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TITLE

An Empirical Model for Perovskite Tetragonality

ABSTRACT

Tetragonal distortions in perovskites are useful for advanced devices, as they can induce functional properties like capacitance, piezoelectricity, pyroelectricity, and ferroelectricity. These distortions are commonly due to either second-order Jahn-Teller effects or antiferrodistortive instabilities. Accurate empirical composition-structure models can significantly reduce the time and cost involved with developing new functional ceramics; however, until now no such model has existed for tetragonal perovskites, the structures of which are further complicated by extrinsic point defects often used to tune electrical properties. In this work, LeBail refinements of X-ray diffraction patterns obtained from $[(\text{Pb}_y\text{Ba}_{1-y})_{(1-3x)}\text{La}_{(2x)}]\text{TiO}_3$ ($P4mm$, No. 99) were conducted to measure lattice constants and reveal tetragonality trends. These trends were combined with a model for unit-cell volume in order to derive a general empirical model, based solely on published ionic radii data, for tetragonal lattice constants of perovskites in $P4mm$ and $P4/mmm$.

INTRODUCTION

Fundamentally, the science of materials is based on processing-structure-property relationships, with composition being a key processing parameter. Indeed, there is a direct link between the degree of tetragonality and the resultant polarization in tetragonal perovskites.[1] As such, predicting and controlling perovskite tetragonality would be useful for the design of materials with specified properties for a whole range of applications including high-K capacitors (e.g., BaTiO₃), pyroelectrics (e.g., Pb_{1-3x}La_{2x}TiO₃), piezoelectrics (e.g., Pb_{1-3x}La_{2x}Zr_yTi_{1-y}O₃), ferroelectrics (e.g., Ba_{1-x}Sr_xTiO₃), and high-temperature superconductors (e.g., YBa₂(Cu_{1-x}Ga_x)₃O₇).[2-5] Unfortunately, no empirical model which can predict the tetragonality of perovskites yet exists.

In 2001, Lufaso and Woodward[6] developed a perovskite structural prediction program (SPuDS) based on the earlier global-instability-index concept of Salinas-Sanchez et al.;[7] however, as powerful as SPuDS is, it does not consider $P4mm$ structures nor any stoichiometry with extrinsic vacancy concentrations or complex compositions. Others have derived methods for predicting cubic perovskite structural stability.[8, 9] Later, methods for predicting lattice constants for orthorhombic perovskites emerged.[10, 11]

For space group $P4/mmm$, the anions retain their ideal positions at 0.5, 0.5, 0 and 0.5, 0, 0.5; however, in the case of $P4mm$ second-order Jahn-Teller (SOJT) distortions (Figure 1) arise. First-order Jahn-Teller (FOJT) distortions are due to incompletely filled electron shells, which are doubly or triply degenerate molecular orbitals. The nature of the FOJT effect is such that distortions are inevitably so weak as to be negligible. On the other hand, SOJT distortions occur when a molecule has filled shells, but where there is only a small energy difference between the highest filled orbital and the lowest empty one. These distortions result in measurable antiparallel

(therefore polar) ionic displacements of cation and anion sublattices and typically yield piezoelectric or ferroelectric behavior. They occur when the HOMO-LUMO gap is small and there is a symmetry-allowed distortion which gives rise to mixing between the two. This distortion is favored because it stabilizes the HOMO while destabilizing the LUMO. SOJT distortions are typically observed for two classes of cations: octahedrally coordinated high-valent d^0 cations (*e.g.*, Ti^{4+} , V^{4+}) and cations containing filled valence s shells (*e.g.*, Pb^{2+}). [12, 13] In the case of $SrTiO_3$, Ti^{4+} is driven off-center within the octahedron as strontium is increasingly replaced with lead. In the extreme case of $PbVO_3$, the d^0 V^{4+} adopts a five-fold coordination whilst the Pb^{2+} cuboctahedral geometry distorts off-center by 19% (Figure 1). [14, 15]

In 2010, Qi et al. [16] used density-functional theory calculations to investigate the tetragonality of 25 ferroelectric perovskites. They found a consistent trend with respect to B-site cation displacements, showing that tetragonality is empirically predictable. In 2011, Kumar and Bhardwaj [17] found a tetragonal trend using a log-log scale of lattice constants versus average radii [18] for several compositions; however, they did not explicitly state which compositions were modeled.

In general, the vertex-sharing nature of perovskite octahedra necessitates either bond stretching or compression to maintain stability. The tolerance factor, t , is a relative measure of the perovskite stability and was first introduced by Goldschmidt [19] in 1926 (Equation 1), where r_A , r_B , and r_X are the published ionic radii of A, B, and X ions, respectively. [18]

$$t_* = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)} \quad (1)$$

This formulation cannot account for the effect of extrinsic vacancies on effective ionic sizes. Recently, Uvic et al.[20-22] derived a tolerance factor (Equation 2), based on the pseudocubic cell volume rather than r_A , which can account for the effect of extrinsic A-site vacancies:

$$t_1 = \frac{a_{pc} - 0.011730139}{0.7209203(r_B + r_X)} - 0.760998 \quad (2)$$

Equation 2 is a better predictor of octahedral distortions in perovskites than is Equation 1; however, it requires the foreknowledge of a_{pc} . As part of this model[20], an empirical relationship between t^* and t_1 for defective perovskites was derived (Equation 3)

$$t_1 = A + Bt_* + Ct_*^2 \quad (3)$$

where the coefficients A, B, and C are in terms of the ideal (i.e., weighted average of Shannon radii) A-site size without extrinsic vacancies, and

$$\begin{aligned} A &= -50.978 + 84.274r_{A(id)0} - 32.411r_{A(id)0}^2 \\ B &= 130.35 - 205.44r_{A(id)0} + 77.539r_{A(id)0}^2 \\ C &= -81.294 + 124.73r_{A(id)0} - 46.185r_{A(id)0}^2 \end{aligned}$$

In the present work, the $[(Pb_yBa_{1-y})(1-3x)La_{(2x)}]TiO_3$ ($0 \leq x \leq 0.05$, $0 \leq y \leq 1.0$) system was investigated in order to develop empirical models for tetragonality. With this formulation, the value of x is equal to the concentration of extrinsic A-site vacancies, [V].

MATERIALS & METHODS

A total of 21 compositions in the system $[(Pb_yBa_{1-y})(1-3x)La_{(2x)}]TiO_3$ ($y = 0.0, 0.25, 0.5, 0.667, 0.75$ and 1.0) ($x = 0.0, 0.01, 0.02, 0.03, 0.04$ and 0.05) were synthesized via the solid-state mixed-oxide

route. Stoichiometric amounts of PbO (99.9%, Thermo Fisher Scientific Inc., Pittsburgh, PA), BaCO₃ (99.9%, Alfa-Aesar, Ward Hill, MA), TiO₂ (99.9%, Aldrich Chemical Co., Milwaukee, WI), and La₂O₃ (99.95%, Alfa-Aesar, Ward Hill, MA) were ball milled with yttria-stabilized ZrO₂ (YSZ) media in deionized water for ~24 hours in a high-density nylon pot. Powders were then dried overnight in an atmospheric drying oven at 80-100°C until the water was evaporated. Calcination was conducted at 1000°C for three hours in a box furnace (1807FL, CM Furnaces Inc., Bloomfield, NJ). No excess PbO was added to account for volatility; however, Pb-containing compositions ($y > 0$) were calcined adjacent to a sacrificial powder bed of the same composition on a pre-contaminated Al₂O₃ lid muffled by an inverted Al₂O₃ crucible (also pre-contaminated) to inhibit both volatility and lead-loss into the crucible walls. After calcination the powders were pulverized by hand using a mortar and pestle.

