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

Supporting Information

Dielectric and photoluminescence properties in a layered perovskite-type organic-inorganic hybrid phase transition compound: $NH_3(CH_2)_5NH_3MnCl_4$

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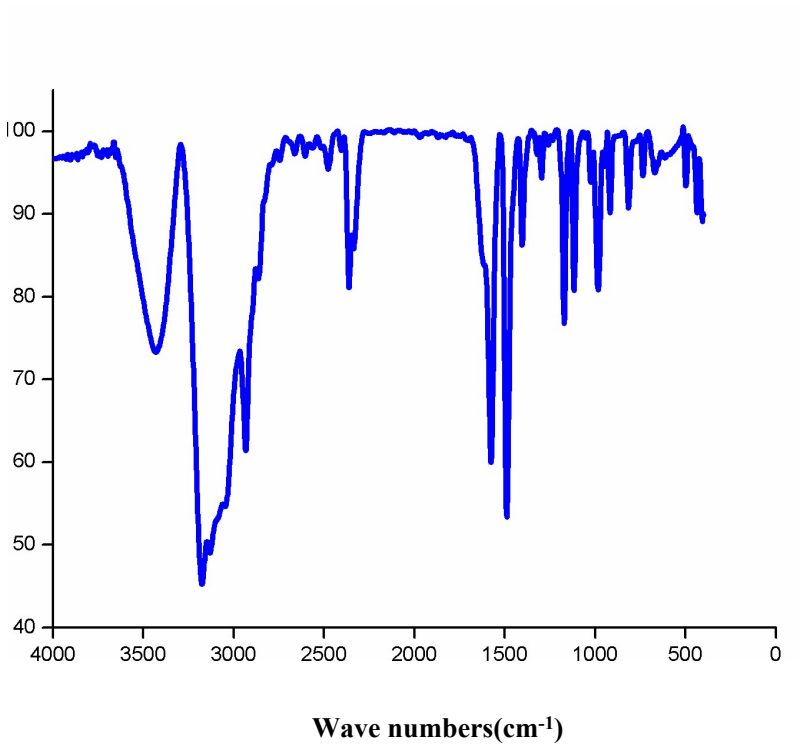

Fig. S1 Infrared (IR) spectra of solid **1** in KBr pellet recorded on a Shimadzu model IR-60 spectrometer at room temperature.

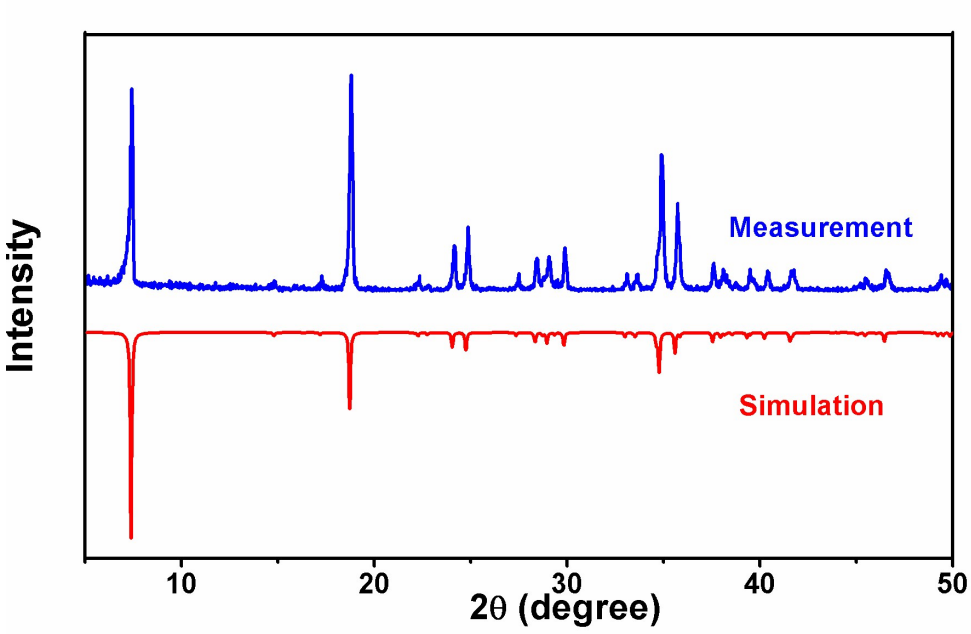

Fig. S2 Experimental powder diffraction (XRPD) pattern matching very well with the simulated pattern in terms of the crystal structures at room temperature.

