Supporting Information

A High-Temperature Halide Perovskite Molecular Ferroelastic with Evident Dielectric Switchings

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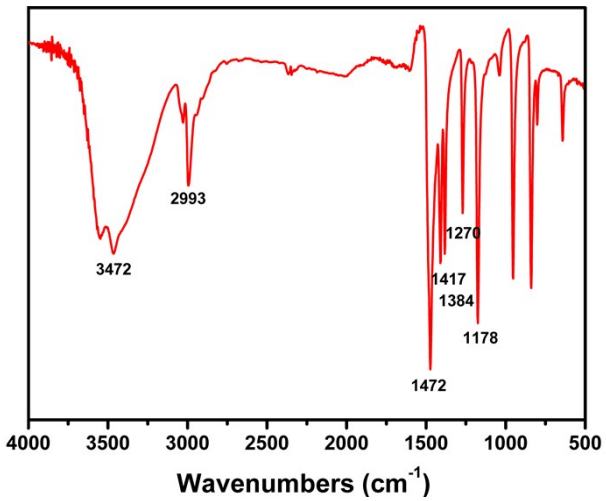

Figure S1. IR spectrum for **1**.

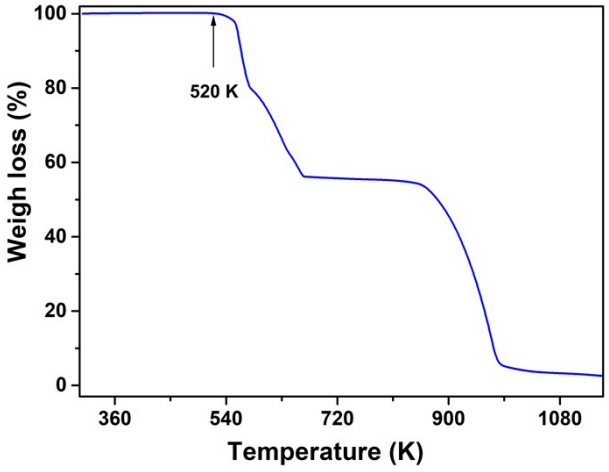

Figure S2. TGA spectrum for **1**.

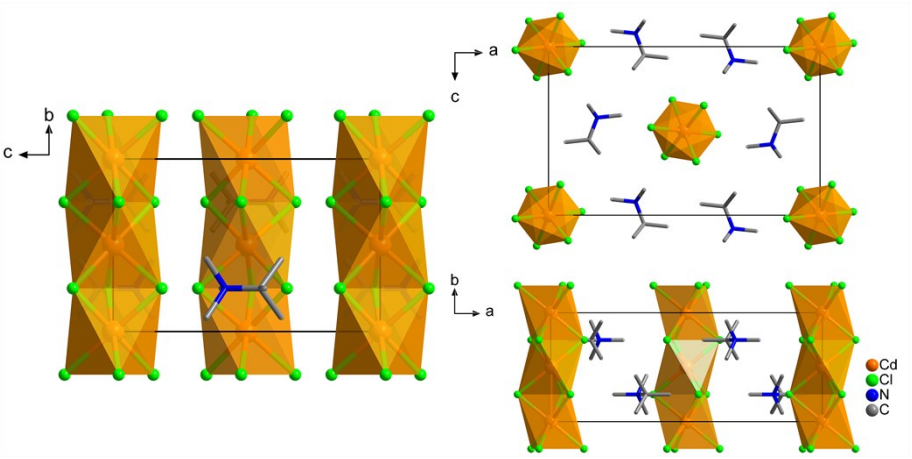

Figure S3. Unit packing structures for **1** at 293 K.

