Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supporting Information

$Sr_9In(VO_4)_7$ as a model ferroelectric in the structural family of β-$Ca_3(PO_4)_2$-type phosphates and vanadates

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Table S1. Structure parameters of $Sr_9In(VO_4)_7$ at 293 K from laboratory X-ray powder diffraction data.

Site	Wyckoff position	*x*	*y*	*z*	*B* (Å^2)
Sr1	18*b*	0.7233(2)	0.8571(2)	0.43262(8)	0.72(3)
Sr2	18*b*	0.6188(2)	0.8230(2)	0.23166(7)	0.60(4)
Sr3	18*b*	0.1281(2)	0.27378(14)	0.32492(7)	0.90(3)
In	6*a*	0.0	0.0	0.0	0.52(4)
V1	6*a*	0.0	0.0	0.27062(13)	1.04(10)
V2	18*b*	0.6845(3)	0.8567(4)	0.13523(10)	0.22(8)
V3	18*b*	0.6572(4)	0.8466(4)	0.03138(11)	0.80(9)
O11	6*a*	0.0	0.0	0.3136(4)	0.8(4)
O12	18*b*	0.0201(10)	0.8680(8)	0.2574(3)	0.6(3)
O21	18*b*	0.7423(13)	0.9231(11)	0.1737(3)	1.6(3)
O22	18*b*	0.7511(14)	0.7594(15)	0.1194(3)	0.6(3)
O23	18*b*	0.7162(13)	0.0034(10)	0.1108(3)	0.2(3)
O24	18*b*	0.5022(10)	0.7625(13)	0.1316(3)	0.2(2)
O31	18*b*	0.5968(11)	0.9446(11)	0.0444(3)	0.2(2)
O32	18*b*	0.5749(11)	0.6844(13)	0.0495(3)	0.5(3)
O33	18*b*	0.8316(11)	0.9199(16)	0.0375(3)	0.2(2)
O34	18*b*	0.6138(9)	0.8171(13)	0.9888(2)	0.1(2)

Space group *R*3*c* (No. 161, origin choice 1); $Z = 6$. $a = 11.18016(9)$ Å, $c = 39.6170(3)$ Å, and $V = 4288.53(5)$ Å^3; $R_{wp} = 5.86$ %, $R_p = 4.52$ %, $R_B = 1.35$ %, and $R_F = 0.62$ %. $\rho_{cal} = 3.968$ g/cm^3.
The occupation factor of all the sites is unity ($g = 1$).

Table S2. Selected Interatomic Distances (Å) and Bond Valence Sum (BVS) in $Sr_9In(VO_4)_7$.

Sr1–O32	2.471(2)	Sr2–O12	2.488(9)
Sr1–O34	2.467(9)	Sr2–O23	2.499(1)
Sr1–O31	2.611(2)	Sr2–O21	2.626(1)
Sr1–O12	2.680(9)	Sr2–O22	2.548(2)
Sr1–O24	2.584(2)	Sr2–O33	2.605(2)
Sr1–O23	2.558(3)	Sr2–O′33	2.684(2)
Sr1–O′24	2.751(3)	Sr2–O32	2.917(2)
Sr1–O22	2.951(4)	Sr2–O31	2.899(1)
<Sr1–O>	**2.634**	<Sr2–O>	**2.658**
BVS($Sr1^{2+}$)	2.13	BVS($Sr2^{2+}$)	2.01
Sr3–O22	2.628(2)	In–O34 (×3)	2.150(1)
Sr3–O23	2.597(1)	In–O43 (×3)	2.207(1)
Sr3–O31	2.567(1)	<In–O>	**2.178**
Sr3–O34	2.677(2)	BVS(In^{3+})	2.85
Sr3–O11	2.690(3)		
Sr3–O′34	2.699(3)	V1–O1	1.703(2)
Sr3–O32	2.707(2)	V1–O12 (×3)	1.683(8)
Sr3–O21	2.781(1)	<V1–O>	**1.688**
Sr3–O12	3.010(1)		
<Sr3–O>	2.707		
BVS($Sr3^{2+}$)	1.92		