Powder X-ray diffraction (XRD) measurements were performed in a diffractometer (Miniflex-600, Rigaku, Woodlands, TX) operating with convergent-beam geometry and Cu K α radiation ($\lambda=1.540593$ Å). Le Bail fits to the XRD data were analyzed using DiffracPLUS TOPAS 4.2 (Bruker AXS Inc., Madison, WI). The background was fitted with a fourth-order Chebychev polynomial, and asymmetry was corrected using the Finger et al. model.[23]

RESULTS & DISCUSSION

Figure 2 demonstrates that the 21 synthesized compositions appeared via XRD to be single-phase tetragonal perovskites. Figure 3 shows how the tetragonality changes as a function of t_1 (Equation 2). Each line in this figure corresponds to a family of compositions, all in space group $P4mm$, with a single Pb/Ba ratio (*i.e.*, y value). The different data points on each line correspond to various

values of x (*i.e.*, vacancy concentrations). These linear relationships are described by Equations 4-9, which all seem to (notionally) converge at $t_1 \sim 0.9640$, corresponding to a (notional) tetragonality of 0.9057.

$$(c/a)_{y=0} = 0.9348(t_1) + 0.0045 \quad (4)$$

$$(c/a)_{y=0.25} = 1.0325(t_1) - 0.0894 \quad (5)$$

$$(c/a)_{y=0.5} = 1.2352(t_1) - 0.2850 \quad (6)$$

$$(c/a)_{y=0.667} = 1.3867(t_1) - 0.4312 \quad (7)$$

$$(c/a)_{y=0.75} = 1.4755(t_1) - 0.5169 \quad (8)$$

$$(c/a)_{y=1} = 1.7130(t_1) - 0.7457 \quad (9)$$

Figure 4 illustrates that the slopes of these linear relationships, m , can be calculated (Equation 10) as a function of the tolerance factor corresponding to $x = 0$ in each case, t_0 (Equation 1 at $x = 0$). Equation 11 can then be used to estimate the tetragonality using the point of convergence, t_1 and a slope defined by Equation 10. Figure 5 demonstrates the fit achieved with this method, which has an average relative absolute error of 0.29%; however, this fit only accounts for the 58 specific cases of $P4mm$ titanate perovskites (*i.e.*, $A(\text{TiO}_3)$); where the open data points are from literature and the filled data points are the 21 titanate compositions synthesized in this work.

$$m = 317.07(t_0)^2 - 683.79(t_0) + 369.6 \quad (10)$$

$$c/a = m(t_1 - 0.964038) + 0.905694 \quad (11)$$

The question then becomes whether or not this method can be extended to other tetragonal compounds. Perhaps the point of convergence (Figure 3) can be used to relate other tetragonal compositional systems. One may naturally shift attention to the effects of changing the B-site cation (Table 1) in an attempt to extend this method and further the understandings of tetragonality. Replacing Ti^{4+} ($r_{\text{Ti}}^{\text{VI}} = 0.605 \text{ \AA}$) with Zr^{4+} ($r_{\text{Zr}}^{\text{VI}} = 0.72 \text{ \AA}$) increases the average B-site cation size and so reduces the tolerance factor, which simultaneously decreases the tetragonality (Figure 6). The inset of Figure 6 shows these 15 $\text{Pb}(\text{Zr}_{1-z}\text{Ti}_z)\text{O}_3$ data points in context with Figure 3.

Assuming, this method may be used for any tetragonal compositional family which shares the same point of convergence. A combined total of 133 various tetragonal compounds in either $P4mm$ or $P4/mmm$ (Table 2) were used in conjunction with this point of convergence to calculate the slopes of their respective c/a vs t_l curves (Figure 7) and to generalize Equation 10:

$$m[t_0, r_B] = m_1 - (m_1 - m_2) \left(\frac{2}{\sqrt{\pi}} \right) \int_0^B e^{-n^2} dn \quad (12)$$

where

$$\begin{aligned} m_1 &= -97.6891 + 337.225 r_B - 279.582 r_B^2 \\ m_2 &= -9.33831 + 33.2458 r_B - 27.5444 r_B^2 \\ B &= \frac{t_0 - (0.573697 + 1.34272 r_B - 1.11274 r_B^2)}{2 \sqrt{-0.0839725 + 0.282206 r_B - 0.233808 r_B^2}} \end{aligned}$$

As a proof of concept, Figure 8 shows the results of this method of estimating c/a using Equations 11 - 12. Table 2 shows the results of this approach for each of the 133 compositions shown in Figure 8. It is noteworthy that Figure 8 includes the otherwise anomalous PbVO_3 outlier compound

($c/a = 1.229$)[15] and three compositions in space group $P4/mmm$ (*i.e.*, SrFeO_3 , $\text{Sr}_{0.9}\text{Bi}_{0.1}\text{FeO}_3$ and CeAlO_3)[24-26] and demonstrates a goodness of fit with an overall average absolute relative error of just 0.64%. The tetragonal lattice constants can then be derived (assuming the absence of any cation ordering) with equations 12 - 13. Equation 13 shows the mathematical relationship between c/a and a_{pc} (assuming one ABX_3 formula unit for the tetragonal compound). **While vacancy ordering can exist in compositions with higher vacancy concentrations and can effect structure/symmetry, the empirical model invoked here [20] remains valid. As the model is based on effective bond lengths, it is sensitive to cation ordering, which affects bond lengths, but not vacancy ordering, which does not.**

Table 3 shows experimental and calculated tetragonal lattice constants using equations 3, 11, 12 and 13; where the calculated c/a (Equation 11) depends on m (Equation 12) and the calculated t_l (Equation 3).

$$\frac{c}{a} = \left(\frac{a_{pc}}{a} \right)^3 \quad (13)$$

It is also of significant interest in the field of electroceramics to relate tetragonality to polarization, which determines the intrinsic component of relative permittivity - a property at the heart of capacitance, pyroelectricity, piezoelectricity, and ferroelectricity. The dipole moment of a compound is a function of ionic charge and the relative separation between the two oppositely charged sublattice centroids. Space group $P4/mmm$ is centrosymmetric, which means that the two sublattice centroids coincide and there is no net dipole moment; however, perovskites in space group $P4mm$ are non-centrosymmetric and have non-zero dipole moments. Table 4 shows the dipole moments derived from experimental positional data of 43 various $P4mm$ tetragonal $\text{A}^{2+}\text{B}^{4+}\text{O}_3$ perovskites, which arise as a direct result of their tetragonal distortions. Figure 9 shows

the relationship between tetragonality and polarization for these compounds. The inset shows the goodness of fit to experimental data, and the trend can be described by equation 14.

$$p \left[\frac{\mu C}{cm^2} \right] = -800467.451 + 3410445.611 \left(\frac{c}{a} \right) - 5806887.936 \left(\frac{c}{a} \right)^2 + 4938557.817 \left(\frac{c}{a} \right)^3 - 2097541.606 \left(\frac{c}{a} \right)^4 + 355895.421 \left(\frac{c}{a} \right)^5 \quad (14)$$

As can be seen in Figure 9 and Table 4, most of the data points which show significant error are based on structural parameters determined via XRD. As XRD is insensitive to oxygen positions, the experimental values of polarization for these compositions is likely to contain a great amount of uncertainty, thereby explaining the errors observed in this work.

There are three additional positional parameters, z , which define the structure of $P4mm$ perovskites: the B-cation displacement (z) in the 1b position and the displacement (z) of anions in both 2c and 1b sites; however, tetragonality is clearly the dominating effect in ultimately determining p . Expanding this model to include compositions in other systems would require additional data; but it is reasonable to assume that each system would follow a similar trend, varying only due to differences in ionic charge, polarizability, or ionic displacements.

CONCLUSION

A total of 21 compositions in the system $[(Pb_yBa_{1-y})(1-3x)La_{(2x)}]TiO_3$ ($y = 0.0, 0.25, 0.5, 0.667, 0.75$ and 1.0) ($x = 0.0, 0.01, 0.02, 0.03, 0.04$ and 0.05) were synthesized via the solid-state mixed-oxide route. LeBail refinements of X-ray diffraction patterns were conducted to observe lattice constants

and reveal c/a ratio trends. A general empirical model, based solely on published ionic radii data, for tetragonal lattice constants of perovskites in $P4mm$ or $P4/mmm$ has been proposed. Furthermore, a general empirical model for the unit-cell polarization of $A^{2+}B^{4+}O_3^{2-}$ perovskites has been derived.

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FIGURE LIST

Figure 1. Tetragonal PbTiO_3 showing the result of SOJT distortions which exist in $P4mm$ perovskite compounds; unlike $P4/mmm$ compounds which maintain ideal cation and anion relative positions. Pb^{2+} is shown at the origin.

