

Electronic Supplementary Information

Synthesis conditions impact on $\text{Sr}_{11}\text{Mo}_4\text{O}_{23}$ electroceramic: crystal structure, stability and transport properties.

Carlos D. Miranda¹, Dimar Villarroel-Rocha², Karim Sapag²,

Carlos A. López^{1*}, José C. Pedregosa¹, José A. Alonso³,

¹INTEQUI, Universidad Nacional de San Luis, CONICET and Facultad de Química, Bioquímica y Farmacia, UNSL, Almirante Brown 1455, San Luis, Argentina.

²INFAP, Universidad Nacional de San Luis, CONICET, Ejército de los Andes 950, San Luis, Argentine.

³Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain.

*calopez@unsl.edu.ar

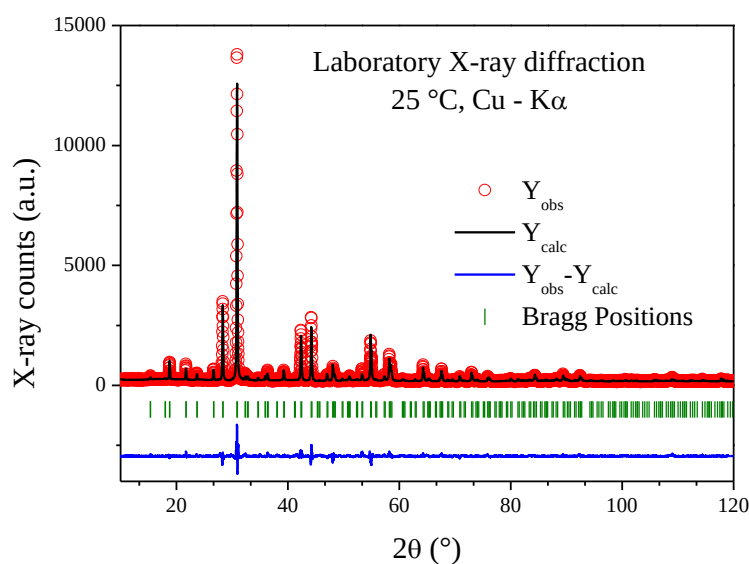


Figure S1: Laboratory XRPR pattern at room temperature, after the Rietveld refinement in a cubic lattice.

Table S1: Crystallographic data for SMO14 phase from the laboratory XRPD refinements at 25 °C. System: Cubic, Space group: $Fd\bar{3}m$. Unit-cell parameters: $a = 16.3982(2)$ Å and $V = 4409.5(1)$ Å³. Reliability Factors: R_p : 7.9%; R_{wp} : 10.2%; χ^2 : 2.9 and R_{Bragg} : 9.2%

Atoms	x	y	z	U_{iso}	Occ. (<1)
Sr1	0.4011(2)	0.12500	0.12500	0.072(2)	
Sr2	0.37500	0.37500	0.37500	0.046(4)	
Sr3	0.2274(1)	0.2274(1)	0.2274(1)	0.060(2)	
Mo1	0.50000	0.50000	0.50000	0.027(2)	
Mo2	0.00000	0.00000	0.00000	0.0470(2)	
O1	0.5017(8)	0.5017(8)	0.6083(6)	0.060 (4)	
O2	0.089(1)	0.0894(1)	0.016(0)	0.12665	0.41(2)
O3	0.00000	0.093(1)	-0.093(1)	0.12665	0.51(2)

Table S2: Crystallographic data for SMO11 phase from the SXRPD refinements at 25 °C. System: Triclinic, Space group: $P\bar{1}$. Unit-cell parameters: $a = 16.4007(8)$ Å, $b = 16.4237(5)$ Å, $c = 16.4090(8)$ Å, $\alpha = 90.084(3)^\circ$, $\beta = 90.449(1)^\circ$, $\gamma = 89.964(4)^\circ$ and $V=4418.9(3)$ Å³. Reliability Factors: R_p : 14.8%; R_{wp} : 19.9%; χ^2 : 5.62 and R_{Bragg} : 43.7%

