



## Journal Name

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## Supplementary Information

Table S1: Bond valence sums for each metal site calculated for structures resulting from refinements against synchrotron X-ray powder diffraction data.

	Sr(II)	Ti(IV)	Zr(IV)	Nb(V)
$\text{Sr}_{0.8}\text{Ti}_{0.6}\text{Nb}_{0.4}\text{O}_3$	2.02	4.01	-	5.20
$\text{Sr}_{0.8}\text{Ti}_{0.54}\text{Zr}_{0.06}\text{Nb}_{0.4}\text{O}_3$	1.96	3.93	5.34	5.10
$\text{Sr}_{0.8}\text{Ti}_{0.48}\text{Zr}_{0.12}\text{Nb}_{0.4}\text{O}_3$	1.91	3.86	5.24	5.00
$\text{Sr}_{0.8}\text{Ti}_{0.36}\text{Zr}_{0.24}\text{Nb}_{0.4}\text{O}_3$	1.82	3.72	5.05	4.83
$\text{Sr}_{0.8}\text{Ti}_{0.24}\text{Zr}_{0.36}\text{Nb}_{0.4}\text{O}_3$	1.76	3.59	4.87	4.65
$\text{Sr}_{0.8}\text{Ti}_{0.12}\text{Zr}_{0.48}\text{Nb}_{0.4}\text{O}_3$	1.72	3.44	4.67	4.46
$\text{Sr}_{0.8}\text{Zr}_{0.6}\text{Nb}_{0.4}\text{O}_3$	1.67	-	4.49	4.29

Table S2: Bond valence sums for each metal site calculated for structures resulting from refinements against neutron powder diffraction data.

	Sr(II)	Ti(IV)	Zr(IV)	Nb(V)
$\text{Sr}_{0.8}\text{Ti}_{0.6}\text{Nb}_{0.4}\text{O}_3$	2.01	4.00	-	5.18
$\text{Sr}_{0.8}\text{Ti}_{0.54}\text{Zr}_{0.06}\text{Nb}_{0.4}\text{O}_3$	1.96	3.93	5.34	5.10
$\text{Sr}_{0.8}\text{Ti}_{0.48}\text{Zr}_{0.12}\text{Nb}_{0.4}\text{O}_3$	1.91	3.86	5.24	5.00
$\text{Sr}_{0.8}\text{Ti}_{0.36}\text{Zr}_{0.24}\text{Nb}_{0.4}\text{O}_3$	1.82	3.72	5.04	4.82
$\text{Sr}_{0.8}\text{Ti}_{0.24}\text{Zr}_{0.36}\text{Nb}_{0.4}\text{O}_3$	1.77	3.57	4.85	4.63
$\text{Sr}_{0.8}\text{Zr}_{0.6}\text{Nb}_{0.4}\text{O}_3$	1.68	-	4.47	4.27

Table S3: Tolerance Factors for  $\text{Sr}_{0.8}\text{Ti}_{0.6-x}\text{Zr}_x\text{Nb}_{0.4}\text{O}_3$  and parent compounds. Tolerance factors are calculated such that the A cation is taken to be 100 % strontium and the B cation is a weighted average of the B cations. Ionic radii are taken from Shannon [37]. \*This is theoretical only as this composition does not form with a perovskite type structure<sup>35</sup>.

Compound	Tolerance Factor
$\text{SrTiO}_3$	1.0091
$\text{Sr}_{0.8}\text{Ti}_{0.6}\text{Nb}_{0.4}\text{O}_3$	1.0019
$\text{Sr}_{0.8}\text{Ti}_{0.54}\text{Zr}_{0.06}\text{Nb}_{0.4}\text{O}_3$	0.9984
$\text{Sr}_{0.8}\text{Ti}_{0.48}\text{Zr}_{0.12}\text{Nb}_{0.4}\text{O}_3$	0.9950
$\text{Sr}_{0.8}\text{Ti}_{0.36}\text{Zr}_{0.24}\text{Nb}_{0.4}\text{O}_3$	0.9881
$\text{Sr}_{0.8}\text{Ti}_{0.24}\text{Zr}_{0.36}\text{Nb}_{0.4}\text{O}_3$	0.9813
$\text{Sr}_{0.8}\text{Ti}_{0.12}\text{Zr}_{0.48}\text{Nb}_{0.4}\text{O}_3$	0.9746
$\text{Sr}_{0.8}\text{Zr}_{0.6}\text{Nb}_{0.4}\text{O}_3$	0.9680
$\text{SrZrO}_3$	0.9531
* $\text{Sr}_{0.5}\text{NbO}_3$	0.9914

Table S4: Phase transition temperatures from cubic ( $Pm\bar{3}m$ ) to tetragonal ( $I4/mcm$ ).