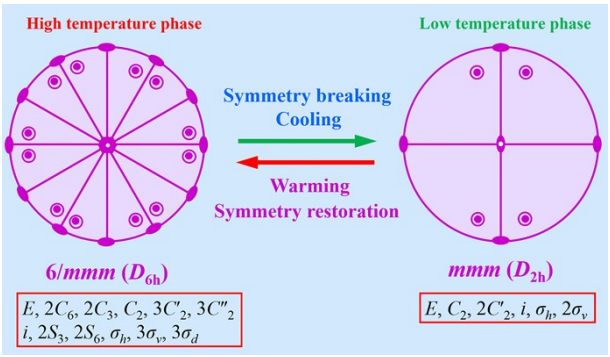

Fig. S4 Symmetry change in **1** of the RTP and HTP.

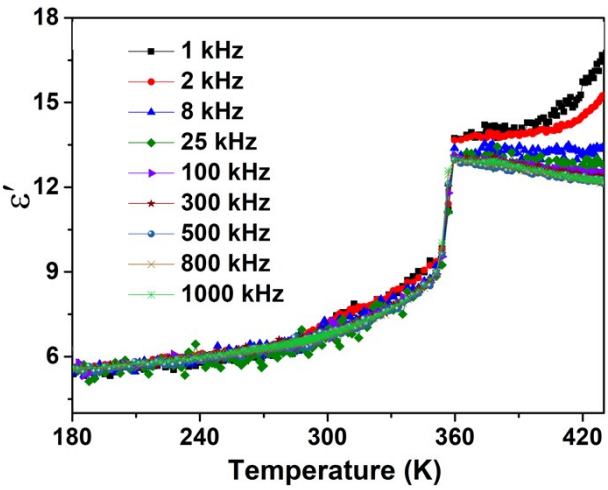

Figure S5. Temperature-dependence of the real part (ε′) of dielectric constant performed on the polycrystalline sample of **1** at muti-frequencies.

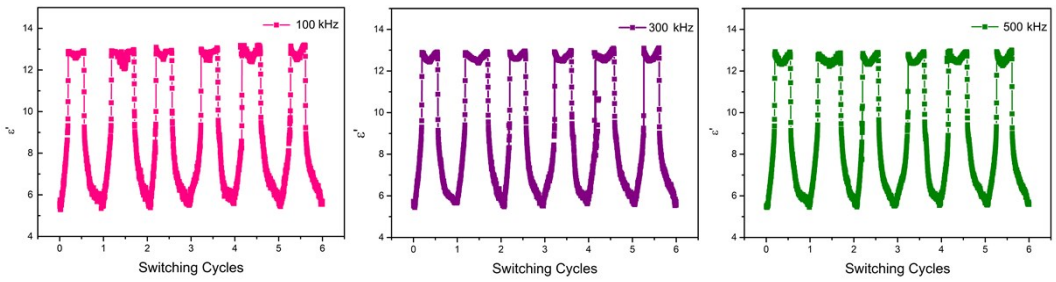

Figure S6. The recoverable dielectric switching of **1** at 100, 300 and 500 kHz as a function of time.

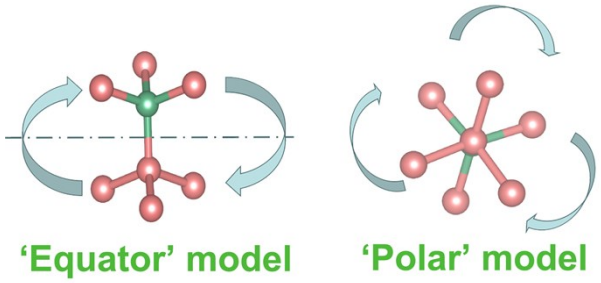

Figure S7. The rotation models used during the DFT calculation for **1**, the neighboring cations and anions are omitted for clarity.

Table S1. Crystal structure and refinement detail of **1**.

