Supporting information for:

Temperature-induced isosymmetric reversible structural phase transition in catena-[pyridinium tris(μ_2-bromo)-cadmium(II)]

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1. IR Spectrum

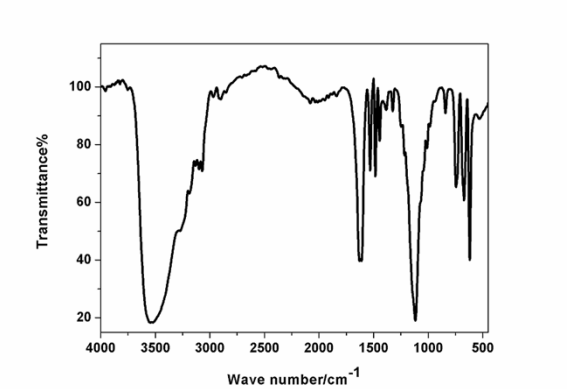

Fig. S1 The IR Spectrum of compound **1** at room temperature.

The IR spectrum of **1** shows strong vibration peaks at 3500, 3078 can attribute to the C-H and N-H and strong vibration peaks at 1632 and 1542 cm^{-1} can attribute to the C=C and c=N， indicating the existence of a protonated pyridinium cation

2. XRPD

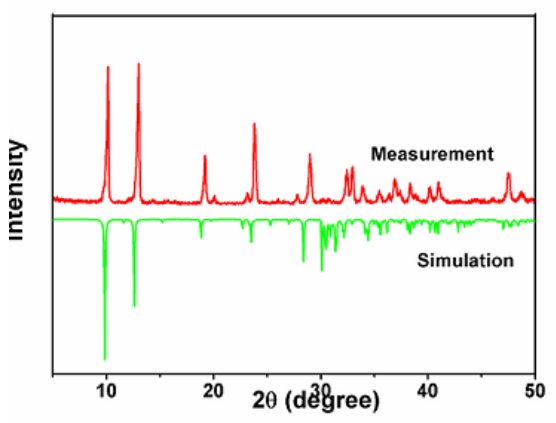

Fig. S2 XRPD powder pattern of **1** and 2 at room temperature.

Compounds **1** was characterized by X-ray powder diffraction (XRPD) at room temperature. As

shown in Fig. **S2**, the diffraction peaks in both experimental and simulated patterns calculated from the single-crystal X-ray data correspond well to each other in position but with different peak intensities, indicating the phase purity of the as-synthesized sample

3. ***Variable-PXRD***

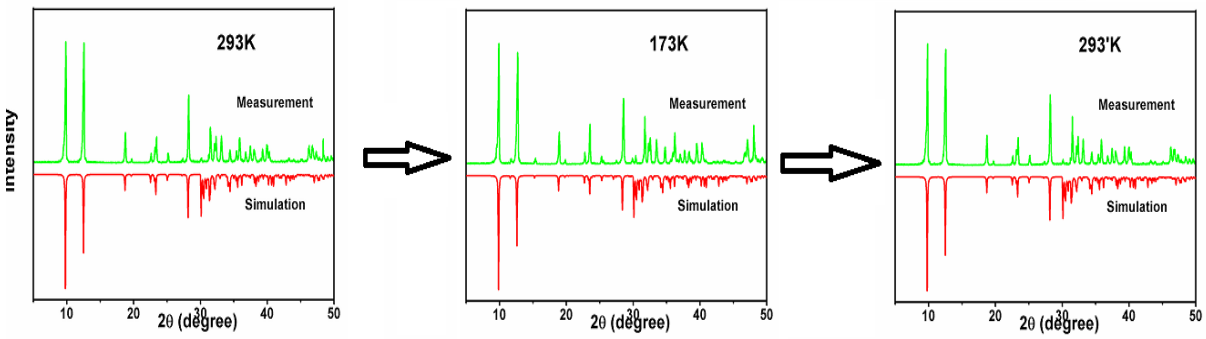

Fig. S3 The variable-temperature powder X-ray diffraction for compound **1** at 293K and 173K. When the temperature increasing from 173K to 293K, we can see the diffraction peaks are identical with the previous RTP and matches well with the simulated ones, which means this is a reproduced process.

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Table S1 Selected bond lengths (Å) and angles (°) for the compound **1** .

Bond lengths（Å）(140K)			
Cd1−Br1	2.748(18)	Cd1−Br1i	2.759(18)
Cd1-Br2	2.760(19)	Cd1-Br2ii	2.798(19)
Cd1-Br3	2.807(18)	Cd1-Br3i	2.815(18)
Bond angles（°）(150K)			
Br1-Cd1-Br2	96.66(5)	Br2^{ii}-Cd1-Br3	81.95(5)
Br1-Cd1-Br3	85.46(6)	Br1^{i}-Cd1-Br3^{i}	85.09(6)
Br1-Cd1-Br1^{i}	97.84(6)	Br2^{ii}-Cd1-Br2	178.23(6)
Br1-Cd1-Br2^{ii}	84.85(5)	Br1-Cd1-Br3^{i}	176.89(5)
Br1-Cd1-Br3^{i}	176.89(5)	Br1^{i}-Cd1-Br2	85.35(6)
Bond lengths（Å）(293K)			
Cd1-Br1	2.7883(6)	Cd1-Br2	2.8075(7)
Bond angles（°）(293K)			
Br1-Cd1-Br2	83.387（3）	Br1^{iv}-Cd1-Br2	96.613(6)
Br1-Cd1-Br1^{iii}	84.75（3）	Br1-Cd1-Br1^{iv}	95.245(8)
Br1^{iii}-Cd1-Br2	83.388(16)	Br1^{v}-Cd1-Br2	96.613(6)

Symmetry codes: (i) 0.5+x, y, 1.5-z; (ii) –0.5+x, y, 1.5-z; (iii) (1-x, y, 0.5-z); (iv) (1-x, 1-y, -0.5+z); (v) (x, 1-y, -z)

Table S2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å$\times 10^3$) U_{eq} is defined as one third of the trace of the orthogonalized *Uij* tensor.

		x/a	y/b	z/c	U(eq)	o.f.
LTP	Cd1	359(1)	396(5)	748(7)	9.93	1.0
	Br1	-214(7)	515(1)	688(6)	13.39	1.0
	Br2	285(5)	393(8)	630(2)	12.59	1.0
	Br3	215(0)	268(2)	695(1)	12.17	1.0
	C1	191(0)	117(3)	495(8)	26.67	1.0
	C2	77(2)	111(9)	556(1)	32.37	1.0
	C3	153(4)	134(1)	624(5)	30.40	1.0
	C4	384(1)	142(9)	503(7)	22.84	1.0
	C5	453(5)	163(4)	571(9)	38.27	1.0
	N1	334(3)	158(4)	629(1)	41.04	1.0
RTP	Cd1	500	500	0	39.94	0.25
	Br1	744(3)	557(5)	250	43.76	0.5
	Br2	500	379(6)	250	44.83	0.25
	C1	1000	751	845(1)	96.32	0.5
	C2	1000	686	936(1)	96.70	0.5
	C3/N	1000	624	838(1)	82.97	0.25/0.25