Composition	Transition Temperature
$\text{Sr}_{0.8}\text{Ti}_{0.6}\text{Nb}_{0.4}\text{O}_3$	90 K
$\text{Sr}_{0.8}\text{Ti}_{0.54}\text{Zr}_{0.06}\text{Nb}_{0.4}\text{O}_3$	< 298 K
$\text{Sr}_{0.8}\text{Ti}_{0.48}\text{Zr}_{0.12}\text{Nb}_{0.4}\text{O}_3$	~ 298 K
$\text{Sr}_{0.8}\text{Ti}_{0.36}\text{Zr}_{0.24}\text{Nb}_{0.4}\text{O}_3$	> 298 K
$\text{Sr}_{0.8}\text{Ti}_{0.24}\text{Zr}_{0.36}\text{Nb}_{0.4}\text{O}_3$	430 K
$\text{Sr}_{0.8}\text{Ti}_{0.12}\text{Zr}_{0.48}\text{Nb}_{0.4}\text{O}_3$	470 K
$\text{Sr}_{0.8}\text{Zr}_{0.6}\text{Nb}_{0.4}\text{O}_3$	610 K

Table S5: Atomic coordinates and isotropic atomic displacement parameters as determined by refinements against synchrotron X-ray powder diffraction data collected at room temperature

Composition	Atom	x	y	z	U <sub>iso</sub>
<b>Sr<sub>0.8</sub>Ti<sub>0.6</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0.5	0.5	0.5	0.00933(8)
	Ti/ Nb	0	0	0	0.01119(8)
	O	0	0	0.5	0.01220(19)
<b>Sr<sub>0.8</sub>Ti<sub>0.54</sub>Zr<sub>0.06</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0.5	0.5	0.5	0.00871(8)
	Ti/ Nb	0	0	0	0.00892(7)
	O	0	0	0.5	0.0125(2)
<b>Sr<sub>0.8</sub>Ti<sub>0.48</sub>Zr<sub>0.12</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0.5	0.5	0.5	0.00970(8)
	Ti/Zr/Nb	0	0	0	0.00933(8)
	O	0	0	0.5	0.0147(2)
<b>Sr<sub>0.8</sub>Ti<sub>0.36</sub>Zr<sub>0.24</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0.5	0.5	0.5	0.01068(7)
	Ti/Zr/Nb	0	0	0	0.00823(6)
	O	0	0	0.5	0.0195(2)
<b>Sr<sub>0.8</sub>Ti<sub>0.24</sub>Zr<sub>0.36</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0	0.5	0.25	0.00997(5)
	Ti/Zr/Nb	0	0	0	0.00673(4)
	O1	0	0	0.25	0.0265(18)
	O2	0.2626(3)	0.7626	0	0.0182(8)
<b>Sr<sub>0.8</sub>Ti<sub>0.12</sub>Zr<sub>0.48</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0	0.5	0.25	0.01053(5)
	Ti/Zr/Nb	0	0	0	0.00642(4)
	O1	0	0	0.25	0.0220(5)
	O2	0.27276(18)	0.77276	0	0.0208(4)
<b>Sr<sub>0.8</sub>Zr<sub>0.6</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0	0.5	0.25	0.01042(5)
	Zr/Nb	0	0	0	0.00621(4)
	O1	0	0	0.25	0.0233(4)
	O2	0.27787(16)	0.77787	0	0.0217(3)

Table S6: Atomic coordinates and isotropic atomic displacement parameters as determined by refinements against neutron powder diffraction data collected at room temperature

Composition	Atom	x	y	z	U <sub>iso</sub>
<b>Sr<sub>0.8</sub>Ti<sub>0.6</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0.5	0.5	0.5	0.0096(7)
	Ti/ Nb	0	0	0	0.014(2)
	O	0	0	0.5	0.0066(3)
<b>Sr<sub>0.8</sub>Ti<sub>0.54</sub>Zr<sub>0.06</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0	0.5	0.25	0.0072(5)
	Ti/Zr/Nb	0	0	0	0.0074(13)
	O	0	0	0.5	0.0098(3)
<b>Sr<sub>0.8</sub>Ti<sub>0.48</sub>Zr<sub>0.12</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0	0.5	0.25	0.0094(4)
	Ti/Zr/Nb	0	0	0	0.0059(8)
	O	0	0	0.5	0.0135(2)
<b>Sr<sub>0.8</sub>Ti<sub>0.36</sub>Zr<sub>0.24</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0	0.5	0.25	0.0127(3)
	Ti/Zr/Nb	0	0	0	0.0087(4)
	O1	0	0	0.25	0.0346(10)
	O2	0.25645(19)	0.75645	0	0.0147(4)
<b>Sr<sub>0.8</sub>Ti<sub>0.24</sub>Zr<sub>0.36</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0	0.5	0.25	0.0156(3)
	Ti/Zr/Nb	0	0	0	0.0102(4)
	O1	0	0	0.25	0.0175(8)
	O2	0.2667(2)	0.7667	0	0.0290(5)
<b>Sr<sub>0.8</sub>Zr<sub>0.6</sub>Nb<sub>0.4</sub>O<sub>3</sub></b>	Sr	0	0.5	0.25	0.0144(3)
	Zr/Nb	0	0	0	0.0056(3)
	O1	0	0	0.25	0.0284(7)
	O2	0.27953(18)	0.77953	0	0.0227(4)