Table-1 Structural parameters and R-factors obtained for *Amm2* and *P4mm* space group after Rietveld refinement.

Space group	**T (K)**	**Thermal Parameter**		**Atomic positions (x,y,z)**				**R-factors**			
		Ba^{2+}/Ca^{2+}	Zr^{4+}/Ti^{4+}	Ba^{2+}/Ca^{2+}	Zr^{4+}/Ti^{4+}	*O1*	*O2*	R_p	R_{wp}	R_B	χ^2
Amm2	253	1.26	0.51	(0,0,0.022)	(0,0,0.54)	(0,0,0.45)	(0.5,0.24,0.29)	5.34	7.78	2.93	1.39
	263	1.27	0.48	(0,0,0.018)	(0,0,0.54)	(0,0,0.44)	(0.5,0.23,0.28)	5.44	7.79	2.94	1.44
	273	1.29	0.54	(0,0,0.028)	(0,0,0.53)	(0,0,0.46)	(0.5,0.21,0.28)	5.04	7.60	2.51	1.23
P4mm	318	1.26	0.57	(0,0,0.06)	(0.5,0.5,0.58)	(0.5,0.5,0.01)	(0,0.5,0.49)	5.11	7.28	2.73	1.31
	323	1.86	0.68	(0,0,0.08)	(0.5,0.5,0.57)	(0.5,0.5,0.003)	(0,0.5,0.51)	5.21	7.58	2.83	1.37
	333	1.92	0.78	(0,0,0.09)	(0.5,0.5,0.59)	(0.5,0.5,-0.04)	(0,0.5,0.52)	4.94	6.98	2.33	1.29

Table-2 Lattice parameters and volume obtained for *Amm2* and *P4mm* space group after Rietveld refinement.

T (K)	*Amm2*			*Pseudo monoclinic with $b_m=c_m$*			*P4mm*		Volume of primitive unit cell
	a	*b*	*c*	a_m	c_m	γ	a_t	c_t	
253	4.069 *Å*	5.791 *Å*	5.783 *Å*	4.069 *Å*	4.092 *Å*	90.079^o	---	---	68.13$Å^3$
263	4.070 *Å*	5.790 *Å*	5.783 *Å*	4.070*Å*	4.092 *Å*	90.069^o	---	---	68.14 *Å*
273	4.072 *Å*	5.788 *Å*	5.782 *Å*	4.072 *Å*	4.091 *Å*	90.049^o	---	---	68.15 $Å^3$
318	---	---	---	---	---	---	4.071 *Å*	4.100 *Å*	67.94 $Å^3$
323	---	---	---	---	---	---	4.072 *Å*	4.101 *Å*	67.99 *Å*
333	---	---	---	---	---	---	4.073 *Å*	4.101 *Å*	68.03 *Å*

Table-3 Lattice parameters, unit cell volume, R-factors and wt% of tetragonal (P4mm) phase obtained for mixed *Amm2+ P4mm* space group after Rietveld refinement

T (K)	Lattice parameter (Å)								Avg. volume of primitive unit cell (Å^3)	Wt % of tetragonal phase	R-factors			
	Amm2			*Pseudo monoclinic with b_m=c_m*			*P4mm*				R_p	R_{wp}	R_B	χ^2
	a	*b*	*c*	a_m	c_m	γ	a_t	c_t						
293	4.066	5.797	5.777	4.066	4.092	90.19^o	4.077	4.099	68.096	27	4.98	6.83	3.13(O), 3.40(T)	1.12
298	4.063	5.792	5.776	4.063	4.089	90.16^o	4.074	4.102	68.004	46	5.18	7.23	3.63(O), 3.93(T)	1.20
303	4.062	5.788	5.774	4.062	4.087	90.13^o	4.070	4.103	67.914	58	5.08	7.20	3.65(O), 4.00(T)	1.13
308	4.070	5.793	5.784	4.070	4.093	90.08^o	4.072	4.104	68.097	63	5.58	8.10	4.16(O), 4.03(T)	1.45
313	4.069	5.788	5.778	4.069	4.089	90.09^o	4.072	4.105	68.068	76	5.11	7.03	3.73(O), 3.43(T)	1.33

Table-4 Structural parameters obtained for mixed *Amm2 +P4mm* space group after Rietveld refinement

T (K)	Thermal Parameter Amm2 P4mm		Atomic positions (x,y,z) (Amm2) (P4mm)			
	Ba^{2+}/Ca^{2+}	Zr^{4+}/Ti^{4+}	Ba^{2+}/Ca^{2+}	Zr^{4+}/Ti^{4+}	*O1*	*O2*
293	1.43 1.37	0.43 0.51	(0,0,0.018) (0,0,0.024)	(0,0,0.53) (0.5,0.5,0.55)	(0,0,0.44) (0.5,0.5,0.01)	(0.5,0.24,0.30) (0,0.5,0.485)
298	1.70 1.59	0.52 0.44	(0,0,0.013) (0,0,0.014)	(0,0,0.54) (0.5,0.5,0.55	(0,0,0.44) (0.5,0.5,0.008)	(0.5,0.23,0.30) (0,0.5,0.478)
303	1.49 1.58	0.46 0.51	(0,0,0.009) (0,0,-0.04)	(0,0,0.52) (0.5,0.5,0.56)	(0,0,0.42) (0.5,0.5,0.010)	(0,0.18,0.31) (0,0.5,0.531)
308	1.44 1.39	0.52 0.51	(0,0,0.001) (0,0,0.053)	(0,0,0.53) (0.5,0.5,0.57)	(0,0,0.43) (0.5,0.5,0.007)	(0,0.25,0.31) (0,0.5,0.514)
313	1.76 1.45	0.57 0.49	(0,0,-0.022) (0,0,0.053)	(0,0,0.49) (0.5,0.5,0.56)	(0,0,0.43) (0.5,0.5,0.025)	(0,0.21,0.33) (0,0.5,0.497)