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Electronic Supplementary Information

Successive high-temperature phase transitions triggered dielectric switching in a one-dimensional hybrid perovskite with blue emission

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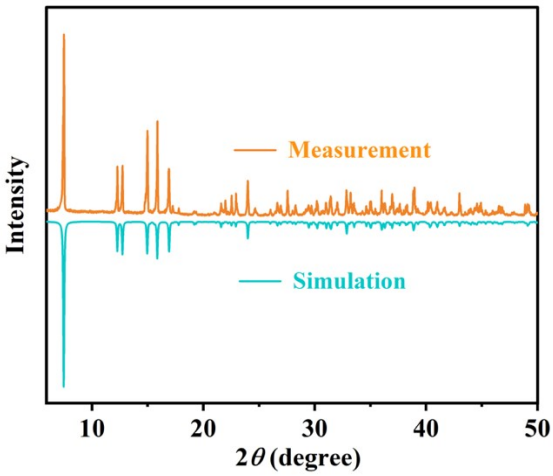

Fig. S1 Experimental PXRD and simulated patterns from single-crystal data of compound **1** at 293 K.

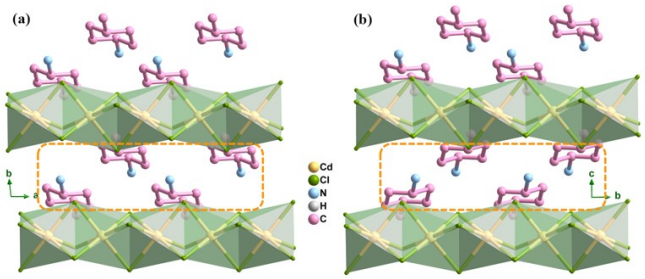

Fig. S2 Packing diagrams of compound **1** at (a) LTP along the *a*-axis and (b) ITP along the *b*-axis.

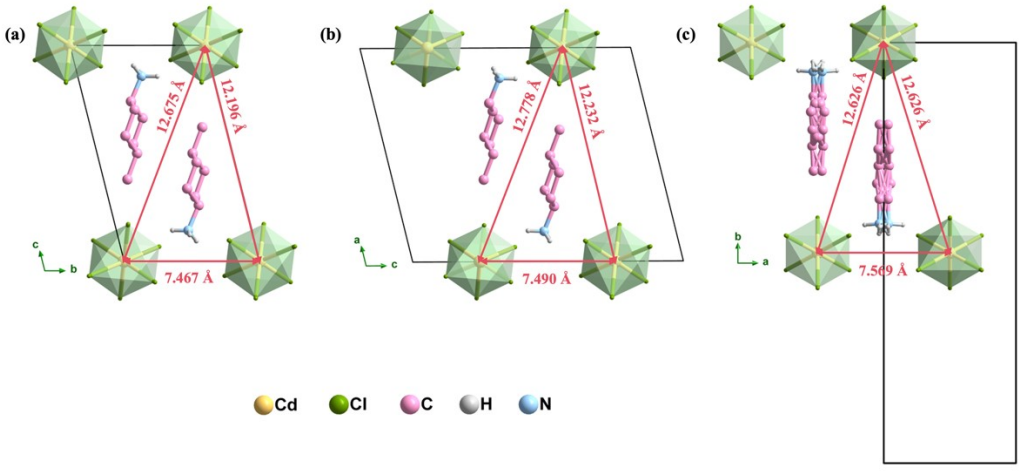

Fig. S3 Packing diagrams of compound **1** at (a) LTP, (b) ITP and (c) HTP. Hydrogen atoms bonded to C atoms are omitted for clarity.

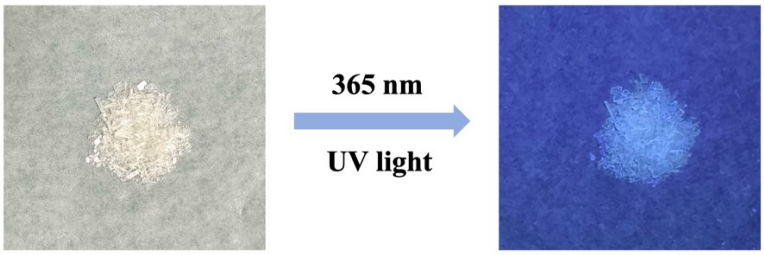

Fig. S4 The luminescence photos of compound **1** under the UV lamp.