Figure 2. X-ray diffraction patterns of 24 synthesized compositions in the system $[(\text{Pb}_y\text{Ba}_{1-y})(1-3x)\text{La}_{(2x)}]\text{TiO}_3$ ($y = 0.0, 0.25, 0.5, 0.667, 0.75$ and 1.0) ($x = 0.0, 0.01, 0.02, 0.03, 0.04$ and 0.05). The patterns are in ascending order with $x = 0$ and $y = 0$ at the bottom.

Figure 3. Tetragonal titanates in the system $[(\text{Pb}_y\text{Ba}_{1-y})(1-3x)\text{La}_{(2x)}]\text{TiO}_3$. The open data points are from literature.[3, 27-31] Data points for varying x between $0 \leq x \leq 0.5$ are shown as: $y = 0.0$ circles, $y = 0.25$ diamonds, $y = 0.50$ triangles, $y = 0.667$ squares, $y = 0.75$ circles and $y = 1.0$ squares; $\text{Pb}_{1-x}\text{Bi}_{2x}\text{TiO}_3$ ($x = 0.025$ and 0.05 squares) and $\text{Ba}_{1-3x}\text{Sm}_{2x}\text{TiO}_3$ ($x = 0.0333$ circle). The notional point of convergence is $(0.964038, 0.905694)$.

Figure 4. Slopes of c/a vs t_0 curves for $(\text{Pb}_{1-y}\text{Ba}_y)\text{TiO}_3$ $0 \leq y \leq 1$, including all 54 titanates in Table 2. The black curve is the fit described by Equation 10.

Figure 5. Calculated tetragonalities of 54 titanate perovskites. The 21 filled data points are from this work and the open data points are from literature.[3, 27-34] These 54 titanates (*i.e.*, $A(\text{TiO}_3)$) are listed in Table 2 (the remaining 79 of the 133 compositions listed in Table 2 are not purely titanates).

Figure 6. Effect of tolerance factor on tetragonality for $\text{Pb}(\text{Zr}_{1-z}\text{Ti}_z)\text{O}_3$ in $P4mm$, with the concentration of Ti^{4+} (z) increasing from left to right, simultaneously increasing both tetragonality and tolerance factor. These seven compositions were selected from Table 1. The inset shows these data points in context with Figure 3.

Figure 7. Slopes of the c/a vs t_1 curves in terms of tolerance factor at $x = 0$ (t_0) derived from the 133 perovskite oxides in Table 2.

Figure 8. Calculated tetragonalities of the 133 perovskite oxides listed in Table 2.

Figure 9. Polarization of 43 of $A^{2+}B^{4+}\text{O}_3$ perovskites as a function of c/a (Table 4) from literature. Circle data points indicate neutron diffraction data, and x data points indicate X-ray diffraction data. Equation 13 is illustrated by the black curve.

Table 1. The effect of the weighted average B-site size on tetragonality of Pb perovskites

Composition	c/a	t_1	r_B Avg. ($\text{\AA}$)	ICSD #
PbTiO ₃	1.064524	1.056747	0.605	183213
PbTiO ₃	1.061888	1.055354	0.605	165498
PbTiO ₃	1.059146	1.05415	0.605	90693
Pb (Zr _{0.1} Ti _{0.9}) O ₃	1.052124	1.048186	0.6165	90694
Pb (Zr _{0.2} Ti _{0.8}) O ₃	1.045019	1.044535	0.628	90695
Pb (Zr _{0.3} Ti _{0.7}) O ₃	1.036852	1.043805	0.6395	90696
Pb (Zr _{0.3} Ti _{0.7}) O ₃	1.042718	1.047756	0.6395	183587
Pb _{0.96} Ce _{0.04} (Zr _{0.3} Ti _{0.7}) O ₃	1.040693	1.04360	0.6395	153294
Pb _{0.96} Nd _{0.04} (Zr _{0.3} Ti _{0.7}) O ₃	1.03006	1.041733	0.6395	153295
Pb (Zr _{0.35} Ti _{0.65}) O ₃	1.039471	1.046321	0.64525	247782
Pb (Zr _{0.4} Ti _{0.6}) O ₃	1.031436	1.038146	0.651	90697
Pb (Zr _{0.4} Ti _{0.6}) O ₃	1.035439	1.038967	0.651	187471
Pb (Zr _{0.45} Ti _{0.55}) O ₃	1.024367	1.036188	0.65675	55700
Pb (Zr _{0.5} Ti _{0.5}) O ₃	1.021153	1.036373	0.6625	155328
Pb (Zr _{0.52} Ti _{0.48}) O ₃	1.021989	1.034568	0.6648	191123

Table 2

Table 2. The 133 tetragonal compositions used for the generalized tetragonality relationship (Figure 8). 58 of these 133 are titanates (i.e., A(TiO₃)).

ICSD #	S.G.	Composition	t_0	slope	t_1	c/a exptl	c/a calc	Error%	a_{pc} calc.	Error%
28621	<i>P4mm</i>	(Pb _{0.2} Ba _{0.8}) (Ti O ₃)	1.0619	0.9819	1.0677	1.0163	1.0075	0.87	3.9904	0.20
54150	<i>P4mm</i>	(Ba _{0.67} Sr _{0.33}) (Ti O ₃)	1.0503	1.1601	1.0487	0.9995	1.0039	0.44	3.9740	0.06
55629	<i>P4/mmm</i>	Ce (Ga O ₃)	0.7071	2.7066	1.0015	1.0018	1.0071	0.53	3.8765	0.03
55700	<i>P4mm</i>	Pb ((Zr _{0.45} Ti _{0.55}) O ₃)	1.0007	1.7397	1.0362	1.0244	1.0312	0.67	4.0071	1.26
80800	<i>P4/mmm</i>	(Sr _{0.9} Bi _{0.1}) (Fe O ₃)	0.7071	0.9126	1.0638	0.9971	0.9968	0.03	3.8542	0.69
88534	<i>P4/mmm</i>	(Ba _{0.272} Sr _{0.728}) (Zr _{0.403} Ti _{0.597}) O ₃	1.0021	1.9132	1.0137	0.9975	1.0007	0.32	3.9983	0.42
90693	<i>P4mm</i>	Pb (Ti O ₃)	1.0272	1.7483	1.0541	1.0591	1.0632	0.39	3.9414	0.95
90694	<i>P4mm</i>	Pb (Zr _{0.1} Ti _{0.9}) O ₃	1.0212	1.9040	1.0482	1.0521	1.0659	1.31	3.9560	0.96
90695	<i>P4mm</i>	Pb (Zr _{0.2} Ti _{0.8}) O ₃	1.0153	1.9857	1.0445	1.0450	1.0655	1.96	3.9706	1.04
90696	<i>P4mm</i>	Pb (Zr _{0.3} Ti _{0.7}) O ₃	1.0094	1.9781	1.0438	1.0369	1.0635	2.57	3.9852	1.22
90697	<i>P4mm</i>	Pb (Zr _{0.4} Ti _{0.6}) O ₃	1.0036	1.8580	1.0381	1.0314	1.0434	1.16	3.9998	1.23
97116	<i>P4/mmm</i>	(Pr _{0.6} Ba _{0.4}) Co O ₃	0.7071	0.7127	1.0623	0.9807	0.9757	0.51	3.8249	1.13
97117	<i>P4/mmm</i>	(Pr _{0.5} Ba _{0.5}) Co O ₃	0.7071	0.6352	1.0675	0.9764	0.9714	0.51	3.8418	0.88
97834	<i>P4mm</i>	(Pb _{0.58} Ca _{0.42}) (Ti O ₃)	1.0044	2.6688	1.0001	1.0180	1.0019	1.59	3.9093	0.16
97836	<i>P4mm</i>	(Pb _{0.61} Ca _{0.39}) (Ti O ₃)	1.0060	2.5927	1.0047	1.0232	1.0112	1.17	3.9116	0.05
98057	<i>P4mm</i>	K _{0.5} Bi _{0.5} (Ti O ₃)	1.0471	1.2222	1.0307	1.0057	0.9871	1.85	3.9695	0.59
150085	<i>P4mm</i>	(Pb _{0.925} La _{0.05}) (Ti O ₃) x=0.025	1.0272	1.7483	1.0425	1.0413	1.0428	0.15	3.9191	1.11
150086	<i>P4mm</i>	(Pb _{0.85} La _{0.1}) (Ti O ₃) x=0.05	1.0272	1.7483	1.0357	1.0306	1.0310	0.04	3.8968	1.43
150087	<i>P4mm</i>	(Pb _{0.775} La _{0.15}) (Ti O ₃) 0.075	1.0272	1.7483	1.0313	1.0204	1.0233	0.28	3.8745	1.84
150088	<i>P4mm</i>	(Pb _{0.7} La _{0.2}) (Ti O ₃) x=0.1	1.0272	1.7483	1.0266	1.0120	1.0151	0.31	3.8522	2.24
150089	<i>P4mm</i>	(Pb _{0.625} La _{0.25}) (Ti O ₃) x=0.125	1.0272	1.7483	1.0221	1.0049	1.0072	0.24	3.8299	2.65
152277	<i>P4mm</i>	Pb (V O ₃)	0.7071	1.6612	1.1594	1.2295	1.2302	0.06	3.9351	3.44
153294	<i>P4mm</i>	(Pb _{0.96} Ce _{0.04}) (Zr _{0.3} Ti _{0.7}) O ₃	1.0094	1.9781	1.0436	1.0407	1.0631	2.15	3.9822	1.29
153295	<i>P4mm</i>	(Pb _{0.96} Nd _{0.04}) (Zr _{0.3} Ti _{0.7}) O ₃	1.0094	1.9781	1.0417	1.0301	1.0594	2.85	3.9807	1.26

