Supplementary Materials

Temperature Evolution of Crystal Structure, Ferroelectricity and Ionic Conductivity of $Ca_9La(VO_4)_7$

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Table S1. Fractional atomic coordinates and isotropic atomic displacement parameters (U_{iso}) for for $Ca_9La(VO_4)_7$.

Atom	Occupancy	*x*	*y*	*z*	U_{iso}*100
*M*1	0.940(2)Ca^{2+}+ 0.060(2)La^{3+}	0.72537(5)	0.86100(5)	0.43097(3)	1.14(2)
*M*2	0.965Ca^{2+}+ 0.035La^{3+}	0.61342(6)	0.82292(5)	0.23341(3)	1.27(2)
*M*3	0.762(1)Ca^{2+}+ 0.238(1)La^{3+}	0.12326(4)	0.26843(4)	0.32431(3)	1.57(2)
*M*5	1Ca^{2+}	0	0	0	1.87(2)
V1	1V	0	0	0.26772(4)	1.03(2)
V2	1V	0.68426(5)	0.85863(5)	0.13405(3)	0.91(2)
V3	1V	0.65417(5)	0.84759(5)	0.03224(3)	0.79(2)
O1	1O	0	0	0.3128(1)	2.0(1)
O2	1O	0.0129(2)	0.8551(2)	0.25628(7)	1.85(8)
O3	1O	0.7078(3)	0.9052(4)	0.17665(7)	3.6(2)
O4	1O	0.7679(2)	0.7688(2)	0.12184(7)	1.98(9)
O5	1O	0.7237(2)	0.0133(2)	0.11202(6)	1.22(7)
O6	1O	0.5074(2)	0.7514(2)	0.12463(8)	1.88(8)
O7	1O	0.5929(2)	0.9585(2)	0.04369(7)	1.83(9)
O8	1O	0.5718(3)	0.6851(3)	0.05079(7)	2.67(9)
O9	1O	0.8288(2)	0.9269(2)	0.04377(7)	1.42(8)
O10	1O	0.6272(3)	0.8214(2)	0.98837(7)	1.83(9)

Table S2. Anisotropic atomic displacement parameters in $Ca_9La(VO_4)_7$.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
*M*1	0.0119(3)	0.0126(3)	0.0105(3)	0.0068(2)	-0.0002(2)	-0.0016(2)
*M*2	0.0134(3)	0.0117(3)	0.0118(3)	0.0054(2)	-0.0034(2)	-0.0014(2)
*M*3	0.0122(2)	0.0208(2)	0.0137(2)	0.00785(15)	-0.0008(1)	0.0053(1)
*M*5	0.0244(3)	0.0244(3)	0.0072(4)	0.0122(2)	0	0
V1	0.0094(2)	0.0094(2)	0.0123(4)	0.0047(1)		
V2	0.0105(2)	0.0099(2)	0.0084(2)	0.0063(2)	0.0026(2)	0.0017(2)
V3	0.0073(2)	0.0087(2)	0.0068(2)	0.0034(2)	0.0000(2)	0.0000(2)
O1	0.0235(12)	0.0235(12)	0.0134(17)	0.0118(6)	0	0
O2	0.0158(10)	0.0126(9)	0.0288(11)	0.0083(8)	0.0085(8)	0.0025(8)
O3	0.0547(17)	0.059(2)	0.0140(11)	0.0438(17)	0.0005(11)	0.0003(11)
O4	0.0255(11)	0.0252(11)	0.0188(10)	0.0202(10)	0.0066(8)	0.0049(9)
O5	0.0108(9)	0.0093(9)	0.0144(9)	0.0035(7)	0.0018(7)	0.0020(7)
O6	0.0123(11)	0.0097(9)	0.0323(12)	0.0039(8)	0.0044(9)	0.0009(8)
O7	0.0237(11)	0.0271(11)	0.0143(9)	0.0205(9)	-0.0026(8)	-0.0053(9)
O8	0.0330(12)	0.0157(11)	0.0218(11)	0.0050(9)	0.008(1)	0.0077(9)
O9	0.0107(9)	0.0138(9)	0.0192(10)	0.0068(8)	-0.0034(8)	-0.0042(8)
O10	0.0261(12)	0.0232(11)	0.0089(10)	0.0147(9)	-0.0021(9)	-0.0018(8)

Table S3. Selected interatomic distances (Å) and angles in the $[VO_4]^{3-}$ tetrahedra for $Ca_9La(VO_4)_7$.

Bond	Distance, Å	Bond	Distance, Å
*M*1-O2	2.524(2)	*M*2-O2	2.392(3)
O5	2.540(3)	O3	2.373(3)
O6	2.528(2)	O4	2.414(3)
O6	2.461(4)	O5	2.364(3)
O7	2.418(3)	O7	2.881(3)
O8	2.318(4)	O8	2.860(3)
O10	2.379(3)	O9	2.449(2)
		O9	2.501(3)
mean	2.458	*mean*	2.529
DI	0.0283	DI	0.0675
*M*3-O1	2.575(9)	*M*5-O6×3	2.297(3)
O2	2.921(3)	O9×3	2.328(2)
O3	2.843(6)	*mean*	2.313
O4	2.506(3)	DI	0.0067
O5	2.410(3)		
O7	2.437(3)	V1-O1	1.722(4)
O8	2.657(3)	O2×3	1.711(3)
O10	2.628(2)	*mean*	1.714
O10	2.704(3)		
mean	2.631		
DI	0.0476		
V2-O3	1.684(3)	V3-O7	1.705(3)
O4	1.704(3)	O8	1.689(3)
O5	1.735(2)	O9	1.709(2)
O6	1.720(2)	O10	1.699(3)
mean	1.711	*mean*	1.701
Angle	Angle, °	Angle	Angle, °
O1-V1-O2×3	104.78(10)	O3-V2-O4	113.13(19)
O2-V1-O2×3	113.72(14)	O3-V2-O5	104.37(16)
		O3-V2-O6	110.90(15)
O7-V3-O8	116.41(14)	O4-V2-O5	118.85(13)
O7-V3-O9	107.92(11)	O4-V2-O6	107.00(12)
O7-V3-O10	106.00(15)	O5-V2-O6	102.03(12)
O8-V3-O9	107.25(14)		
O8-V3-O10	106.24(12)		
O9-V3-O10	113.20(14)		