Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Structural phase transitions coupled with prominent dielectric anomalies and dielectric relaxation in a one-dimensional organic–inorganic hybrid compound $[C_3H_4NS][CdCl_3]$

Guang-Quan Mei,*[a] and Wei-Qiang Liao[b]

[a]Key Laboratory of Jiangxi University for Applied Chemistry and Chemical Biology, Yichun University, Yichun 336000, China. E-mail: yc_mgq@163.com

[b]Ordered Matter Science Research Center, Southeast University, Nanjing 211189, PR China

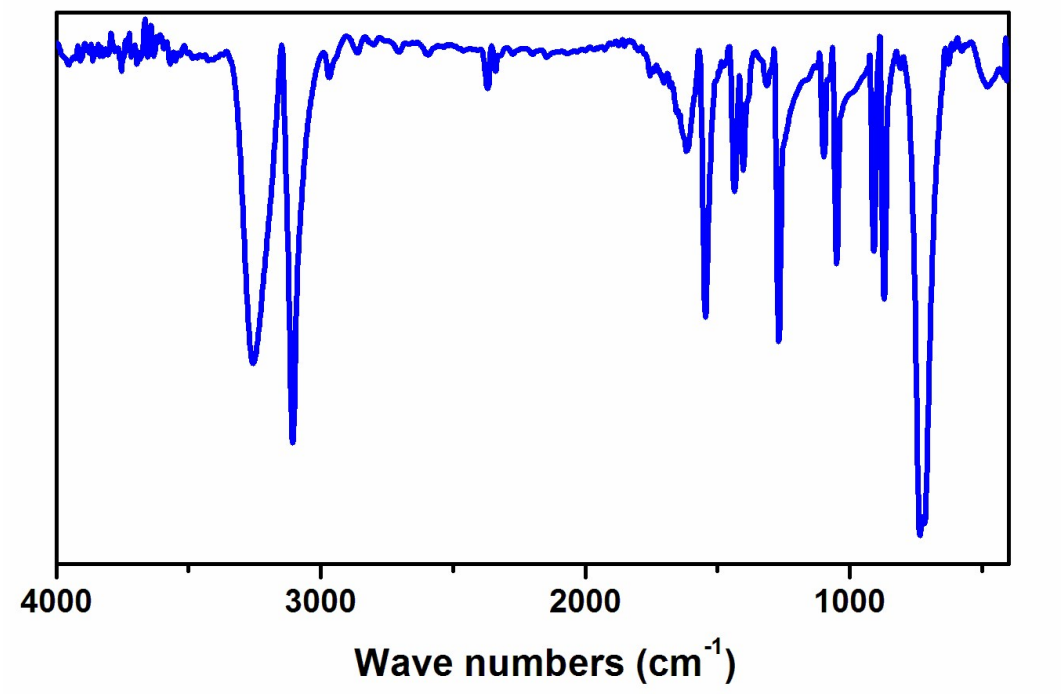

Fig. S1 Infrared (IR) spectra of solid **1** in KBr pellet recorded on a Shimadzu model IR-60 spectrometer at room temperature.

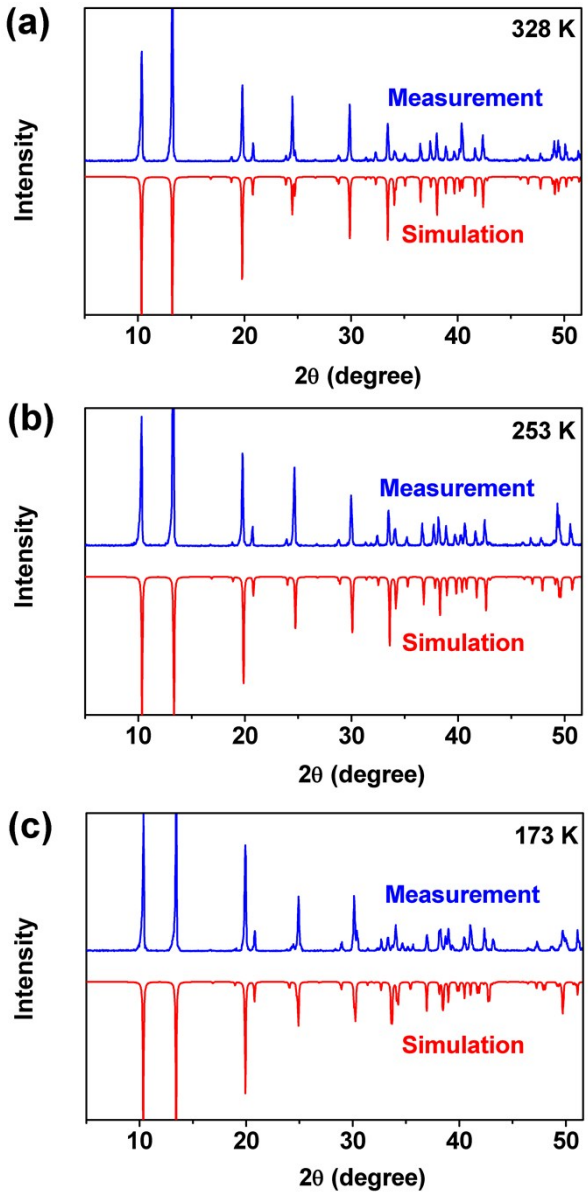

Fig. S2 X-ray powder diffraction (XRPD) of **1** at (a) 328, (b) 253, and (c) 173 K.