Table S1. Selected bond lengths [Å] and angles [°] for **1** at 173 and 333 K.

LTP(173K)	Mn(1)-Cl(2)	2.502
	Mn(1)-Cl(1)	2.591
	Cl(1)#3-Mn(1)-Cl(1)	92.06
	Cl(1)#4-Mn(1)-Cl(1)	87.94
	Mn(1)#5-Cl(1)-Mn(1)	164.8
HTP(333K)	Mn(1)-Cl(2)	2.493
	Mn(1)-Cl(1)	2.592
	Cl(1)#2-Mn(1)-Cl(1)	92.16
	Cl(1)-Mn(1)-Cl(1)	87.84
	Mn(1)-Cl(1)-Mn(1)	168.8

Symmetry transformations used to generate equivalent atoms:

#1 -*x*+1,-*y*+1/2,*z*; #2 -*x*+1/2,-*y*+1/2,-*z*+3/2; #3 *x*,*y*+1/2,-*z*+1

#4 -*x*+1/2,-*y*+0,*z*+1/2， #5 -*x*+1/2,-*y*+0,*z*-1/2 #6 *x*,-*y*+3/2,*z*

#7 -*x*,-*y*+1,-*z*+2 #8 -*x*+1/2,-*y*+1,*z*+1/2 #9 *x*-1/2,*y*,-*z*+3/2

#10 -*x*+1/2,-*y*+1,*z*-1/2

Table S2. Hydrogen-Bond Geometry (Å, deg) for the weak N–H···Cl and C–H···Cl interactions at 173K and 333K in **1**.

	D–H···A	D···H	H···A	D···A	D–H···A
LTP(173K)	N(1)-H(1E) ...Cl(2)	0.89	2.34	3.203	164.8
	N(1)-H(1D)...Cl(1)	0.89	2.41	3.271	161.9
	N(1)-H(1C)...Cl(2)	0.89	2.42	3.290	165.7
	N(1)-H(1C)...Cl(1)	0.89	2.96	3.401	112.4
	C(1)-H(1B)...Cl(2)	0.97	2.81	3.684	150.9
	C(1)-H(1A)...Cl(2)	0.97	2.81	3.676	149.7
HTP(333K)	N(1)-H(1A)... Cl(1)	0.900	2.615	3.459	156.5
	N(1)-H(1A)... Cl(1)	0.900	2.791	3.246	112.6
	N(1)-H(1C)...Cl(1)	0.900	2.518	3.409	156.3
	N(1)-H(1C)...Cl(1)	0.900	2.380	3.224	128.1
	C(1)-H(1D)... Cl(2)	0.960	2.729	3.581	148.2
	C(1)-H(1E)... Cl(2)	0.943	2.835	3.699	152.9

Symmetry transformations used to generate equivalent atoms:

#1 *x*,-*y*+3/2,*z* #2 -*x*,-*y*+1,-*z*+2 #3 -*x*+1/2,-*y*+1,*z*+1/2

#4 *x*-1/2,*y*,-*z*+3/2 #5 -*x*+1/2,-*y*+1,*z*-1/2 #6 *x*,*y*,*z*-1

#7 -*x*+1/2, -*y*+1/2, -*z*+1/2 #8 -*x*+1/2, -*y*, *z*-1/2

#9 *x*, *y*-1/2, -*z*+1 #10 *x*, *y*+1/2, -*z*+1