154107	<i>P4/mmm</i>	Nd Ba Co ₂ O ₆	0.7071	0.6409	1.0608	0.9782	0.9677	1.07	3.8398	0.70
155328	<i>P4mm</i>	Pb ((Zr _{0.5} Ti _{0.5}) O ₃)	0.9979	1.5580	1.0364	1.0212	1.0184	0.27	4.0144	1.37
155329	<i>P4mm</i>	Pb ((Zr _{0.5} Ti _{0.5}) O ₃)	0.9979	1.5580	1.0364	1.0156	1.0184	0.28	4.0144	1.37
156987	<i>P4mm</i>	(Pb _{0.97} Cd _{0.03}) (Ti O ₃)	1.0233	1.8820	1.0518	1.0673	1.0708	0.33	3.9359	1.01
156988	<i>P4mm</i>	(Pb _{0.94} Cd _{0.06}) (Ti O ₃)	1.0194	2.0258	1.0539	1.0681	1.0878	1.85	3.9304	1.22
157807	<i>P4mm</i>	(Pb _{0.333} Ba _{0.667}) (Ti O ₃)	1.0563	1.0601	1.0546	1.0284	1.0017	2.60	3.9824	0.06
158886	<i>P4/mmm</i>	Pr Ba (Mn ₂ O ₆)	0.7071	1.6327	1.0253	0.9972	1.0057	0.85	3.8837	0.12
158890	<i>P4/mmm</i>	Nd Ba (Mn ₂ O ₆)	0.7071	1.6814	1.0201	0.9939	1.0000	0.62	3.8817	0.01
161317	<i>P4mm</i>	(Ba _{0.985} Na _{0.015}) ((Ti _{0.985} Nb _{0.015}) O ₃)	1.0688	0.9047	1.0746	1.0044	1.0057	0.14	4.0023	0.20
161710	<i>P4mm</i>	(Pb _{0.95} Bi _{0.05}) (Ti O ₃)	1.0272	1.7483	1.0518	1.0556	1.0591	0.33	3.9404	0.90
161711	<i>P4mm</i>	(Pb _{0.9} Bi _{0.1}) (Ti O ₃)	1.0272	1.7483	1.0490	1.0517	1.0543	0.25	3.9394	0.83
164352	<i>P4mm</i>	(Pb _{0.85} La _{0.1}) (Ti O ₃) x=0.05	1.0272	1.7483	1.0366	1.0291	1.0325	0.33	3.8968	1.46
164977	<i>P4mm</i>	(Ba _{0.996} Y _{0.004}) (Ti O ₃)	1.0706	0.8883	1.0737	1.0104	1.0031	0.72	4.0018	0.13
165130	<i>P4mm</i>	Pb ((Fe _{0.012} Ti _{0.988}) O ₃)	0.7071	1.6611	1.0615	1.0530	1.0676	1.39	3.9411	1.21
165131	<i>P4mm</i>	(Pb _{0.7} Sr _{0.3}) ((Fe _{0.012} Ti _{0.988}) O ₃)	0.7071	1.7336	1.0222	1.0031	1.0065	0.34	3.9211	0.32
165498	<i>P4mm</i>	Pb (Ti O ₃)	1.0272	1.7483	1.0554	1.0619	1.0653	0.33	3.9414	1.00
166283	<i>P4/mmm</i>	Ce (Al O ₃)	0.7071	2.3952	1.0073	1.0049	1.0094	0.45	3.8078	0.90
169562	<i>P4/mmm</i>	Nd Ba (Co _{1.5} Fe _{0.5}) O ₆	0.7071	0.6627	1.0687	0.9809	0.9750	0.60	3.8414	1.00
169563	<i>P4/mmm</i>	Nd Ba (Co Fe) O ₆	0.7071	0.6876	1.0755	0.9847	0.9823	0.24	3.8429	1.26
169568	<i>P4/mmm</i>	Gd Ba (Co Fe) O ₆	0.7071	0.7353	1.0636	0.9791	0.9789	0.02	3.8350	1.05
169588	<i>P4mm</i>	(Bi _{0.69} Pb _{0.31}) ((Fe _{0.69} Ti _{0.31}) O ₃)	0.7071	1.5167	1.1514	1.1874	1.1899	0.21	3.8969	3.47
169589	<i>P4mm</i>	(Bi _{0.6} Pb _{0.4}) ((Fe _{0.6} Ti _{0.4}) O ₃)	0.7071	1.3073	1.1370	1.1624	1.1318	2.64	3.8911	3.38
169590	<i>P4mm</i>	(Bi _{0.5} Pb _{0.5}) ((Fe _{0.5} Ti _{0.5}) O ₃)	0.7071	1.3550	1.1212	1.1352	1.1187	1.45	3.8970	2.98
169591	<i>P4mm</i>	(Bi _{0.4} Pb _{0.6}) ((Fe _{0.4} Ti _{0.6}) O ₃)	0.7071	1.4508	1.1064	1.1167	1.1123	0.40	3.9053	2.55
169592	<i>P4mm</i>	(Bi _{0.3} Pb _{0.7}) ((Fe _{0.3} Ti _{0.7}) O ₃)	0.7071	1.5477	1.0926	1.0963	1.1047	0.77	3.9144	2.13
169593	<i>P4mm</i>	(Bi _{0.2} Pb _{0.8}) ((Fe _{0.2} Ti _{0.8}) O ₃)	0.7071	1.5406	1.0795	1.0821	1.0835	0.13	3.9234	1.73
169594	<i>P4mm</i>	(Bi _{0.1} Pb _{0.9}) ((Fe _{0.1} Ti _{0.9}) O ₃)	0.7071	1.6976	1.0669	1.0709	1.0804	0.88	3.9324	1.35