Atoms	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}	Occ. (<1)
Sr11	0.354 (4)	0.122 (4)	0.614 (4)	0.0205 (17)*	
Sr12	0.864 (4)	0.614 (4)	0.623 (4)	0.0205 (17)*	
Sr13	0.868 (3)	0.601 (3)	0.131 (3)	0.0205 (17)*	
Sr14	0.121 (4)	0.402 (4)	0.133 (4)	0.0205 (17)*	
Sr15	0.648 (4)	0.352 (4)	0.142 (4)	0.0205 (17)*	
Sr16	0.643 (4)	0.846 (4)	0.632 (4)	0.0205 (17)*	
Sr17	0.132 (4)	0.910 (4)	0.638 (4)	0.0205 (17)*	
Sr18	0.135 (4)	0.123 (4)	0.401 (4)	0.0205 (17)*	
Sr19	0.124 (4)	0.629 (4)	0.361 (4)	0.0205 (17)*	
Sr110	0.651 (3)	0.621 (4)	0.884 (3)	0.0205 (17)*	
Sr111	0.635 (4)	0.119 (4)	0.909 (4)	0.0205 (17)*	
Sr112	0.864 (4)	0.652 (4)	0.373 (4)	0.0205 (17)*	
Sr113	0.382 (4)	0.097 (4)	0.861 (4)	0.0205 (17)*	
Sr114	0.086 (3)	0.855 (4)	0.389 (3)	0.0205 (17)*	
Sr115	0.652 (4)	0.386 (4)	0.898 (4)	0.0205 (17)*	
Sr116	0.865 (4)	0.387 (4)	0.108 (4)	0.0205 (17)*	
Sr117	0.387 (4)	0.852 (4)	0.651 (4)	0.0205 (17)*	
Sr118	0.399 (4)	0.641 (4)	0.621 (4)	0.0205 (17)*	
Sr119	0.852 (4)	0.118 (4)	0.122 (4)	0.0205 (17)*	
Sr120	0.142 (4)	0.139 (4)	0.857 (4)	0.0205 (17)*	
Sr121	0.636 (4)	0.615 (4)	0.408 (4)	0.0205 (17)*	
Sr122	0.862 (3)	0.153 (4)	0.869 (4)	0.0205 (17)*	
Sr123	0.392 (4)	0.596 (4)	0.383 (4)	0.0205 (17)*	
Sr124	0.393 (4)	0.142 (4)	0.123 (4)	0.0205 (17)*	
Sr21	0.373 (4)	0.372 (3)	0.377 (4)	0.017 (4)*	
Sr22	0.375 (4)	0.877 (4)	0.876 (4)	0.017 (4)*	

