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Rapid dielectric bistable switching materials without time/temperature responsive blind area in the linarite-like type molecular large-size single crystals

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Table S1 Selected structural data for 1under 293K

Bond lengths / Å and bond angles / °			
Cd(1)-O(1)	2.234(3)	Cd(1)-O(1)#1	2.234(3)
Cd(1)-O(1)#2	2.234(3)	Cd(1)-O(1)#3	2.234(3)
Cd(1)-Cl(1)#4	2.6260(6)	Cd(1)-Cl(1)#1	2.6260(6)
Cd(1)-Cl(1)#5	2.6260(6)	Cd(1)-Cl(1)	2.6260(6)
Cl(1)-Cd(1)#7	2.6260(6)	S(1)-O(1)#4	1.492(4)
S(1)-O(2)	1.401(2)	S(1)-O(2)#4	1.401(2)
S(1)-O(1)#3	1.492(4)	S(1)-O(1)	1.492(4)
S(1)-O(1)#6	1.492(4)		
O(1)-Cd(1)-O(1)#1	180.00(18)	O(1)-Cd(1)-O(1)#2	165.20(19)
O(1)#1-Cd(1)-O(1)#2	14.80(19)	O(1)-Cd(1)-O(1)#3	14.80(19)
O(1)#1-Cd(1)-O(1)#3	165.20(19)	O(1)#2-Cd(1)-O(1)#3	180.0

Hydrogen bonds / Å and °				
D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1C)...O(2)#8	0.89	1.82	2.637(3)	151.7

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z #2 x,-y+1,-z #3 -x+1,y,z #4 -x+1,y,-z+1/2 #5 x,-y+1,z-1/2 #6 x,y,-z+1/2 #7 -x+1,-y+1,z+1/2 #8 x-1/2,y-1/2,z

Table S2 Selected structural data for 1 under 193k

Bond lengths / Å and bond angles / °			
Cd(1)-O(2)	2.269(3)	Cd(1)-O(2)#1	2.269(3)
Cd(1)-Cl(1)	2.6287(15)	Cd(1)-Cl(1)#1	2.6287(15)
Cd(1)-Cl(2)	2.6348(14)	Cd(1)-Cl(2)#1	2.6348(14)
Cl(2)-Cd(1)#2	2.6348(14)	Cl(1)-Cd(1)#2	2.6287(15)
S(1)-O(3)	1.450(3)	S(1)-O(2)#3	1.470(2)
S(1)-O(2)	1.470(2)	S(1)-O(1)	1.488(3)
O(7)#2-Cl(1)-O(7)	109.72(11)	O(7)#2-Cl(1)-O(10)	108.94(7)
O(7)-Cl(1)-O(10)	108.94(7)	O(7)#2-Cl(1)-O(9)	109.86(4)

Hydrogen bonds / Å and °				
D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1C)...O(3)#4	0.90	1.84	2.609(5)	142.7
N(2)-H(2C)...O(1)#5	0.90	1.78	2.648(5)	159.9

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z #2 -x+1,y+1/2,-z #3 x,-y+1/2,z #4 x+1/2,y,-z+1/2 #5 x+1/2,y,-z-1/2

Table S3 Selected structural data for 2 under 293K

Bond lengths / Å and bond angles / °			
Cd(1)-O(1)	2.260(4)	Cd(1)-O(1)#1	2.260(4)
Cd(1)-O(1)#2	2.260(4)	Cd(1)-O(1)#3	2.260(4)
Cd(1)-Br(1)#4	2.7667(11)	Cd(1)-Br(1)#1	2.7667(11)
Cd(1)-Br(1)#5	2.7667(11)	Cd(1)-Br(1)	2.7667(11)
Br(1)-Cd(1)#7	2.7667(11)	S(1)-O(2)#4	1.448(3)
S(1)-O(2)	1.448(3)	S(1)-O(1)#2	1.457(4)
S(1)-O(1)#6	1.457(4)	S(1)-O(1)#4	1.457(4)
S(1)-O(1)	1.457(4)		
O(1)-Cd(1)-O(1)#1	180.0	O(1)-Cd(1)-O(1)#2	6.2(5)
O(1)#1-Cd(1)-O(1)#2	173.8(5)	O(1)-Cd(1)-O(1)#3	173.8(5)
O(1)#1-Cd(1)-O(1)#3	6.2(5)	O(1)#2-Cd(1)-O(1)#3	180.00(19)