169595	<i>P4mm</i>	(Bi _{0.7} Pb _{0.3}) ((Fe _{0.7} Ti _{0.3}) O ₃)	0.7071	1.5210	1.1521	1.1875	1.1917	0.35	3.8967	3.47
169597	<i>P4mm</i>	(Bi _{0.71} Pb _{0.29}) ((Fe _{0.71} Ti _{0.29}) O ₃)	0.7071	1.4963	1.1529	1.1876	1.1882	0.06	3.8952	3.50
169599	<i>P4mm</i>	(Bi _{0.72} Pb _{0.28}) ((Fe _{0.72} Ti _{0.28}) O ₃)	0.7071	1.5005	1.1537	1.1876	1.1903	0.22	3.8950	3.50
181726	<i>P4mm</i>	(Bi _{0.85} Nd _{0.15}) (Fe O ₃)	0.7071	0.8187	1.0919	1.0118	1.0104	0.14	3.8374	2.09
183213	<i>P4mm</i>	Pb (Ti O ₃)	1.0272	1.7483	1.0567	1.0645	1.0678	0.31	3.9414	1.05
183587	<i>P4mm</i>	Pb (Zr _{0.3} Ti _{0.7}) O ₃	1.0094	1.9781	1.0478	1.0427	1.0713	2.74	3.9852	1.36
184861	<i>P4mmm</i>	Sr (Fe O ₃)	0.7071	1.1543	1.0477	1.0039	1.0023	0.16	3.8626	0.09
186228	<i>P4mm</i>	Ba _{0.9} K _{0.05} Bi _{0.05} (Ti O ₃)	1.0683	0.9108	1.0720	1.0103	1.0040	0.62	3.9993	0.13
186229	<i>P4mm</i>	(Ba _{0.85} K _{0.075} Bi _{0.075}) (Ti O ₃)	1.0671	0.9227	1.0693	1.0111	1.0028	0.82	3.9976	0.08
186230	<i>P4mm</i>	(Ba _{0.8} K _{0.1} Bi _{0.1}) (Ti O ₃)	1.0659	0.9353	1.0671	1.0116	1.0021	0.93	3.9960	0.04
186683	<i>P4mmm</i>	(Ba _{0.5} Sr _{0.5}) (Ti _{0.946} Fe _{0.046}) O ₃	0.7071	1.3078	1.0457	0.9987	1.0125	1.39	3.9520	0.10
186684	<i>P4mmm</i>	(Ba _{0.5} Sr _{0.5}) (Ti _{0.876} Fe _{0.081}) O ₃	0.7071	0.9177	1.0798	0.9995	1.0119	1.25	3.9212	0.95
186685	<i>P4mmm</i>	(Ba _{0.5} Sr _{0.5}) (Ti _{0.849} Fe _{0.139}) O ₃	0.7071	1.0005	1.0577	0.9994	0.9994	0.00	3.9275	0.83
186686	<i>P4mmm</i>	(Ba _{0.5} Sr _{0.5}) (Ti _{0.806} Fe _{0.183}) O ₃	0.7071	0.7059	1.0946	0.9992	0.9979	0.14	3.9021	1.49
186687	<i>P4mmm</i>	(Ba _{0.5} Sr _{0.5}) (Ti _{0.624} Fe _{0.402}) O ₃	0.7071	1.3185	1.0376	0.9995	1.0026	0.32	3.9529	0.47
187081	<i>P4mm</i>	(Ba _{0.91} Ca _{0.11}) (Ti O ₃)	1.0715	0.8802	1.0729	1.0041	1.0015	0.26	4.0039	0.05
187471	<i>P4mm</i>	Pb (Zr _{0.4} Ti _{0.6}) O ₃	1.0036	1.8580	1.0390	1.0354	1.0449	0.92	3.9998	1.26
187472	<i>P4mm</i>	(Pb _{0.9} Ba _{0.1}) ((Zr _{0.40} Ti _{0.60}) O ₃)	1.0078	1.6752	1.0393	1.0291	1.0318	0.26	4.0059	1.12
187472	<i>P4mm</i>	(Pb _{0.9} Ba _{0.1}) ((Zr _{0.40} Ti _{0.60}) O ₃)	1.0078	1.6752	1.0393	1.0291	1.0318	0.26	4.0059	1.12
187473	<i>P4mm</i>	(Pb _{0.8} Ba _{0.2}) ((Zr _{0.40} Ti _{0.60}) O ₃)	1.0121	1.5102	1.0457	1.0224	1.0290	0.64	4.0121	1.19
187473	<i>P4mm</i>	(Pb _{0.8} Ba _{0.2}) ((Zr _{0.40} Ti _{0.60}) O ₃)	1.0121	1.5102	1.0457	1.0224	1.0290	0.64	4.0121	1.19
187474	<i>P4mm</i>	(Pb _{0.7} Ba _{0.3}) ((Zr _{0.40} Ti _{0.60}) O ₃)	1.0163	1.3632	1.0453	1.0157	1.0165	0.07	4.0182	1.03
187474	<i>P4mm</i>	(Pb _{0.7} Ba _{0.3}) ((Zr _{0.40} Ti _{0.60}) O ₃)	1.0163	1.3632	1.0453	1.0157	1.0165	0.07	4.0182	1.03
187475	<i>P4mm</i>	(Pb _{0.6} Ba _{0.4}) ((Zr _{0.40} Ti _{0.60}) O ₃)	1.0206	1.2340	1.0468	1.0095	1.0078	0.17	4.0243	0.93
187475	<i>P4mm</i>	(Pb _{0.6} Ba _{0.4}) ((Zr _{0.40} Ti _{0.60}) O ₃)	1.0206	1.2340	1.0468	1.0095	1.0078	0.17	4.0243	0.93
187635	<i>P4mm</i>	Pb (V O ₃)	0.7071	1.6612	1.1566	1.2210	1.2256	0.38	3.9351	3.34
188645	<i>P4mm</i>	(Ba _{0.9} Sm _{0.067}) (Ti O ₃)	1.0706	0.8883	1.0692	1.0040	0.9991	0.49	3.9629	0.94

188784	<i>P4mm</i>	(Ba _{0.95} Sr _{0.05}) (Ti O ₃)	1.0675	0.9181	1.0697	1.0093	1.0027	0.65	3.9983	0.08
188785	<i>P4mm</i>	(Ba _{0.9} Sr _{0.1}) (Ti O ₃)	1.0645	0.9514	1.0657	1.0080	1.0024	0.56	3.9939	0.04
188786	<i>P4mm</i>	(Ba _{0.85} Sr _{0.15}) (Ti O ₃)	1.0614	0.9887	1.0609	1.0068	1.0015	0.52	3.9896	0.02
188985	<i>P4mm</i>	(Bi _{0.6} Sr _{0.4}) (Mn O ₃)	0.7071	0.8842	1.0495	0.9747	0.9813	0.68	3.8568	0.64
188986	<i>P4mm</i>	(Bi _{0.55} Sr _{0.45}) (Mn O ₃)	0.7071	0.8869	1.0413	0.9693	0.9742	0.50	3.8565	0.36
188987	<i>P4mm</i>	(Bi _{0.5} Sr _{0.5}) (Mn O ₃)	0.7071	0.8897	1.0360	0.9706	0.9697	0.09	3.8563	0.18
188988	<i>P4mm</i>	(Bi _{0.45} Sr _{0.55}) (Mn O ₃)	0.7071	0.8925	1.0343	0.9737	0.9684	0.54	3.8560	0.12
189052	<i>P4/mmm</i>	Pr Ba Co ₂ O ₆	0.7071	0.6352	1.0611	0.9847	0.9673	1.76	3.8418	0.65
189232	<i>P4/mmm</i>	Sm Ba (Co _{1.2} Fe _{0.8}) O ₆	0.7071	0.7198	1.0641	0.9766	0.9777	0.11	3.8347	1.05
189382	<i>P4mm</i>	(Ba _{0.96} La _{0.027}) (Ti O ₃) x=0.0135	1.0706	0.8883	1.0683	1.0030	0.9983	0.47	3.9885	0.27
191123	<i>P4mm</i>	Pb ((Zr _{0.52} Ti _{0.48}) O ₃)	0.9967	1.4562	1.0346	1.0220	1.0084	1.33	4.0173	1.35
191126	<i>P4mm</i>	Pb ((Zr _{0.52} Ti _{0.48}) O ₃)	0.9967	1.4562	1.0382	1.0083	1.0136	0.53	4.0173	1.48
192240	<i>P4mm</i>	(Bi _{0.6} Ca _{0.4}) (Fe O ₃)	0.7071	1.2788	1.0404	0.9991	1.0033	0.42	3.8732	1.18
192241	<i>P4mm</i>	(Bi _{0.5} Ca _{0.5}) (Fe O ₃)	0.7071	1.4048	1.0298	0.9971	0.9981	0.10	3.8676	0.95
192848	<i>P4mm</i>	(Bi _{0.6} Pb _{0.4}) ((Fe _{0.6} Ti _{0.4}) O ₃)	0.7071	1.3073	1.1524	1.1552	1.1520	0.28	3.8911	3.89
192849	<i>P4mm</i>	(Bi _{0.57} La _{0.03} Pb _{0.4}) ((Fe _{0.6} Ti _{0.4}) O ₃)	0.7071	1.3323	1.1255	1.1308	1.1208	0.89	3.8897	3.03
193390	<i>P4mm</i>	(Bi _{0.465} Na _{0.465} Ba _{0.07}) (Ti O ₃)	1.0067	2.5627	1.0001	1.0006	0.9982	0.24	3.9125	0.24
237599	<i>P4mm</i>	(Bi _{0.9} Sm _{0.1}) (Fe _{0.5} Co _{0.5}) O ₃	0.7071	1.5245	1.1868	1.2611	1.2453	1.25	3.8659	4.41
240256	<i>P4mm</i>	Pb V O ₃	0.7071	1.6612	1.1560	1.2290	1.2247	0.35	3.9351	3.33
245945	<i>P4mm</i>	Ba (Ti O ₃)	1.0706	0.8883	1.0738	1.0082	1.0032	0.50	4.0026	0.11
247691	<i>P4mm</i>	(Bi _{0.8} La _{0.2}) (Fe _{0.9} Ti _{0.1}) O ₃	0.7071	0.7767	1.1012	1.0101	1.0123	0.21	3.8420	2.58
247692	<i>P4mm</i>	(Bi _{0.8} La _{0.2}) (Fe _{0.85} Ti _{0.15}) O ₃	0.7071	0.7487	1.0942	1.0031	1.0031	0.00	3.8408	2.51
247747	<i>P4mm</i>	(La _{0.21} Pb _{0.79}) (Fe _{0.18} Ti _{0.82}) O ₃	0.7071	1.4590	1.0466	1.0157	1.0262	1.03	3.9289	0.50
247748	<i>P4mm</i>	(La _{0.12} Pb _{0.88}) (Fe _{0.10} Ti _{0.90}) O ₃	0.7071	1.6519	1.0503	1.0399	1.0482	0.80	3.9344	0.72
247782	<i>P4mm</i>	Pb (Zr _{0.35} Ti _{0.65}) O ₃	1.0065	1.9344	1.0463	1.0395	1.0649	2.44	3.9925	1.41
248396	<i>P4mm</i>	(Ba _{0.96} Nd _{0.04}) Ti O ₃ x=0.02	1.0706	0.8883	1.0658	1.0052	0.9961	0.91	3.9957	0.00
249001	<i>P4/mmm</i>	(Ce _{0.016} Sr _{0.984}) (Fe O ₃)	0.7071	1.1211	1.0492	0.9975	1.0011	0.37	3.8647	0.10