Sr23	0.884 (4)	0.876 (4)	0.377 (4)	0.017 (4)*	
Sr24	0.882 (4)	0.379 (4)	0.882 (4)	0.017 (4)*	
Sr31	0.218 (4)	0.229 (4)	0.243 (3)	0.020 (2)*	
Sr32	0.525 (4)	0.012 (4)	0.728 (3)	0.020 (2)*	
Sr33	0.033 (3)	0.741 (4)	0.527 (3)	0.020 (2)*	
Sr34	0.738 (3)	0.533 (3)	0.030 (3)	0.020 (2)*	
Sr35	0.969 (3)	0.493 (4)	0.276 (3)	0.020 (2)*	
Sr36	0.511 (3)	0.280 (3)	0.974 (3)	0.020 (2)*	
Sr37	0.270 (3)	0.973 (3)	0.488 (4)	0.020 (2)*	
Sr38	0.226 (4)	0.734 (4)	0.710 (3)	0.020 (2)*	
Sr39	0.521 (4)	0.515 (4)	0.233 (3)	0.020 (2)*	
Sr310	0.051 (3)	0.258 (3)	0.023 (3)	0.020 (2)*	
Sr311	0.973 (4)	0.991 (4)	0.773 (4)	0.020 (2)*	
Sr312	0.475 (3)	0.769 (4)	0.471 (3)	0.020 (2)*	
Sr313	0.726 (4)	0.232 (4)	0.734 (4)	0.020 (2)*	
Sr314	0.225 (4)	0.540 (4)	0.515 (4)	0.020 (2)*	
Sr315	0.763 (4)	0.975 (4)	0.991 (4)	0.020 (2)*	
Sr316	0.728 (3)	0.733 (4)	0.260 (3)	0.020 (2)*	
Mo101	0.50000	0.50000	0.50000	0.014 (2)*	
Mo102	0.255 (4)	0.756 (4)	−0.002 (4)	0.014 (2)*	
Mo103	0.748 (4)	0.005 (4)	0.258 (4)	0.014 (2)*	
Mo104	0.005 (4)	0.247 (4)	0.762 (4)	0.014 (2)*	
Mo105	0.50000	0.00000	0.00000	0.014 (2)*	
Mo106	0.247 (4)	0.249 (4)	0.504 (4)	0.014 (2)*	
Mo107	0.760 (3)	0.492 (4)	0.767 (3)	0.014 (2)*	
Mo108	0.00000	0.50000	0.00000	0.014 (2)*	
Mo109	0.500 (3)	0.256 (4)	0.253 (4)	0.014 (2)*	
Mo110	0.00000	0.00000	0.50000	0.014 (2)*	
Mo201	0.00000	0.00000	0.00000	0.017 (3)*	
Mo202	0.746 (3)	0.251 (4)	0.503 (4)	0.017 (3)*	
Mo203	0.269 (4)	0.500 (4)	0.764 (3)	0.017 (3)*	

Mo204	0.501 (4)	0.753 (4)	0.245 (4)	0.017 (3)*	
Mo205	0.00000	0.50000	0.50000	0.017 (3)*	
Mo206	0.758 (4)	0.750 (4)	0.003 (4)	0.017 (3)*	
Mo207	0.270 (3)	0.001 (4)	0.251 (3)	0.017 (3)*	
Mo208	0.50000	0.00000	0.50000	0.017 (3)*	
Mo209	0.020 (3)	0.752 (4)	0.757 (4)	0.017 (3)*	
Mo210	0.50000	0.50000	0.00000	0.017 (3)*	
O101	0.49870	0.49870	0.61180	0.013 (3)*	
O102	0.25130	0.75130	0.11180	0.013 (3)*	
O103	0.75130	0.99870	0.13820	0.013 (3)*	
O104	0.99870	0.25130	0.63820	0.013 (3)*	
O105	0.61180	0.49870	0.49870	0.013 (3)*	
O106	0.11180	0.25130	0.75130	0.013 (3)*	
O107	0.13820	0.75130	0.99870	0.013 (3)*	
O108	0.63820	0.99870	0.25130	0.013 (3)*	
O109	0.49870	0.61180	0.49870	0.013 (3)*	
O110	0.75130	0.11180	0.25130	0.013 (3)*	
O111	0.99870	0.13820	0.75130	0.013 (3)*	
O112	0.25130	0.63820	0.99870	0.013 (3)*	
O113	0.24870	0.74870	0.88820	0.013 (3)*	
O114	0.74870	0.00130	0.36180	0.013 (3)*	
O115	0.00130	0.24870	0.86180	0.013 (3)*	
O116	0.24870	0.86180	0.00130	0.013 (3)*	
O117	0.00130	0.36180	0.74870	0.013 (3)*	
O118	0.74870	0.88820	0.24870	0.013 (3)*	
O119	0.36180	0.74870	0.00130	0.013 (3)*	
O120	0.86180	0.00130	0.24870	0.013 (3)*	
O121	0.88820	0.24870	0.74870	0.013 (3)*	
O122	0.49870	0.99870	0.11180	0.013 (3)*	
O123	0.25130	0.25130	0.61180	0.013 (3)*	
O124	0.75130	0.49870	0.63820	0.013 (3)*	

