Supporting Information

Reversible high temperature dielectric switch in a 2H-perovskite compound: $[Me_3NCH_2CH_3]CdCl_3$

Dong-Sheng Sun, Yao-Zu Zhang, Ji-Xing Gao, Xiu-Ni Hua, Xiao-Gang Chen, Guang-Quan Mei* and Wei-Qiang Liao*

IR analyses: The most intensive band at 956.69 cm^{-1} is attributed to C-C in-plane stretching and 3024.38 cm^{-1} is due to C-H stretching vibrations. At 1485.19 cm^{-1}, it can be assigned to C-N stretching vibrations. The quaternary ammonium salt has no characteristic absorption peak. When the methyl group is connected to the N cation, the stretching vibration frequency shifts to a high frequency.

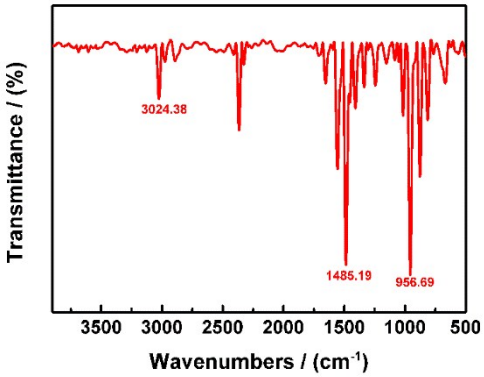

Fig. S1 The IR spectrum of compound **1**.

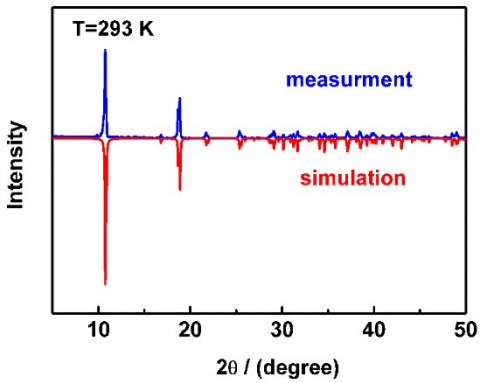

Fig. S2 The powder X-ray diffraction (PXRD) pattern of compound **1** at 293 K.

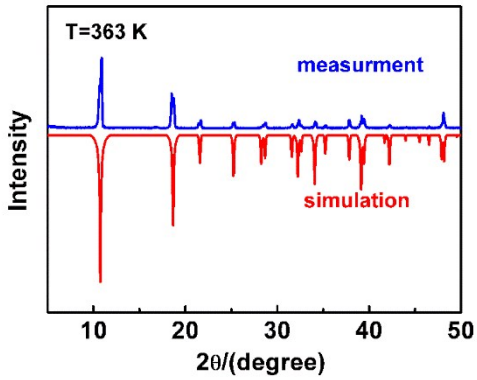

Fig. S3 The powder X-ray diffraction (PXRD) pattern of compound **1** at 363 K.

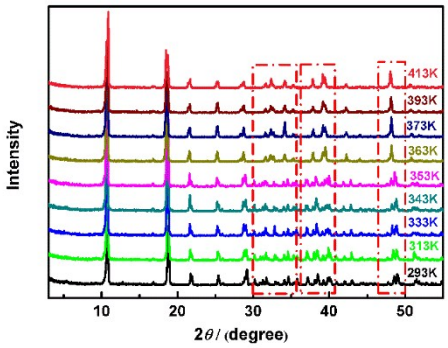

Fig. S4 Variable-temperature PXRD patterns of **1** measured in the heating mode.

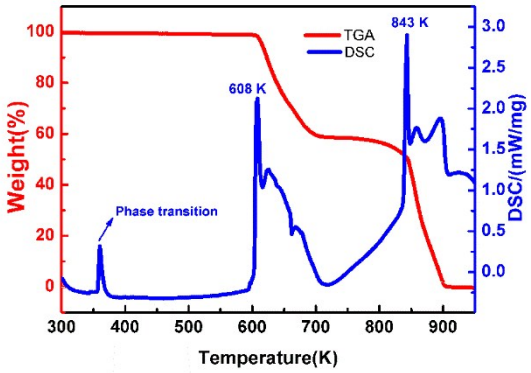

Fig. S5 The TGA-DSC curves of compound **1** with heating rate 10 K min^{-1}.

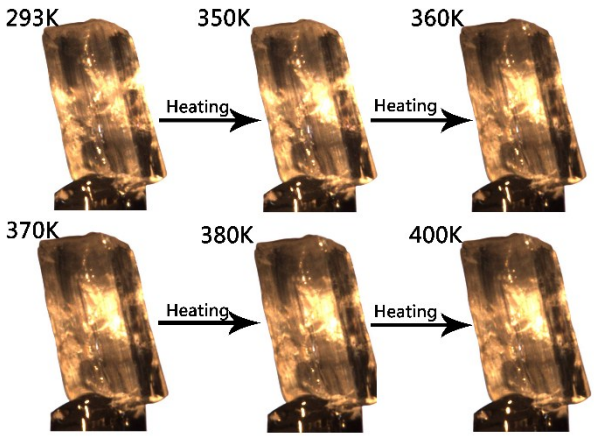

Fig. S6 The photos of single crystal at temperatures of 293 K, 350 K, 360 K, 370 K, 380 K and 400 K.