290401	<i>P4mm</i>	(Bi _{0.65} Pb _{0.35}) (Fe _{0.65} Ti _{0.35}) O ₃	0.7071	0.8991	1.1197	1.0391	1.0457	0.63	3.8710	3.17
290951	<i>P4mm</i>	(Bi _{0.8} Ba _{0.2}) (Fe _{0.97} Co _{0.03}) O ₃	0.7071	0.6507	1.1459	1.0176	1.0241	0.63	3.8673	3.15
291165	<i>P4mm</i>	(Pb _{0.05} Ba _{0.95}) (Ti O ₃)	1.0684	0.9090	1.0725	1.0123	1.0043	0.79	3.9995	0.14
Ganguly ³	<i>Pm-3m</i>	(Ba _{0.9} La _{0.066667}) (Ti O ₃) x=0.033333	1.0706	0.8883	1.0652	1.0000	0.9956	0.44	3.9667	0.71
Ganguly ³	<i>P4mm</i>	(Ba _{0.94} La _{0.04}) (Ti O ₃) x=0.02	1.0706	0.8883	1.0677	1.0000	0.9978	0.22	3.9811	0.44
Ganguly ³	<i>P4mm</i>	(Ba _{0.96} La _{0.0267}) (Ti O ₃) x=0.013333	1.0706	0.8883	1.0683	1.0030	0.9983	0.47	3.9883	0.28
This Work	<i>P4mm</i>	Ba (Ti O ₃) x=0	1.0706	0.8883	1.0727	1.0075	1.0023	0.52	4.0026	0.08
This Work	<i>P4mm</i>	(Ba _{0.88} La _{0.08}) (Ti O ₃) x=0.04	1.0706	0.8883	1.0647	1.0002	0.9951	0.51	3.9596	0.87
This Work	<i>P4mm</i>	(Ba _{0.91} La _{0.06}) (Ti O ₃) x=0.03	1.0706	0.8883	1.0584	0.9961	0.9895	0.66	3.9703	0.38
This Work	<i>P4mm</i>	(Ba _{0.94} La _{0.04}) (Ti O ₃) x=0.02	1.0706	0.8883	1.0684	1.0008	0.9984	0.23	3.9811	0.46
This Work	<i>P4mm</i>	(Ba _{0.97} La _{0.02}) (Ti O ₃) x=0.01	1.0706	0.8883	1.0716	1.0038	1.0012	0.25	3.9918	0.30
This Work	<i>P4mm</i>	(Pb _{0.22} Ba _{0.66} La _{0.08}) (Ti O ₃) x=0.04	1.0598	1.0102	1.0581	1.0057	1.0007	0.50	3.9461	0.97
This Work	<i>P4mm</i>	(Pb _{0.235} Ba _{0.705} La _{0.04}) (Ti O ₃) x=0.02	1.0598	1.0102	1.0692	1.0122	1.0119	0.03	3.9667	0.85
This Work	<i>P4mm</i>	(Pb _{0.25} Ba _{0.75}) (Ti O ₃) x=0	1.0598	1.0102	1.0680	1.0198	1.0107	0.89	3.9873	0.29
This Work	<i>P4mm</i>	(Pb _{0.455} Ba _{0.455} La _{0.06}) (Ti O ₃) x=0.03	1.0489	1.1866	1.0527	1.0162	1.0108	0.53	3.9217	1.40
This Work	<i>P4mm</i>	(Pb _{0.485} Ba _{0.485} La _{0.02}) (Ti O ₃) x=0.01	1.0489	1.1866	1.0599	1.0232	1.0194	0.37	3.9552	0.81
This Work	<i>P4mm</i>	(Pb _{0.5867} Ba _{0.2933} La _{0.08}) (Ti O ₃) x=0.04	1.0417	1.3406	1.0448	1.0189	1.0140	0.48	3.9237	1.07
This Work	<i>P4mm</i>	(Pb _{0.6067} Ba _{0.3033} La _{0.06}) (Ti O ₃) x=0.03	1.0417	1.3406	1.0485	1.0229	1.0190	0.38	3.9332	0.96
This Work	<i>P4mm</i>	(Pb _{0.6267} Ba _{0.3133} La _{0.04}) (Ti O ₃) x=0.02	1.0417	1.3406	1.0500	1.0239	1.0210	0.29	3.9428	0.78
This Work	<i>P4mm</i>	(Pb _{0.6375} Ba _{0.2125} La _{0.1}) (Ti O ₃) x=0.05	1.0381	1.4296	1.0396	1.0186	1.0137	0.48	3.9098	1.24
This Work	<i>P4mm</i>	(Pb _{0.6467} Ba _{0.3233} La _{0.02}) (Ti O ₃) x=0.01	1.0417	1.3406	1.0560	1.0299	1.0290	0.09	3.9523	0.75
This Work	<i>P4mm</i>	(Pb _{0.66} Ba _{0.22} La _{0.08}) (Ti O ₃) x=0.04	1.0381	1.4296	1.0423	1.0217	1.0176	0.40	3.9192	1.10

This Work	<i>P4mm</i>	(Pb _{0.667} Ba _{0.333}) (Ti O ₃) x=0	1.0417	1.3406	1.0587	1.0400	1.0325	0.72	3.9618	0.60
This Work	<i>P4mm</i>	(Pb _{0.6825} Ba _{0.2275} La _{0.06}) (Ti O ₃) x=0.03	1.0381	1.4296	1.0462	1.0249	1.0232	0.16	3.9286	1.00
This Work	<i>P4mm</i>	(Pb _{0.705} Ba _{0.235} La _{0.04}) (Ti O ₃) x=0.02	1.0381	1.4296	1.0492	1.0275	1.0274	0.01	3.9380	0.87
This Work	<i>P4mm</i>	(Pb _{0.7275} Ba _{0.2425} La _{0.02}) (Ti O ₃) x=0.01	1.0381	1.4296	1.0527	1.0370	1.0325	0.44	3.9473	0.75
This Work	<i>P4mm</i>	(Pb _{0.75} Ba _{0.25}) (Ti O ₃) x=0	1.0381	1.4296	1.0570	1.0456	1.0386	0.66	3.9567	0.67
This Work	<i>P4mm</i>	(Pb _{0.82} La _{0.12}) (Ti O ₃) x=0.06	1.0272	1.7483	1.0341	1.0260	1.0281	0.20	3.8879	1.60
Mean Relative Errors %								0.64		1.13

Table 3

Table 3. Various experimental and calculated tetragonal lattice constants from equations 3, 11, 12 and 13.