O125	0.61180	0.99870	0.99870	0.013 (3)*	
O126	0.13820	0.25130	0.49870	0.013 (3)*	
O127	0.63820	0.49870	0.75130	0.013 (3)*	
O128	0.49870	0.11180	0.99870	0.013 (3)*	
O129	0.75130	0.61180	0.75130	0.013 (3)*	
O130	0.25130	0.13820	0.49870	0.013 (3)*	
O131	0.24870	0.24870	0.38820	0.013 (3)*	
O132	0.74870	0.50130	0.86180	0.013 (3)*	
O133	0.24870	0.36180	0.50130	0.013 (3)*	
O134	0.74870	0.38820	0.74870	0.013 (3)*	
O135	0.36180	0.24870	0.50130	0.013 (3)*	
O136	0.86180	0.50130	0.74870	0.013 (3)*	
O137	0.99870	0.49870	0.11180	0.013 (3)*	
O138	0.49870	0.25130	0.13820	0.013 (3)*	
O139	0.11180	0.49870	0.99870	0.013 (3)*	
O140	0.61180	0.25130	0.25130	0.013 (3)*	
O141	0.99870	0.61180	0.99870	0.013 (3)*	
O142	0.49870	0.13820	0.25130	0.013 (3)*	
O143	0.50130	0.24870	0.36180	0.013 (3)*	
O144	0.50130	0.36180	0.24870	0.013 (3)*	
O145	0.38820	0.24870	0.24870	0.013 (3)*	
O146	0.99870	0.99870	0.61180	0.013 (3)*	
O147	0.11180	0.99870	0.49870	0.013 (3)*	
O148	0.99870	0.11180	0.49870	0.013 (3)*	
O201	0.07920	0.07920	0.00440	0.123 (12)*	0.49995
O202	0.67080	0.17080	0.50440	0.123 (12)*	0.49995
O203	0.17080	0.57920	0.74560	0.123 (12)*	0.49995
O204	0.57920	0.67080	0.24560	0.123 (12)*	0.49995
O205	0.00440	0.07920	0.07920	0.123 (12)*	0.49995
O206	0.50440	0.67080	0.17080	0.123 (12)*	0.49995
O207	0.74560	0.17080	0.57920	0.123 (12)*	0.49995

O208	0.24560	0.57920	0.67080	0.123 (12)*	0.49995
O209	0.07920	0.00440	0.07920	0.123 (12)*	0.49995
O210	0.17080	0.50440	0.67080	0.123 (12)*	0.49995
O211	0.57920	0.74560	0.17080	0.123 (12)*	0.49995
O212	0.67080	0.24560	0.57920	0.123 (12)*	0.49995
O213	0.82920	0.32920	0.49560	0.123 (12)*	0.49995
O214	0.32920	0.42080	0.75440	0.123 (12)*	0.49995
O215	0.42080	0.82920	0.25440	0.123 (12)*	0.49995
O216	0.82920	0.25440	0.42080	0.123 (12)*	0.49995
O217	0.42080	0.75440	0.32920	0.123 (12)*	0.49995
O218	0.32920	0.49560	0.82920	0.123 (12)*	0.49995
O219	0.75440	0.32920	0.42080	0.123 (12)*	0.49995
O220	0.25440	0.42080	0.82920	0.123 (12)*	0.49995
O221	0.49560	0.82920	0.32920	0.123 (12)*	0.49995
O222	0.07920	0.57920	0.50440	0.123 (12)*	0.49995
O223	0.67080	0.67080	0.00440	0.123 (12)*	0.49995
O224	0.17080	0.07920	0.24560	0.123 (12)*	0.49995
O225	0.00440	0.57920	0.57920	0.123 (12)*	0.49995
O226	0.74560	0.67080	0.07920	0.123 (12)*	0.49995
O227	0.24560	0.07920	0.17080	0.123 (12)*	0.49995
O228	0.07920	0.50440	0.57920	0.123 (12)*	0.49995
O229	0.17080	0.00440	0.17080	0.123 (12)*	0.49995
O230	0.67080	0.74560	0.07920	0.123 (12)*	0.49995
O231	0.82920	0.82920	0.99560	0.123 (12)*	0.49995
O232	0.32920	0.92080	0.25440	0.123 (12)*	0.49995
O233	0.82920	0.75440	0.92080	0.123 (12)*	0.49995
O234	0.32920	0.99560	0.32920	0.123 (12)*	0.49995
O235	0.75440	0.82920	0.92080	0.123 (12)*	0.49995
O236	0.25440	0.92080	0.32920	0.123 (12)*	0.49995
O237	0.57920	0.07920	0.50440	0.123 (12)*	0.49995
O238	0.07920	0.67080	0.74560	0.123 (12)*	0.49995