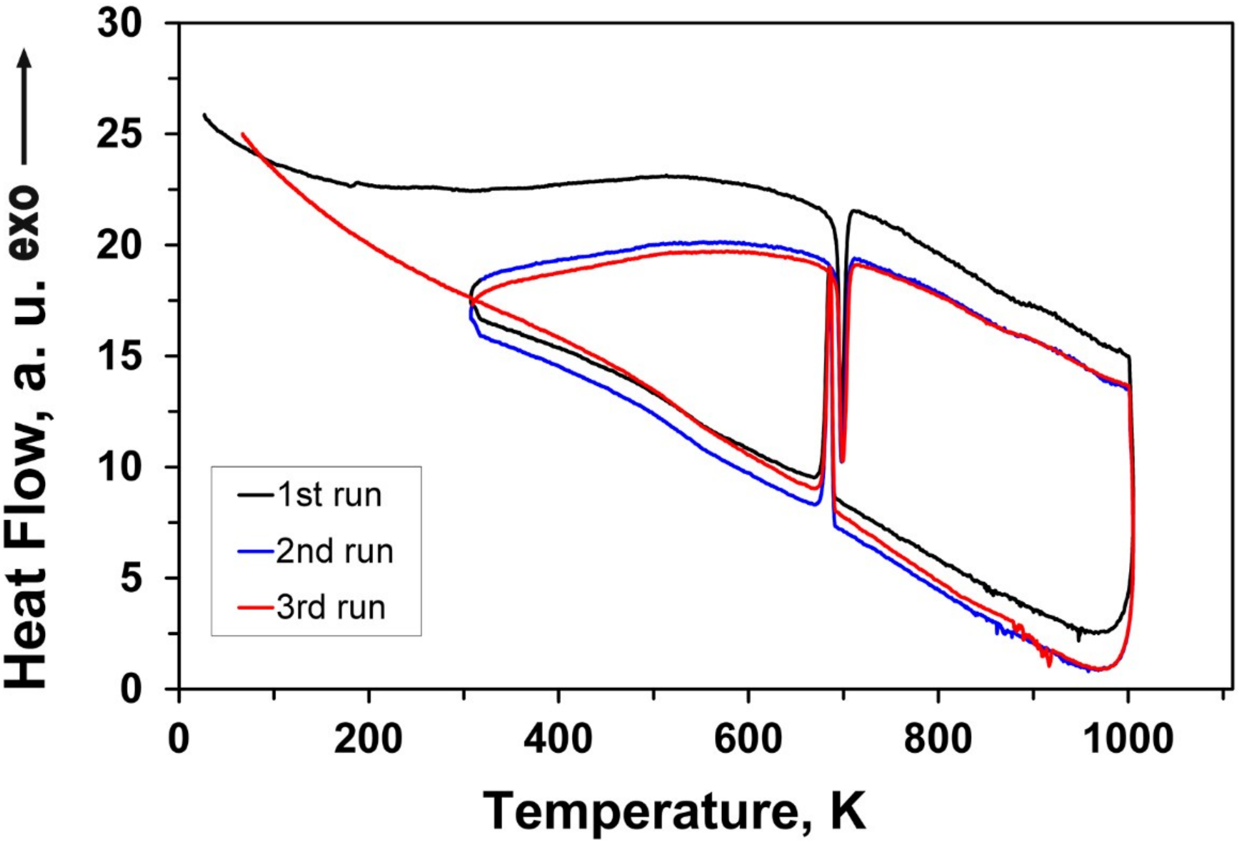

Fig. S1. The heating/cooling DTA curves of $Sr_9In(VO_4)_7$ (the heating/cooling rate was 10 K min^{-1}). Three heating/cooling cycles were run to verify the reproducibility.

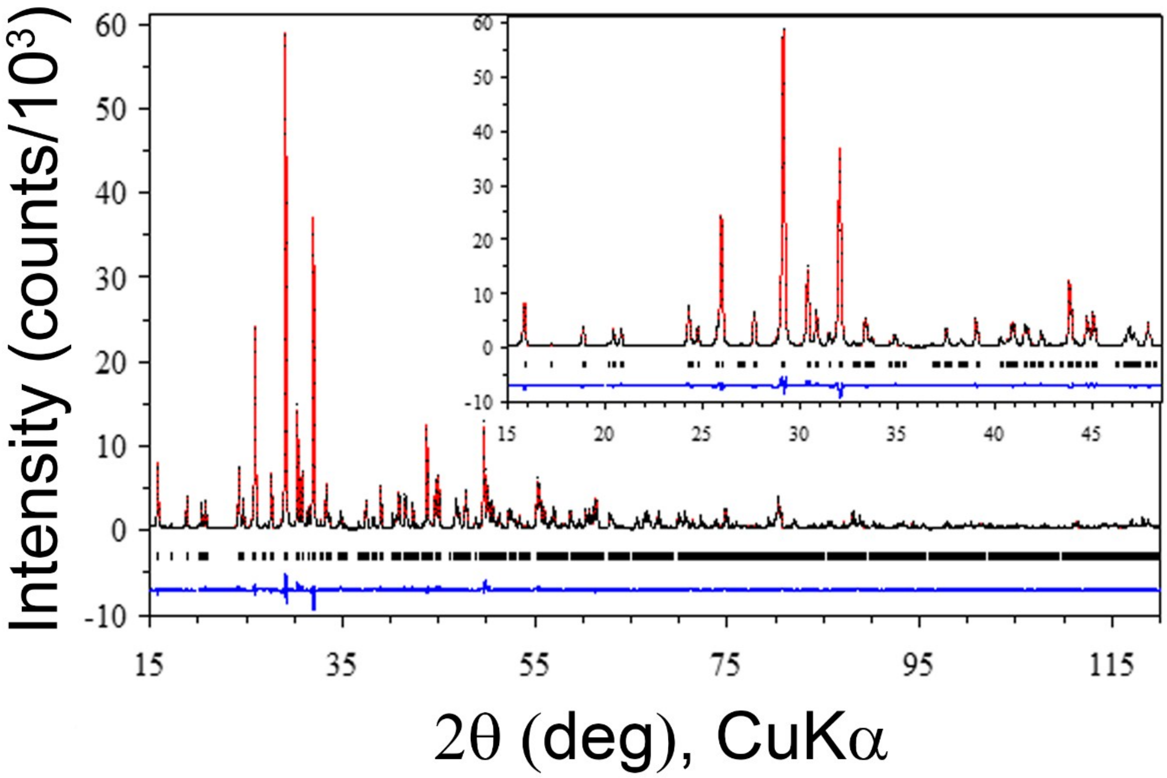

Fig. S2. The XRD data for $Sr_9In(VO_4)_7$ in whole region of data collection.