ICSD#	Compound	a (Exptl.) (Å)	a (Calc.) (Å)	Error%	c (Exptl.) (Å)	c (Calc.) (Å)	Error%
28621	(Pb _{0.2} Ba _{0.8}) (Ti O ₃)	3.9770	4.0198	1.08	4.0420	4.0500	0.20
54150	(Ba _{0.67} Sr _{0.33}) (Ti O ₃)	3.9724	4.0165	1.11	3.9703	4.0322	1.56
55629	Ce (Ga O ₃)	3.8730	3.8594	0.35	3.8800	3.8869	0.18
55700	Pb ((Zr _{0.45} Ti _{0.55}) O ₃)	4.0260	4.0254	0.01	4.1241	4.1511	0.65
80800	(Sr _{0.9} Bi _{0.1}) (Fe O ₃)	3.8848	3.8595	0.65	3.8735	3.8469	0.69
88534	(Ba _{0.272} Sr _{0.728}) (Zr _{0.403} Ti _{0.597}) O ₃	4.0184	4.0536	0.88	4.0084	4.0563	1.20
90693	Pb (Ti O ₃)	3.9039	3.8998	0.11	4.1348	4.1464	0.28
90694	Pb (Zr _{0.1} Ti _{0.9}) O ₃	3.9272	3.9150	0.31	4.1319	4.1730	1.00
90695	Pb (Zr _{0.2} Ti _{0.8}) O ₃	3.9539	3.9341	0.50	4.1319	4.1920	1.45
90696	Pb (Zr _{0.3} Ti _{0.7}) O ₃	3.9862	3.9556	0.77	4.1331	4.2067	1.78
90697	Pb (Zr _{0.4} Ti _{0.6}) O ₃	4.0081	4.0000	0.20	4.1341	4.1736	0.95
97116	(Pr _{0.6} Ba _{0.4}) Co O ₃	3.8939	3.8358	1.49	3.8189	3.7426	2.00
97117	(Pr _{0.5} Ba _{0.5}) Co O ₃	3.9069	3.8785	0.73	3.8145	3.7676	1.23
97834	(Pb _{0.58} Ca _{0.42}) (Ti O ₃)	3.8800	3.9191	1.01	3.9500	3.9265	0.59
97836	(Pb _{0.61} Ca _{0.39}) (Ti O ₃)	3.8800	3.9114	0.81	3.9700	3.9554	0.37
98057	K _{0.5} Bi _{0.5} (Ti O ₃)	3.9388	4.0351	2.45	3.9613	3.9832	0.55
150085	(Pb _{0.925} La _{0.05}) (Ti O ₃) x=0.025	3.9099	3.9140	0.10	4.0712	4.0816	0.26
150086	(Pb _{0.85} La _{0.1}) (Ti O ₃) x=0.05	3.9139	3.9191	0.13	4.0337	4.0407	0.17
150087	(Pb _{0.775} La _{0.15}) (Ti O ₃) 0.075	3.9207	3.9207	0.00	4.0007	4.0120	0.28
150088	(Pb _{0.7} La _{0.2}) (Ti O ₃) x=0.1	3.9250	3.9243	0.02	3.9720	3.9836	0.29
150089	(Pb _{0.625} La _{0.25}) (Ti O ₃) x=0.125	3.9279	3.9289	0.03	3.9470	3.9574	0.26
152277	Pb (V O ₃)	3.8039	3.7071	2.55	4.6768	4.5604	2.49
153294	(Pb _{0.96} Ce _{0.04}) (Zr _{0.3} Ti _{0.7}) O ₃	3.9810	3.9512	0.75	4.1430	4.2004	1.39

153295	(Pb _{0.96} Nd _{0.04}) (Zr _{0.3} Ti _{0.7}) O ₃	3.9920	3.9534	0.97	4.1120	4.1882	1.85
154107	Nd Ba Co ₂ O ₆	3.8952	3.8791	0.41	3.8104	3.7539	1.48
155328	Pb ((Zr _{0.5} Ti _{0.5}) O ₃)	4.0420	4.0521	0.25	4.1275	4.1266	0.02
155329	Pb ((Zr _{0.5} Ti _{0.5}) O ₃)	4.0494	4.0520	0.06	4.1125	4.1266	0.34
156987	(Pb _{0.97} Cd _{0.03}) (Ti O ₃)	3.8907	3.8815	0.24	4.1524	4.1564	0.10
156988	(Pb _{0.94} Cd _{0.06}) (Ti O ₃)	3.8927	3.8518	1.05	4.1576	4.1899	0.78
157807	(Pb _{0.333} Ba _{0.667}) (Ti O ₃)	3.9430	4.0250	2.08	4.0550	4.0317	0.57
158886	Pr Ba (Mn ₂ O ₆)	3.8921	3.8863	0.15	3.8813	3.9084	0.70
158890	Nd Ba (Mn ₂ O ₆)	3.8893	3.8896	0.01	3.8655	3.8897	0.63
161317	(Ba _{0.985} Na _{0.015}) ((Ti _{0.985} Nb _{0.015}) O ₃)	4.0047	4.0233	0.46	4.0221	4.0462	0.60
161710	(Pb _{0.95} Bi _{0.05}) (Ti O ₃)	3.9050	3.9043	0.02	4.1220	4.1349	0.31
161711	(Pb _{0.9} Bi _{0.1}) (Ti O ₃)	3.9060	3.9097	0.09	4.1080	4.1220	0.34
164352	(Pb _{0.85} La _{0.1}) (Ti O ₃) x=0.05	3.9170	3.9172	0.01	4.0310	4.0446	0.34
164977	(Ba _{0.996} Y _{0.004}) (Ti O ₃)	3.9932	4.0242	0.78	4.0346	4.0368	0.05
165130	Pb ((Fe _{0.012} Ti _{0.988}) O ₃)	3.9212	3.8941	0.69	4.1289	4.1572	0.69
165131	(Pb _{0.7} Sr _{0.3}) ((Fe _{0.012} Ti _{0.988}) O ₃)	3.9298	3.9425	0.32	3.9420	3.9681	0.66
165498	Pb (Ti O ₃)	3.9022	3.8972	0.13	4.1437	4.1518	0.20
166283	Ce (Al O ₃)	3.7676	3.7404	0.72	3.7860	3.7756	0.28
169562	Nd Ba (Co _{1.5} Fe _{0.5}) O ₆	3.9050	3.8713	0.86	3.8305	3.7747	1.46
169563	Nd Ba (Co Fe) O ₆	3.9120	3.8637	1.23	3.8520	3.7954	1.47
169568	Gd Ba (Co Fe) O ₆	3.9030	3.8512	1.33	3.8215	3.7699	1.35
169588	(Bi _{0.69} Pb _{0.31}) ((Fe _{0.69} Ti _{0.31}) O ₃)	3.8122	3.6961	3.05	4.5266	4.3981	2.84
169589	(Bi _{0.6} Pb _{0.4}) ((Fe _{0.6} Ti _{0.4}) O ₃)	3.8301	3.7524	2.03	4.4523	4.2469	4.61
169590	(Bi _{0.5} Pb _{0.5}) ((Fe _{0.5} Ti _{0.5}) O ₃)	3.8506	3.7752	1.96	4.3711	4.2233	3.38
169591	(Bi _{0.4} Pb _{0.6}) ((Fe _{0.4} Ti _{0.6}) O ₃)	3.8628	3.7937	1.79	4.3137	4.2198	2.18
169592	(Bi _{0.3} Pb _{0.7}) ((Fe _{0.3} Ti _{0.7}) O ₃)	3.8789	3.8144	1.66	4.2526	4.2139	0.91
169593	(Bi _{0.2} Pb _{0.8}) ((Fe _{0.2} Ti _{0.8}) O ₃)	3.8889	3.8512	0.97	4.2082	4.1729	0.84