O239	0.50440	0.07920	0.57920	0.123 (12)*	0.49995
O240	0.00440	0.67080	0.67080	0.123 (12)*	0.49995
O241	0.57920	0.00440	0.57920	0.123 (12)*	0.49995
O242	0.07920	0.74560	0.67080	0.123 (12)*	0.49995
O243	0.92080	0.82920	0.75440	0.123 (12)*	0.49995
O244	0.92080	0.75440	0.82920	0.123 (12)*	0.49995
O245	0.99560	0.82920	0.82920	0.123 (12)*	0.49995
O246	0.57920	0.57920	0.00440	0.123 (12)*	0.49995
O247	0.50440	0.57920	0.07920	0.123 (12)*	0.49995
O248	0.57920	0.50440	0.07920	0.123 (12)*	0.49995
O301	0.00000	0.07740	0.92260	0.123 (12)*	0.49995
O302	0.75000	0.17260	0.42260	0.123 (12)*	0.49995
O303	0.25000	0.57740	0.82740	0.123 (12)*	0.49995
O304	0.50000	0.67260	0.32740	0.123 (12)*	0.49995
O305	0.92260	0.00000	0.07740	0.123 (12)*	0.49995
O306	0.42260	0.75000	0.17260	0.123 (12)*	0.49995
O307	0.82740	0.25000	0.57740	0.123 (12)*	0.49995
O308	0.32740	0.50000	0.67260	0.123 (12)*	0.49995
O309	0.07740	0.92260	0.00000	0.123 (12)*	0.49995
O310	0.17260	0.42260	0.75000	0.123 (12)*	0.49995
O311	0.57740	0.82740	0.25000	0.123 (12)*	0.49995
O312	0.67260	0.32740	0.50000	0.123 (12)*	0.49995
O313	0.00000	0.57740	0.42260	0.123 (12)*	0.49995
O314	0.75000	0.67260	0.92260	0.123 (12)*	0.49995
O315	0.25000	0.07740	0.32740	0.123 (12)*	0.49995
O316	0.50000	0.17260	0.82740	0.123 (12)*	0.49995
O317	0.92260	0.50000	0.57740	0.123 (12)*	0.49995
O318	0.42260	0.25000	0.67260	0.123 (12)*	0.49995
O319	0.82740	0.75000	0.07740	0.123 (12)*	0.49995
O320	0.32740	0.00000	0.17260	0.123 (12)*	0.49995
O321	0.07740	0.42260	0.50000	0.123 (12)*	0.49995

O322	0.17260	0.92260	0.25000	0.123 (12)*	0.49995
O323	0.57740	0.32740	0.75000	0.123 (12)*	0.49995
O324	0.67260	0.82740	0.00000	0.123 (12)*	0.49995
O325	0.50000	0.07740	0.42260	0.123 (12)*	0.49995
O326	0.25000	0.17260	0.92260	0.123 (12)*	0.49995
O327	0.75000	0.57740	0.32740	0.123 (12)*	0.49995
O328	0.00000	0.67260	0.82740	0.123 (12)*	0.49995
O329	0.42260	0.00000	0.57740	0.123 (12)*	0.49995
O330	0.92260	0.75000	0.67260	0.123 (12)*	0.49995
O331	0.32740	0.25000	0.07740	0.123 (12)*	0.49995
O332	0.82740	0.50000	0.17260	0.123 (12)*	0.49995
O333	0.57740	0.92260	0.50000	0.123 (12)*	0.49995
O334	0.67260	0.42260	0.25000	0.123 (12)*	0.49995
O335	0.07740	0.82740	0.75000	0.123 (12)*	0.49995
O336	0.17260	0.32740	0.00000	0.123 (12)*	0.49995
O337	0.50000	0.57740	0.92260	0.123 (12)*	0.49995
O338	0.25000	0.67260	0.42260	0.123 (12)*	0.49995
O339	0.75000	0.07740	0.82740	0.123 (12)*	0.49995
O340	0.00000	0.17260	0.32740	0.123 (12)*	0.49995
O341	0.42260	0.50000	0.07740	0.123 (12)*	0.49995
O342	0.92260	0.25000	0.17260	0.123 (12)*	0.49995
O343	0.32740	0.75000	0.57740	0.123 (12)*	0.49995
O344	0.82740	0.00000	0.67260	0.123 (12)*	0.49995
O345	0.57740	0.42260	0.00000	0.123 (12)*	0.49995
O346	0.67260	0.92260	0.75000	0.123 (12)*	0.49995
O347	0.07740	0.32740	0.25000	0.123 (12)*	0.49995
O348	0.17260	0.82740	0.50000	0.123 (12)*	0.49995