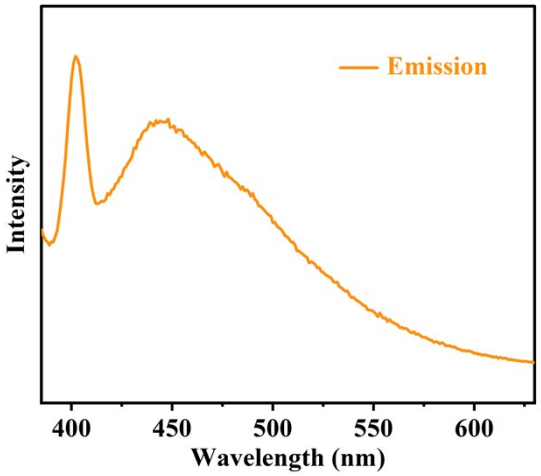

Fig. S5 PL emission spectra of *trans*-4-methylcyclohexanamine hydrochloride.

Table S1 Crystal data and structure refinement for compound **1**

	LTP	**ITP**		**HTP**
Empirical formula		$[C_7H_{16}N][CdCl_3]$		
Formula weight		332.96		
CCDC number	2348074	2348075	2348076	2348077
Temperature [K]	293	388	400	448
Crystal system	triclinic	monoclinic	monoclinic	orthorhombic
Space group	$P\bar{1}$	$P2_1/c$	$P2_1/c$	$Cmcm$
a [Å]	6.6055(7)	12.229(2)	12.2318(12)	7.5694(14)
b [Å]	7.4668(10)	6.6525(11)	6.6515(6)	24.091(4)
c [Å]	12.1960(16)	15.025(2)	15.0423(12)	6.6715(12)
α [°]	103.927(5)	90	90	90
β [°]	90.111(4)	103.592(6)	103.610(3)	90
γ [°]	95.743(4)	90	90	90
Volume [Å^3]	580.71(13)	1188.1(4)	1189.47(19)	1216.6(4)
Z	2	4	4	4
ρ_{calc} [gcm^{-3}]	1.904	1.861	1.859	1.818
μ [mm^{-1}]	2.522	2.466	2.463	2.408
F(000)	328	656	656	656
Goodness-of-fit on F^2	1.043	1.042	1.049	1.088
Final R indexes	R_1 = 0.0347	R_1 = 0.0309	R_1 = 0.0356	R_1 = 0.0326
[$I \geq 2\sigma(I)$]	wR_2 = 0.0890	wR_2 = 0.0739	wR_2 = 0.0811	wR_2 = 0.0853
Final R indexes	R_1 = 0.0379	R_1 = 0.0401	R_1 = 0.0503	R_1 = 0.0370
[all data]	wR_2 = 0.0934	wR_2 = 0.0806	wR_2 = 0.0905	wR_2 = 0.0898

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

Cd1–Cd2	3.3028(4)	Cd1–Cd2$^{\#1}$	3.3028(4)
Cd1–Cl2$^{\#2}$	2.6396(8)	Cd1–Cl2	2.6396(8)
Cd1–Cl3	2.6664(9)	Cd1–Cl3$^{\#2}$	2.6664(9)
Cd1–Cl1	2.6103(8)	Cd1–Cl1$^{\#2}$	2.6103(8)
Cd2–Cl2	2.6114(8)	Cd2–Cl2$^{\#3}$	2.6114(8)
Cd2–Cl3$^{\#3}$	2.6560(8)	Cd2–Cl3	2.6560(8)
Cd2–Cl1$^{\#3}$	2.6505(8)	Cd2–Cl1	2.6505(8)
Cl2–Cd1–Cl3	93.64(3)	Cl2–Cd1–Cl3	86.36(3)
Cl1–Cd1–Cl2	96.30(3)	Cl1–Cd1–Cl2	83.70(3)
Cl1–Cd1–Cl3	95.12(3)	Cl1–Cd1–Cl3	84.88(3)
Cl2–Cd2–Cl3	87.15(3)	Cl2–Cd2–Cl3	92.85(3)
Cl2–Cd2–Cl1	96.53(3)	Cl2–Cd2–Cl1	83.47(3)
Cl1–Cd2–Cl3	84.30(3)	Cl1–Cd2–Cl3	95.70(3)

Symmetry transformations used to generate equivalent atoms: #1: -1+X, +Y, +Z; #2: 1-X, -Y, -Z; #3: 1+X, +Y, +Z; #4: 2-X, -Y, -Z.

