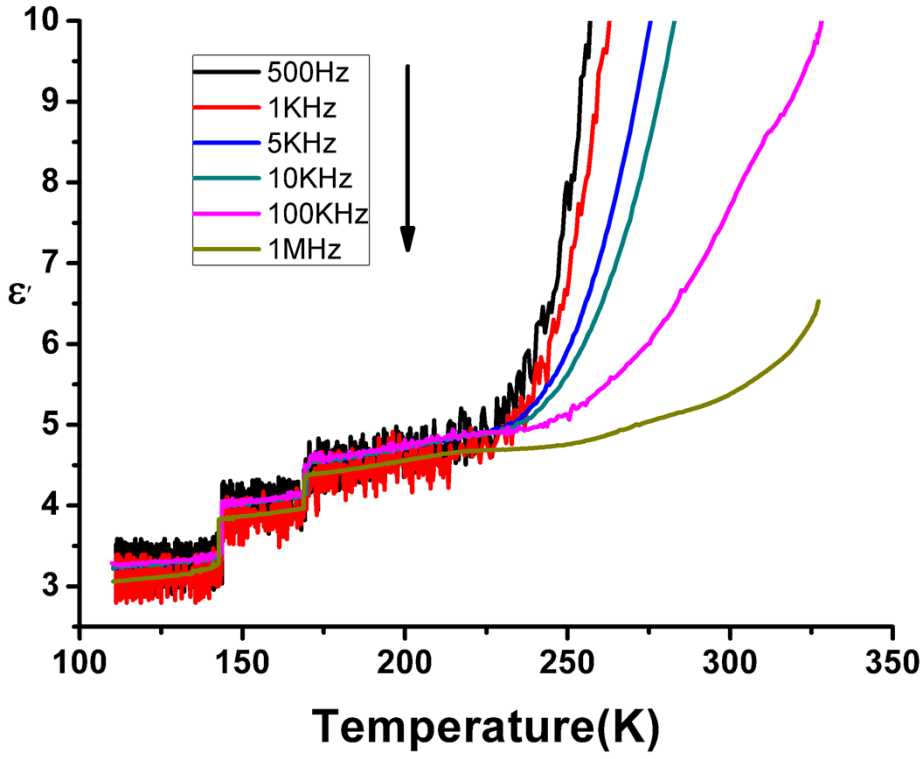

Figure S5 Dependence of the dielectric constants of complex 1 on temperature from 100K to 320K at different frequency ranges.

Table S1. Hydrogen Bond Lengths (Å) and Bond Angles (°) (291K)

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
N(2) –H(2A) ···O(2) #1	0.91	2.42	3.099(9)	132
N(2) –H(2A) ···O(5) #1	0.91	2.37	3.083(6)	135
1 N(2) –H(2A) ···O(8) #1	0.91	2.21	2.917(5)	134

Symmetry codes: #1: 1/2-x, 1/2+y, z

Table S2. Hydrogen Bond Lengths (Å) and Bond Angles (°) (170K)

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
N(1) –H(1C) ···O(1)	0.93	2.36	3.045(8)	131
N(1) –H(1C) ···O(1')	0.93	2.36	3.027(9)	129
N(1) –H(1C) ···O(6)	0.93	2.30	3.035(4)	135
N(1) –H(1C) ···O(7)	0.93	2.17	2.883(4)	132

Table S3. Hydrogen Bond Lengths (Å) and Bond Angles (°) (100K)

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
N(1) –H(1C) ···O(4) #1	0.93	2.34	3.016(7)	129
N(1) –H(1C) ···O(6) #2	0.93	2.28	3.030(7)	138
N(1) –H(1C) ···O(7) #2	0.93	2.18	2.872(7)	130
N(3) –H(3C) ···O(15)	0.93	2.33	3.019(7)	131
N(3) –H(3C) ···O(10) #2	0.93	2.15	2.867(7)	133
N(3) –H(3C) ···O(11) #2	0.93	2.33	3.033(7)	132

Symmetry codes: #1: -1+x, y, z; #2. -1+x,1/2-y,1/2+z