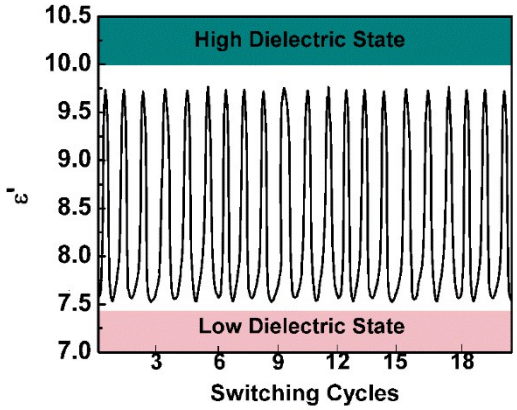

Fig. S7 The ε'-switching of the polycrystalline sample of compound **1** at 1 MHz showing completely reversible behavior within 21 "ON"/"OFF" cycles.

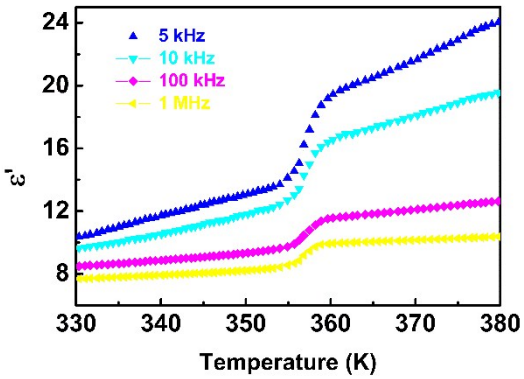

Fig. S8 The temperature-dependent dielectric constant (ε') of the compound **1** measured in a frequency range of 5 to 1000 kHz.

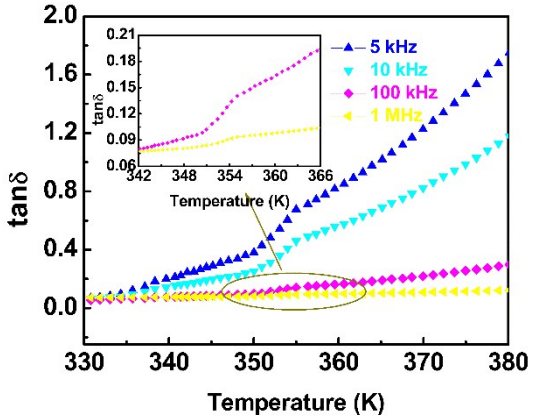

Fig. S9 The dielectric loss (*tan δ*) of the compound **1** measured in a frequency range of 5 to 1000 kHz.

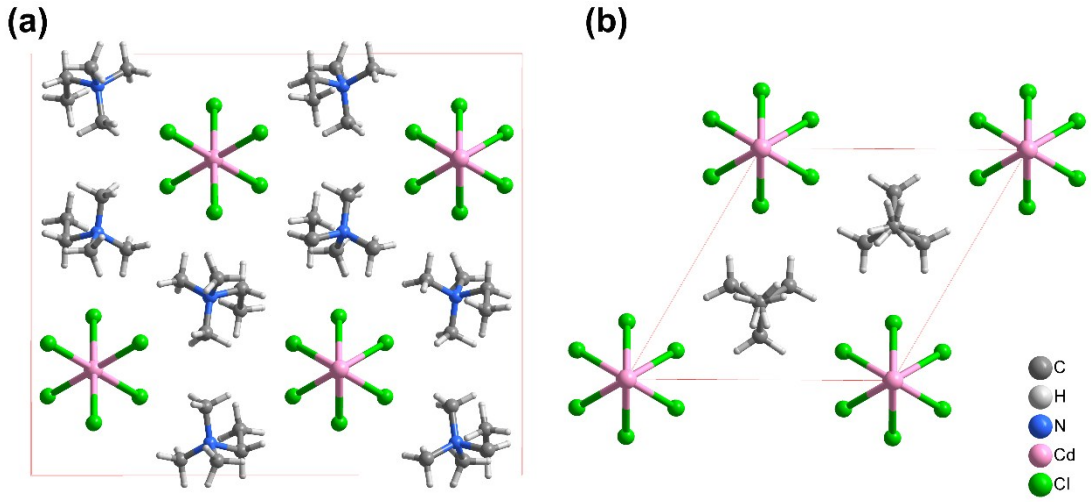

Fig. S10 The packing diagram structures of **1** at (a) 293 K and (b) 363 K.

Table S1 Crystal Data and Structure Refinement Details of **1**.