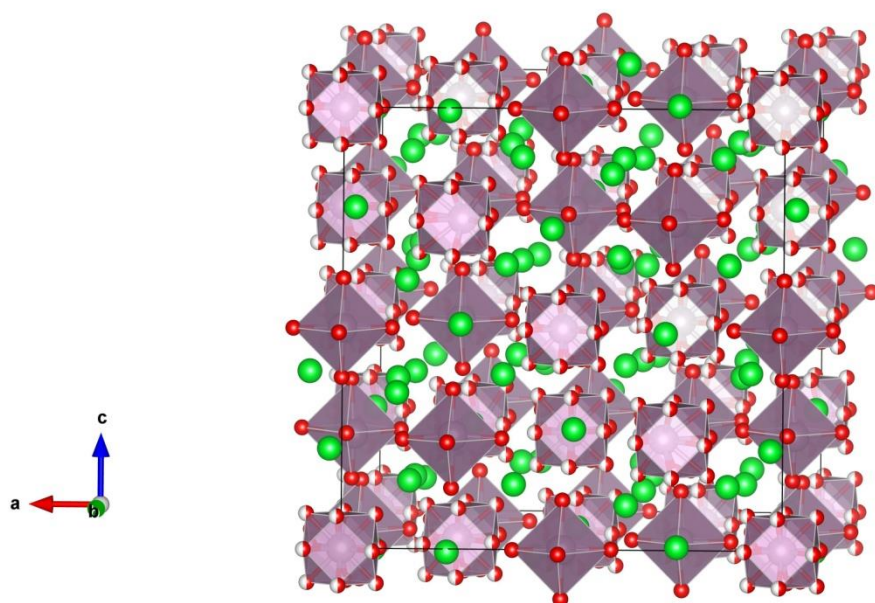


Figure S2: View of triclinic crystal structure of SMO11 at 25 °C.

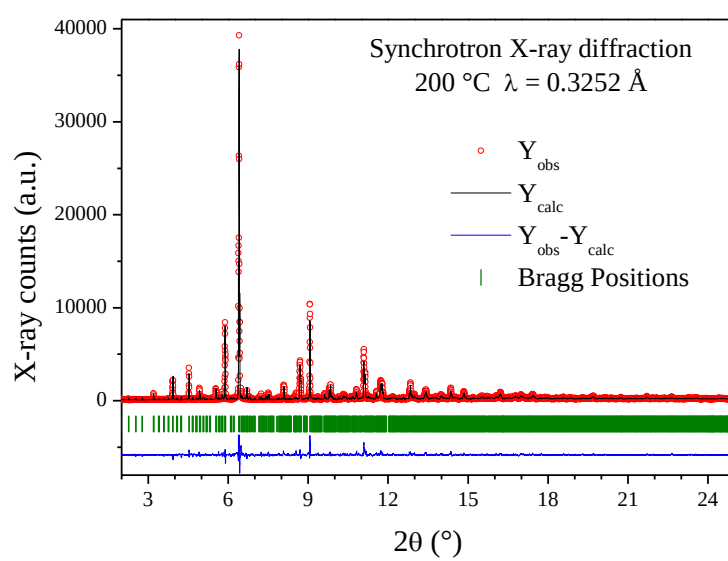


Figure S3: SXRPR pattern at 200 °C, after the Rietveld refinement in $P\bar{1}$ space group.