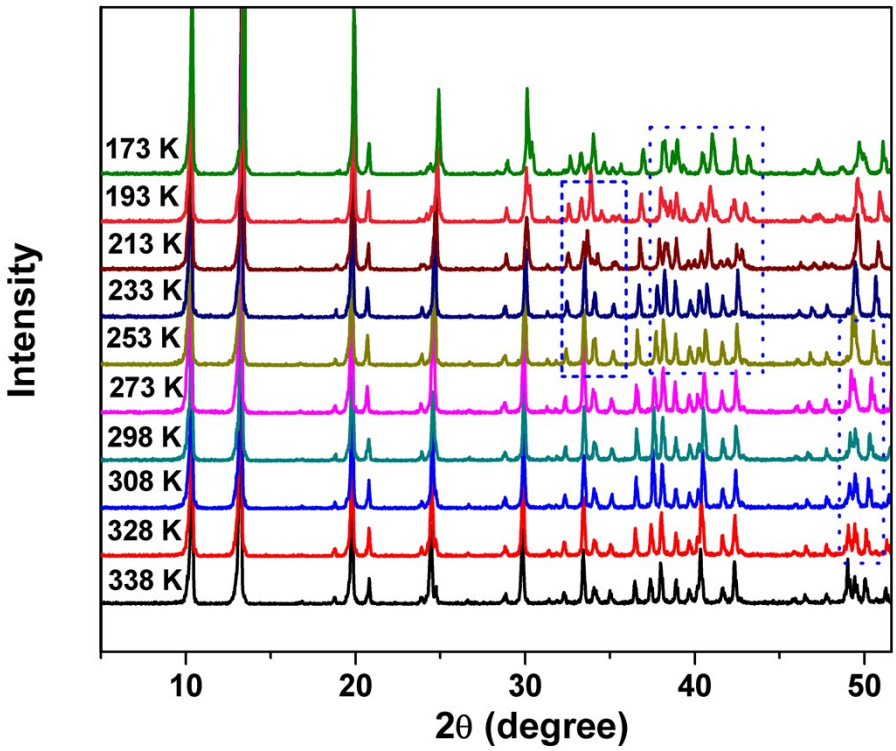

Fig. S3 Variable-temperature XRPD patterns of **1** at selected temperatures.

Table S1. Selected bond lengths [Å] and angles [°] for **1**[a] at 328, 253 and 173 K.

328 K	Cd1–Cl1	2.6411(12)	Cd1–Cl2	2.6411(16)
	Cl1–Cd1–Cl2	83.87(3)	Cl1–Cd1–Cl2^{i}	96.13(9)
	Cl1–Cd1–Cl1^{ii}	85.2(2)	Cl1–Cd1–Cl1^{iii}	94.8(2)
	Cl1–Cd1–Cl1^{i}	180.0	Cl2–Cd1–Cl2^{i}	180.00(5)
253 K	Cd1–Cl1	2.634 (7)	Cd1–Cl2	2.636(10)
	Cl1–Cd1–Cl2	83.99(2)	Cl1–Cd1–Cl2^{iv}	96.01(15)
	Cl1–Cd1–Cl1^{v}	85.30(19)	Cl1–Cd1–Cl1^{vi}	94.70(19)
	Cl1–Cd1–Cl1^{iv}	180.00(4)	Cl2–Cd1–Cl2^{iv}	180.00(4)
173 K	Cd1–Cl1	2.631(2)	Cd2–Cl1	2.628(2)
	Cd1–Cl2	2.638(9)	Cd2–Cl2	2.645(9)
	Cl1–Cd1–Cl2	84.15(7)	Cl1–Cd1–Cl2^{vii}	95.9(3)
	Cl1–Cd1–Cl1^{viii}	85.3(3)	Cl1–Cd1–Cl1^{vii}	94.7(3)
	Cl1–Cd1–Cl1^{ix}	180.0	Cl2–Cd1–Cl2^{vii}	180.00(9)
	Cl1–Cd2–Cl2	84.07(7)	Cl1–Cd2–Cl2^{x}	95.9(3)

Cl1–Cd2–Cl1^{viii}	85.4(3)	Cl1–Cd2–Cl1^{x}	94.6(3)
Cl1–Cd2–Cl1^{xi}	180.00(12)	Cl2–Cd2–Cl2^{x}	180.00(9)

[a]Symmetry codes:
(i) $-x + 1, -y + 2, z - 1/2$; (ii) $-x + 1, y, -z + 1/2$; (iii) $x, -y + 2, -z$; (iv) $-x + 2, -y + 1, z - 1/2$; (v) $-x + 2, y, -z + 1/2$; (vi) $x, -y + 1, -z$; (vii) $-x, y, -z + 1$; (viii) $x, -y + 2, z$; (ix) $-x, -y + 2, -z + 1$; (x) $-x, y, -z$; (xi) $-x, -y + 2, z$.

Table S2. Hydrogen-Bond Geometry (**Å**, deg) for the weak N–H···Cl at 328, 253 and 173 K in **1**[b].

	D–H···A	H···A	D···A	D–H···A
328 K	N1–H1···Cl2^{i}	3.117	3.8047	134.7
253 K	N1–H1···Cl2^{ii}	3.076	3.7441	132.7
173 K	N1–H1···Cl2^{iii}	3.048	3.7350	134.3
	N2–H2···Cl2^{iv}	3.061	3.7274	132.6

[b]Symmetry codes:
(i) $x - 1/2, y - 1/2, z + 1$; (ii) $-x + 1, -y + 1, z - 1/2$; (iii) $-x + 1, y - 1, -z$; (iv) $-x + 1, y - 1, -z + 1$.