Hydrogen bonds / Å and °				
D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1C)...O(2)#8	0.89	1.82	2.637(3)	151.7

Table S4 Selected structural data for 2 under 223k

Bond lengths / Å and bond angles / °			
Cd(1)-O(1)	2.257(11)	Cd(1)-O(1)#1	2.257(11)
Cd(1)-Br(1)#2	2.7554(17)	Cd(1)-Br(1)#3	2.7554(17)
Cd(1)-Br(1)#1	2.7554(17)	Cd(1)-Br(1)	2.7554(17)
Br(1)-Cd(1)#4	2.6348(14)		
S(1)-O(2)	1.439(12)	S(1)-O(2)#2	1.439(12)
S(1)-O(1)	1.460(12)	S(1)-O(1)#5	1.460(12)
O(7)#1-Cl(1)-O(1)	180.0		

Hydrogen bonds / Å and °				
D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1C)...O(2)#8	0.99	1.71	2.64(2)	154.6

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z+1 #2 -x,y,z #3 x,-y+1,-z+1 #4 -x,-y+1,z-1/2 #5 x,y,-z+3/2 #6 x,y,-z+1/2 #7 -x+1,y,z #8 -x+1,-y+1,-z+1

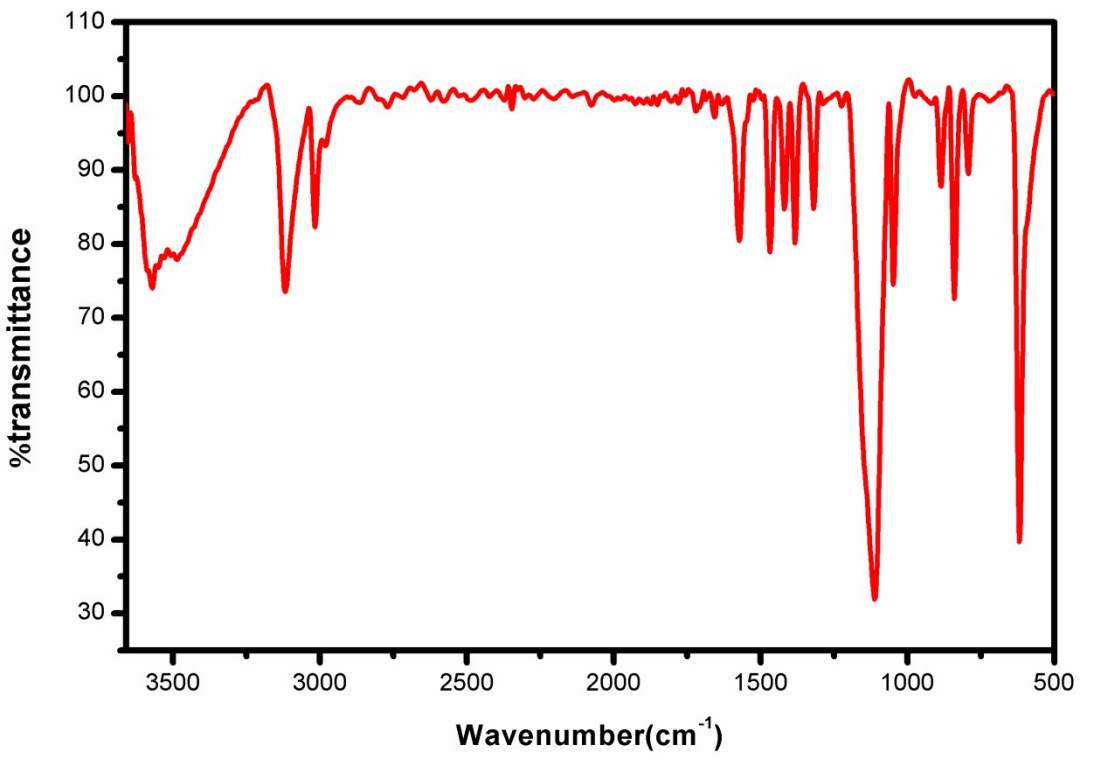

Fig.S1 The IR spectrum for compound 1

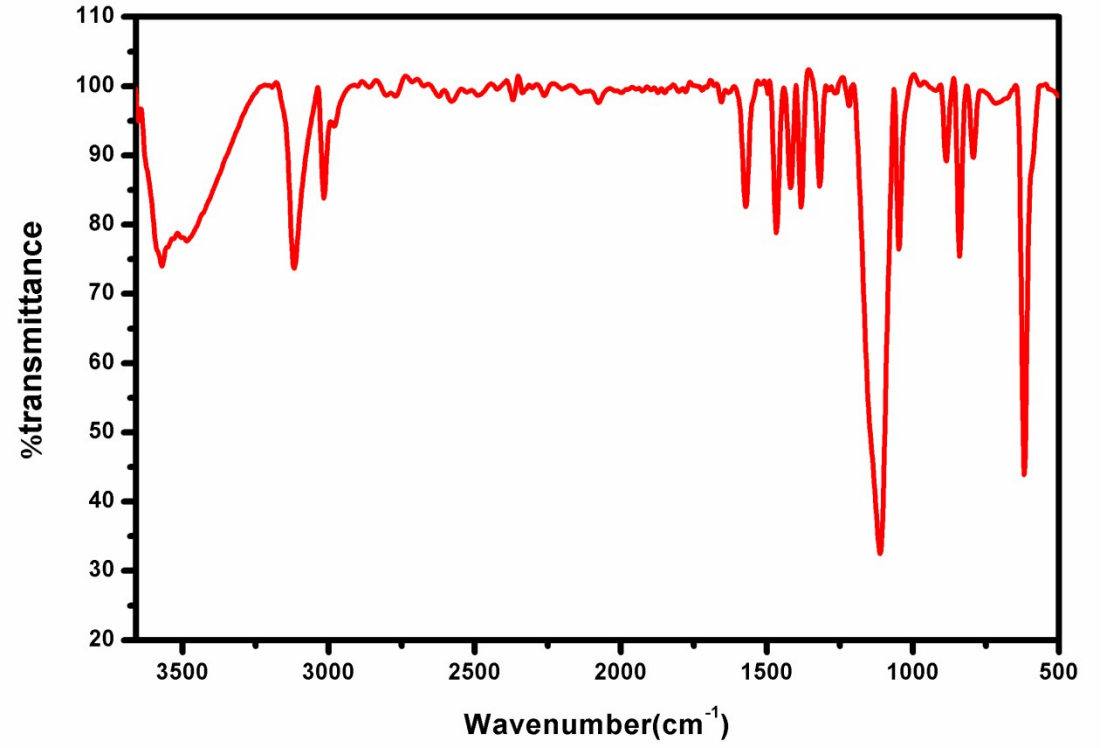

Fig.S2 The IR spectrum for compound 2

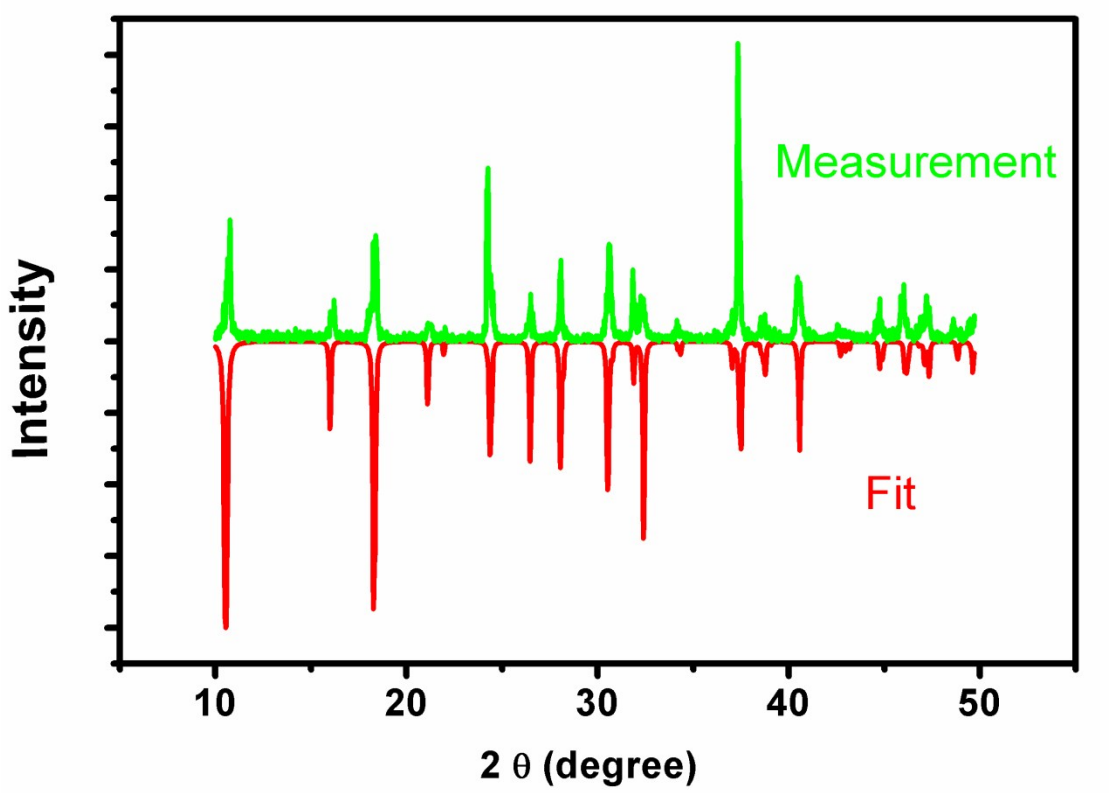

Fig.S3 The powder X-ray diffraction (PXRD) pattern for compound 1

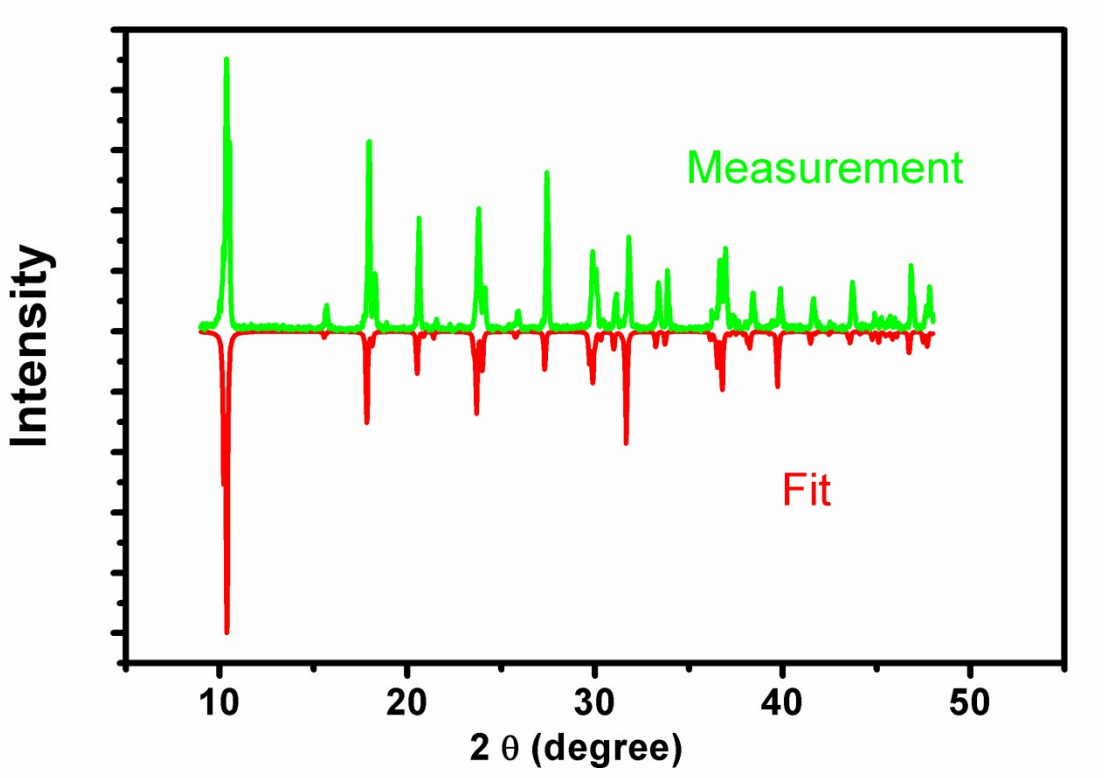