Table S3 Selected bond lengths [Å] and bond angles [°] for compound **1** at 388 K

Cd1–Cd1$^{\#1}$	3.3269(6)	Cd1–Cd1$^{\#2}$	3.3268(5)
Cd1–Cl1$^{\#2}$	2.6409(10)	Cd1–Cl1	2.6306(10)
Cd1–Cl3$^{\#2}$	2.6823(10)	Cd1–Cl3	2.6603(10)
Cd1–Cl2$^{\#1}$	2.6396(10)	Cd1–Cl2	2.6258(10)
Cl1–Cd1–Cl3	96.09(3)	Cl2–Cd1–Cl1	95.65(3)
Cl1–Cd1–Cl3	83.95(3)	Cl2–Cd1–Cl1	97.89(3)
Cl1–Cd1–Cl3	95.35(3)	Cl2–Cd1–Cl1	83.25(3)
Cl1–Cd1–Cl3	84.58(3)	Cl2–Cd1–Cl3	94.92(3)
Cl1–Cd1–Cl2	83.19(3)	Cl2–Cd1–Cl3	86.62(3)
Cl2–Cd1–Cl3	86.44(3)	Cl2–Cd1–Cl3	92.01(3)

Symmetry transformations used to generate equivalent atoms: #1: 2-X, -0.5+Y, 0.5-Z; #2: 2-X, 0.5+Y, 0.5-Z.

Table S4 Selected bond lengths [Å] and bond angles [°] for compound **1** at 400 K

Cd1–Cd1$^{\#1}$	3.3264(3)	Cd1–Cd1$^{\#2}$	3.3264(3)
Cd1–Cl1	2.6280(10)	Cd1–Cl1$^{\#1}$	2.6386(11)
Cd1–Cl3$^{\#2}$	2.6377(10)	Cd1–Cl3	2.6247(10)
Cd1–Cl2	2.6624(10)	Cd1–Cl2$^{\#1}$	2.6848(10)
Cl1–Cd1–Cl3	83.13(3)	Cl3–Cd1–Cl1	97.97(3)
Cl1–Cd1–Cl2	84.64(3)	Cl3–Cd1–Cl1	95.70(3)
Cl1–Cd1–Cl2	96.02(3)	Cl3–Cd1–Cl2	94.92(3)
Cl1–Cd1–Cl2	95.31(3)	Cl3–Cd1–Cl2	92.02(3)
Cl1–Cd1–Cl2	83.99(3)	Cl3–Cd1–Cl2	86.63(3)
Symmetry transformations used to generate equivalent atoms: #1: 2-X, -0.5+Y, 1.5-Z; #2: 2-X, 0.5+Y, 1.5-Z.			

Table S5 Selected bond lengths [Å] and bond angles [°] for compound **1** at 448 K

Cd1–Cd1$^{\#1}$	3.3358(6)	Cd1–Cd1$^{\#2}$	3.3358(6)
Cd1–Cl2	2.6602(7)	Cd1–Cl2$^{\#3}$	2.6602(7)
Cd1–Cl2$^{\#4}$	2.6602(7)	Cd1–Cl2$^{\#5}$	2.6602(7)
Cd1–Cl1$^{\#4}$	2.6229(10)	Cd1–Cl1	2.6228(10)
Cl2–Cd1–Cl2	86.28(3)	Cl1–Cd1–Cl2	96.35(2)
Cl2–Cd1–Cl2	93.72(3)	Cl1–Cd1–Cl2	83.65(2)
Symmetry transformations used to generate equivalent atoms: #1: 1-X, 1-Y, -0.5+Z; #2: 1-X, 1-Y, 0.5+Z; #3: 1-X, 1-Y, 1-Z; #4: +X, 1-Y, -0.5+Z; #5: 1-X, +Y, 1.5-Z.			