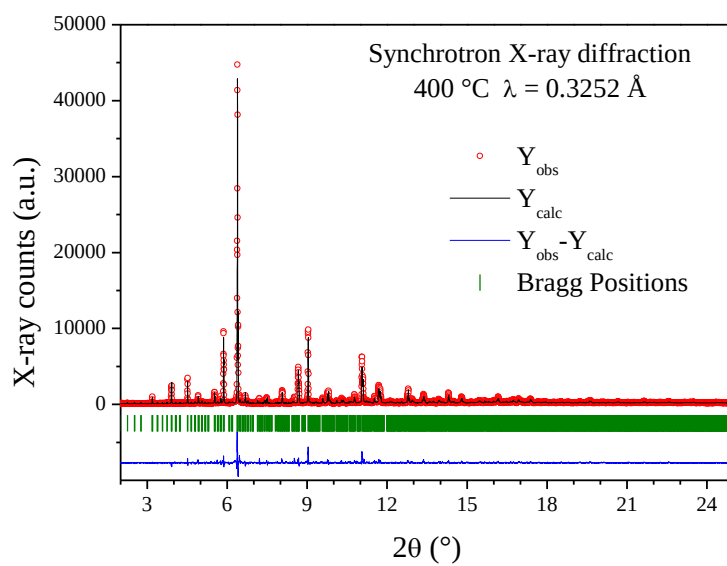


Figure S4: SXRPR pattern at 400 °C, after the Rietveld refinement in $P\bar{1}$ space group.

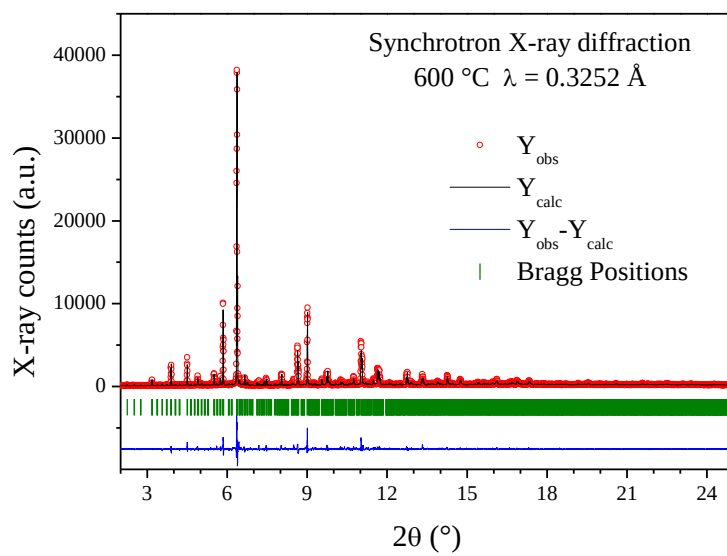


Figure S5: SXRPR pattern at 600 °C, after the Rietveld refinement in $P\bar{1}$ space group.