Fig.S4 The powder X-ray diffraction (PXRD) pattern for compound 2

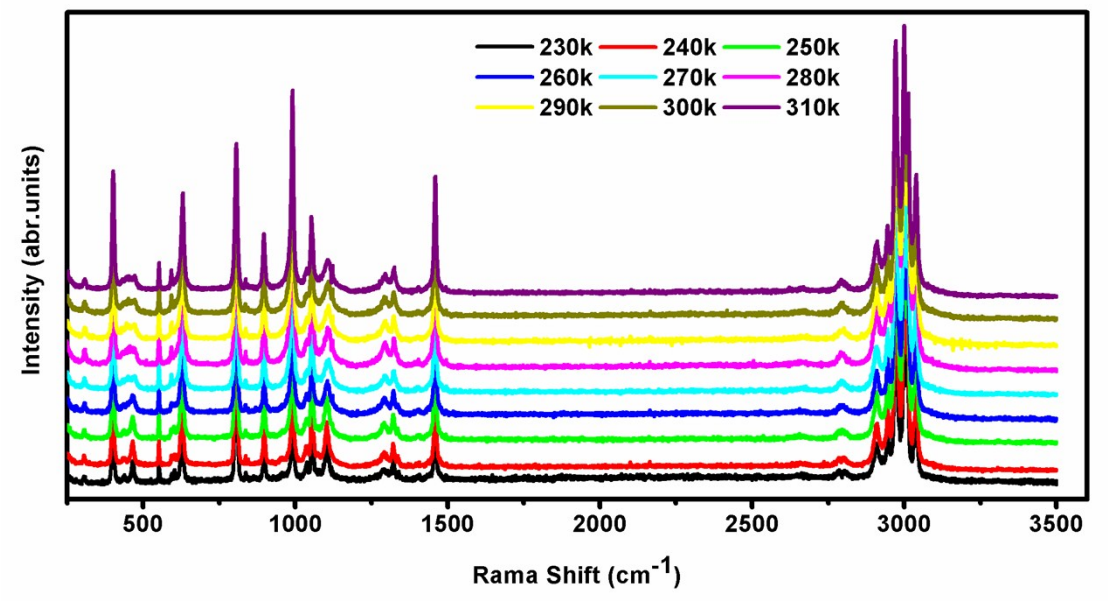

Fig.S5 Raman spectra of compound 1 at various temperatures in the 250-3500 cm^{-1} spectral ranges.

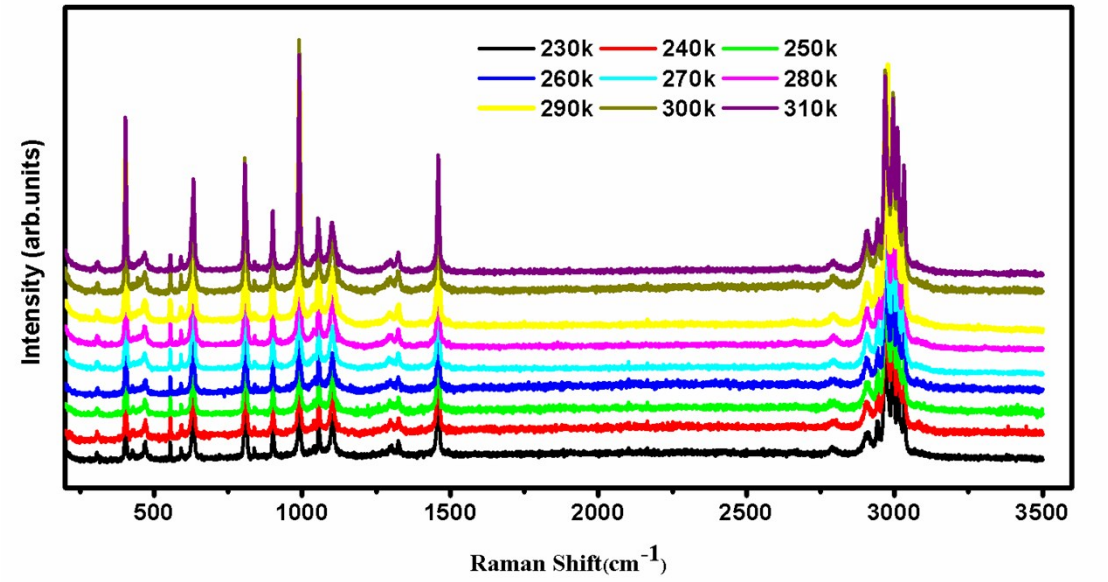

Fig.S6 Raman spectra of compound 2 at various temperatures in the 250-3500 cm^{-1} spectral ranges.