Temperature (K)	293 K	373 K
Crystal system	Orthorhombic	Hexagonal
Space group	*Pnma*	$P6_3/mmc$
a/ Å	16.9323 (13)	10.1902 (5)
b/ Å	6.7865 (4)	10.1902 (5)
c/ Å	10.5059 (5)	6.8314 (5)
Volume/(Å^3)	1207.24 (13)	614.34 (8)
Z	4	2
Mr	334.98	398.91
Mu/mm^{-1}	2.427	2.405
Radiation type	Mo-Kα; λ = 0.71073 Å	Mo-Kα; λ = 0.71073 Å
Dcalc / g cm^{-3}	1.843	2.157
F(000)	664	378
GOF	1.03	1.07
R_1[I > 2σ (I)]	0.05	0.054
wR_2 [I > 2σ (I)]	0.165	0.177
R_{int}	0.06	0.076

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

Cd1−Cl1	2.6826 (15)	Cl3−Cd1^{ii}	2.6218 (12)
Cd1−Cl2	2.6589 (12)	N1−C3	1.470 (12)
Cd1−Cl3	2.6218 (12)	N1−C1	1.473 (11)
Cd1−Cl3^{i}	2.6217 (12)	N1−C2^{iv}	1.489 (10)
Cd1−Cd1^{i}	3.3932 (2)	N1−C2	1.489 (10)
Cd1−Cd1^{ii}	3.3932 (2)	C3−C4	1.446 (15)
Cl1−Cd1^{iii}	2.6826 (15)	C3−C5^{iv}	1.541 (12)
Cl2−Cd1^{ii}	2.6589 (12)	C3−C5	1.541 (12)
Cl3−Cd1−Cl2	83.74 (4)	C3−N1−C1	117.2 (7)
Cl3−Cd1−Cl2^{i}	96.26 (4)	C3−N1−C2^{iv}	110.2 (6)
Cl3−Cd1−Cl1	95.69 (5)	C1−N1−C2^{iv}	107.9 (6)
Cl2−Cd1−Cl1	97.55 (4)	C3−N1−C2	110.2 (6)
Cl3^{i}−Cd1−Cl3	180.0	C1—N1—C2	107.9 (6)
Cl1−Cd1−Cl1^{i}	180.0	C4—C3—N1	117.5 (9)
Cl3−Cd1−Cd1^{iii}	130.33 (2)	C4—C3—C5^{iv}	110.9 (8)
Cl2−Cd1−Cd1^{iii}	129.65 (2)	N1—C3—C5	110.1 (7)

Symmetry codes: (i) –x, –y, –z+2; (ii) –x, y+1/2, –z+2; (iii) –x, y–1/2, –z+2; (iv) x, –y+1/2, z.

Table S3. Bond lengths [Å] and bond angles [°] for **1** at 373 K.

Cd1−Cl1	2.6587 (5)	Cd1−Cl1^{v}	2.6587 (5)

Cd1−Cl1^{i}	2.6587 (5)	Cd1−Cd1^{vi}	3.4157 (3)
Cd1−Cl1^{iii}	2.6587 (5)	Cd1−Cd1^{vii}	3.4157 (3)
Cd1−Cl1^{iv}	2.6587 (5)		
Cl1^{i}−Cd1−Cl1	96.833 (14)	Cl1^{i}−Cd1−Cd1^{vi}	129.969 (9)
Cl1^{i}−Cd1−Cl1^{ii}	180.0	Cl1^{ii}−Cd1−Cd1^{vi}	50.031 (10)
Cl1^{ii}−Cd1−Cl1	83.167 (14)	Cd1^{vi}−Cl1−Cd1	79.938 (19)
Cl1^{ii}−Cd1−Cl1^{iii}	96.831 (14)	Cd1^{vi}−Cd1−Cd1^{vii}	180.0
Cl1^{ii}−Cd1−Cl1^{iv}	83.169 (14)	Cd1^{vi}−Cl1−Cd1^{vii}	79.938 (19)
Cl1^{iii}−Cd1−Cl1^{iv}	180.0	Cl1^{iii}−Cd1−Cd1^{v}	83.168 (14)
Cl1−Cd1−Cd1^{v}	180.0		

Symmetry codes: (i) x−y, x−1, −z; (ii) −x+y+2, −x+1, z; (iii) y+1, −x+y+1, −z; (iv) −y+1, x−y−1, z; (v) −x+2, −y, −z; (vi) −x+2, −y, z+1/2; (vii) −x+2, −y, z−1/2.