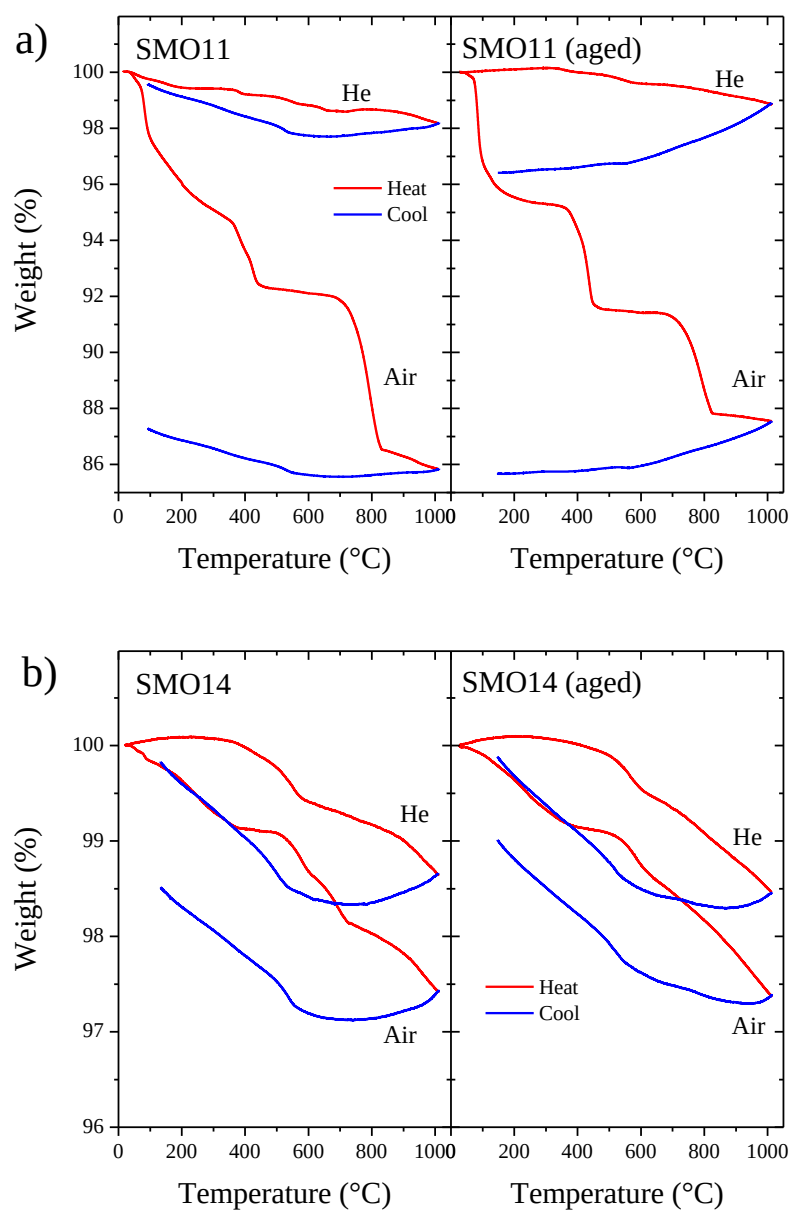


Figure S6: TGA data of fresh and aged for a) SMO11 and b) SMO14.

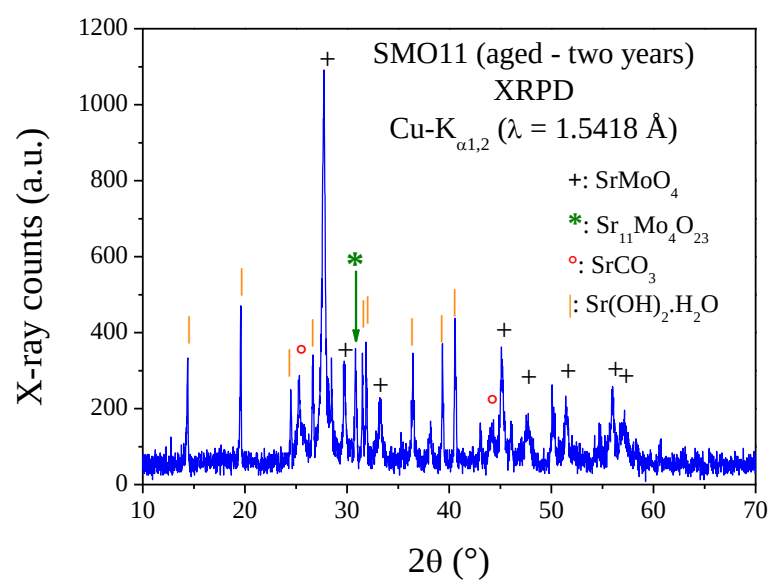


Figure S7: XRPD pattern of SMO11 aged two years.