	293 K	363 K
Empirical formula	$[Me_3NCH_2CH_3][CdCl_3]$	$[Me_3NCH_2CH_3][CdCl_3]$
Formula weight	306.93	306.93
Crystal system	orthorhombic	hexagonal
Space group	*Pbca*	$P6_3/mmc$
a (Å)	16.0893(6)	9.5032(3)
b (Å)	6.8295(3)	9.5032(3)
c (Å)	18.8185(8)	6.8345(4)
α (deg)	90	90
β (deg)	90	90
γ (deg)	90	120
Volume ($Å_3$), *Z*	2067.81(15), 8	534.54(5) , 2
D_{calcd} / g cm^{-3}	1.972	1.906
F(000)	1200.0	299.8
Goodness-of-fit on F_2	1.030	1.008
Tmin/Tmax	0.403/0.568	0.579/0.415
R_1[a] (> 2σ)	0.0555	0.0423
wR_2[b] (> 2σ)	0.1704	0.1219

Table S2 Selected bond lengths [Å] and angles [°] for **1** at 293 K and 363 K.

	Cd1—Cl3	2.6338 (18)	Cd1—Cd1^{i}	3.4148 (1)
	Cd1—Cl3^{i}	2.6522 (18)	Cd1—Cd1^{ii}	3.4148 (1)
	Cd1—Cl2^{i}	2.6563 (18)	Cl1—Cd1^{i}	2.6579 (19)
	Cd1—Cl1^{ii}	2.6579 (19)	Cl2—Cd1^{ii}	2.6563 (18)
	Cd1—Cl1	2.6595 (19)	Cl3—Cd1^{ii}	2.6521 (18)
	Cd1—Cl2	2.6775 (18)		
293 K				
	Cl3—Cd1—Cl3^{i}	96.90 (8)	Cl2^{i}—Cd1—Cl1	83.57 (6)
	Cl3—Cd1—Cl2^{i}	179.71 (6)	Cl1^{ii}—Cd1—Cl1	179.60 (7)
	Cl3^{i}—Cd1—Cl2^{i}	83.26 (6)	Cl3—Cd1—Cl2	83.20 (6)
	Cl3—Cd1—Cl1^{ii}	82.94 (6)	Cl3^{i}—Cd1—Cl2	179.22 (6)
	Cl3^{i}—Cd1—Cl1^{ii}	97.59 (6)	Cl2^{i}—Cd1—Cl2	96.65 (7)
	Cl2^{i}—Cd1—Cl1^{ii}	96.81 (6)	Cl1^{ii}—Cd1—Cl2	83.20 (6)
	Cl3—Cd1—Cl1	96.68 (6)	Cl1—Cd1—Cl2	96.66 (6)
	Cl3^{i}—Cd1—Cl1	82.56 (6)		

	Cd1—Cl1^{vi}	2.6606 (11)	Cd1—Cl1^{x}	2.6606 (11)
	Cd1—Cl1^{vii}	2.6606 (11)	Cd1—Cd1^{xi}	3.4173 (2)
	Cd1—Cl1^{viii}	2.6606 (11)	Cd1—Cd1^{xii}	3.4173 (2)
	Cd1—Cl1^{ix}	2.6606 (11)	Cl1—Cd1^{xi}	2.6606 (11)
	Cd1—Cl1	2.6606 (11)		
363 K	Cl1^{vi}—Cd1—Cl1^{vii}	180.000 (18)	Cl1^{viii}—Cd1—Cl1	96.81 (3)
	Cl1^{vi}—Cd1—Cl1^{viii}	83.19 (3)	Cl1^{ix}—Cd1—Cl1	83.19 (3)
	Cl1^{vii}—Cd1—Cl1^{viii}	96.81 (3)	Cl1^{vi}—Cd1—Cl1^{x}	83.19 (3)
	Cl1^{vi}—Cd1—Cl1^{ix}	96.81 (3)	Cl1^{vii}—Cd1—Cl1^{x}	96.81 (3)
	Cl1^{vii}—Cd1—Cl1^{ix}	83.19 (3)	Cl1^{viii}—Cd1—Cl1^{x}	83.19 (3)
	Cl1^{viii}—Cd1—Cl1^{ix}	180.00 (5)	Cl1^{ix}—Cd1—Cl1^{x}	96.81 (3)
	Cl1^{vi}—Cd1—Cl1	96.81 (3)	Cl1—Cd1—Cl1^{x}	180.0
	Cl1^{vii}—Cd1—Cl1	83.19 (3)		

Symmetry codes:

293 K (i) −x+1/2, y−1/2, z; (ii) −x+1/2, y+1/2, z.

363 K (i) x, y, −z+3/2; (ii) −y+1, x−y, z; (iii) −y+1, x−y, −z+3/2; (iv) −x+y+1, −x+1, −z+3/2; (v) −x+y+1, −x+1, z; (vi) x−y, x−1, −z; (vii) −x+y+2, −x+1, z; (viii) y+1, −x+y+1, −z; (ix) −y+1, x−y−1, z; (x) −x+2, −y, −z; (xi) −x+2, −y, z+1/2; (xii) −x+2, −y, z−1/2.