169594	(Bi _{0.1} Pb _{0.9}) ((Fe _{0.1} Ti _{0.9}) O ₃)	3.8962	3.8670	0.75	4.1726	4.1778	0.13
169595	(Bi _{0.7} Pb _{0.3}) ((Fe _{0.7} Ti _{0.3}) O ₃)	3.8118	3.6939	3.09	4.5266	4.4020	2.75
169597	(Bi _{0.71} Pb _{0.29}) ((Fe _{0.71} Ti _{0.29}) O ₃)	3.8117	3.6956	3.05	4.5267	4.3913	2.99
169599	(Bi _{0.72} Pb _{0.28}) ((Fe _{0.72} Ti _{0.28}) O ₃)	3.8116	3.6932	3.11	4.5268	4.3958	2.89
181726	(Bi _{0.85} Nd _{0.15}) (Fe O ₃)	3.9042	3.8131	2.33	3.9503	3.8527	2.47
183213	Pb (Ti O ₃)	3.9009	3.8942	0.17	4.1526	4.1582	0.13
183587	Pb (Zr _{0.3} Ti _{0.7}) O ₃	3.9843	3.9459	0.96	4.1545	4.2273	1.75
184861	Sr (Fe O ₃)	3.8540	3.8624	0.22	3.8690	3.8713	0.06
186228	Ba _{0.9} K _{0.05} Bi _{0.05} (Ti O ₃)	3.9909	4.0239	0.83	4.0321	4.0401	0.20
186229	(Ba _{0.85} K _{0.075} Bi _{0.075}) (Ti O ₃)	3.9861	4.0259	1.00	4.0303	4.0373	0.17
186230	(Ba _{0.8} K _{0.1} Bi _{0.1}) (Ti O ₃)	3.9824	4.0271	1.12	4.0285	4.0356	0.18
186683	(Ba _{0.5} Sr _{0.5}) (Ti _{0.946} Fe _{0.046}) O ₃	3.9576	3.9803	0.57	3.9524	4.0302	1.97
186684	(Ba _{0.5} Sr _{0.5}) (Ti _{0.876} Fe _{0.081}) O ₃	3.9596	3.9418	0.45	3.9575	3.9887	0.79
186685	(Ba _{0.5} Sr _{0.5}) (Ti _{0.849} Fe _{0.139}) O ₃	3.9610	3.9663	0.13	3.9586	3.9638	0.13
186686	(Ba _{0.5} Sr _{0.5}) (Ti _{0.806} Fe _{0.183}) O ₃	3.9620	3.9361	0.65	3.9590	3.9277	0.79
186687	(Ba _{0.5} Sr _{0.5}) (Ti _{0.624} Fe _{0.402}) O ₃	3.9722	3.9947	0.56	3.9701	4.0051	0.88
187081	(Ba _{0.91} Ca _{0.11}) (Ti O ₃)	4.0003	4.0254	0.63	4.0169	4.0315	0.36
187471	Pb (Zr _{0.4} Ti _{0.6}) O ₃	4.0041	3.9981	0.15	4.1460	4.1776	0.76
187472	(Pb _{0.9} Ba _{0.1}) ((Zr _{0.40} Ti _{0.60}) O ₃)	4.0128	4.0244	0.29	4.1297	4.1526	0.55
187472	(Pb _{0.9} Ba _{0.1}) ((Zr _{0.40} Ti _{0.60}) O ₃)	4.0128	4.0244	0.29	4.1297	4.1526	0.55
187473	(Pb _{0.8} Ba _{0.2}) ((Zr _{0.40} Ti _{0.60}) O ₃)	4.0306	4.0372	0.16	4.1210	4.1541	0.80
187473	(Pb _{0.8} Ba _{0.2}) ((Zr _{0.40} Ti _{0.60}) O ₃)	4.0306	4.0372	0.16	4.1210	4.1541	0.80
187474	(Pb _{0.7} Ba _{0.3}) ((Zr _{0.40} Ti _{0.60}) O ₃)	4.0389	4.0622	0.58	4.1025	4.1290	0.65
187474	(Pb _{0.7} Ba _{0.3}) ((Zr _{0.40} Ti _{0.60}) O ₃)	4.0389	4.0622	0.58	4.1025	4.1290	0.65
187475	(Pb _{0.6} Ba _{0.4}) ((Zr _{0.40} Ti _{0.60}) O ₃)	4.0493	4.0815	0.80	4.0879	4.1134	0.62
187475	(Pb _{0.6} Ba _{0.4}) ((Zr _{0.40} Ti _{0.60}) O ₃)	4.0493	4.0815	0.80	4.0879	4.1134	0.62
187635	Pb (V O ₃)	3.8091	3.7117	2.56	4.6508	4.5490	2.19

188645	(Ba _{0.9} Sm _{0.067}) (Ti O ₃)	3.9953	4.0119	0.42	4.0114	4.0085	0.07
188784	(Ba _{0.95} Sr _{0.05}) (Ti O ₃)	3.9890	4.0259	0.93	4.0260	4.0368	0.27
188785	(Ba _{0.9} Sr _{0.1}) (Ti O ₃)	3.9850	4.0269	1.05	4.0170	4.0365	0.49
188786	(Ba _{0.85} Sr _{0.15}) (Ti O ₃)	3.9800	4.0277	1.20	4.0070	4.0338	0.67
188985	(Bi _{0.6} Sr _{0.4}) (Mn O ₃)	3.9151	3.8849	0.77	3.8158	3.8122	0.10
188986	(Bi _{0.55} Sr _{0.45}) (Mn O ₃)	3.9107	3.8938	0.43	3.7908	3.7933	0.06
188987	(Bi _{0.5} Sr _{0.5}) (Mn O ₃)	3.9017	3.8993	0.06	3.7869	3.7811	0.15
188988	(Bi _{0.45} Sr _{0.55}) (Mn O ₃)	3.8952	3.9004	0.13	3.7928	3.7773	0.41
189052	Pr Ba Co ₂ O ₆	3.8870	3.8839	0.08	3.8275	3.7570	1.84
189232	Sm Ba (Co _{1.2} Fe _{0.8}) O ₆	3.9060	3.8525	1.37	3.8145	3.7666	1.26
189382	(Ba _{0.96} La _{0.027}) (Ti O ₃) x=0.0135	3.9953	4.0317	0.91	4.0073	4.0249	0.44
191123	Pb ((Zr _{0.52} Ti _{0.48}) O ₃)	4.0429	4.0693	0.65	4.1318	4.1035	0.68
191126	Pb ((Zr _{0.52} Ti _{0.48}) O ₃)	4.0663	4.0623	0.10	4.1001	4.1177	0.43
192240	(Bi _{0.6} Ca _{0.4}) (Fe O ₃)	3.9207	3.8618	1.50	3.9173	3.8745	1.09
192241	(Bi _{0.5} Ca _{0.5}) (Fe O ₃)	3.9086	3.8571	1.32	3.8973	3.8497	1.22
192848	(Bi _{0.6} Pb _{0.4}) ((Fe _{0.6} Ti _{0.4}) O ₃)	3.8585	3.7304	3.32	4.4573	4.2972	3.59
192849	(Bi _{0.57} La _{0.03} Pb _{0.4}) ((Fe _{0.6} Ti _{0.4}) O ₃)	3.8502	3.7622	2.29	4.3538	4.2165	3.15
193390	(Bi _{0.465} Na _{0.465} Ba _{0.07}) (Ti O ₃)	3.9025	3.9302	0.71	3.9048	3.9231	0.47
237599	(Bi _{0.9} Sm _{0.1}) (Fe _{0.5} Co _{0.5}) O ₃	3.7432	3.5926	4.02	4.7207	4.4739	5.23
240256	Pb V O ₃	3.8001	3.7127	2.30	4.6703	4.5467	2.65
245945	Ba (Ti O ₃)	3.9961	4.0238	0.69	4.0290	4.0366	0.19
247691	(Bi _{0.8} La _{0.2}) (Fe _{0.9} Ti _{0.1}) O ₃	3.9304	3.8206	2.79	3.9702	3.8674	2.59
247692	(Bi _{0.8} La _{0.2}) (Fe _{0.85} Ti _{0.15}) O ₃	3.9355	3.8306	2.67	3.9477	3.8425	2.66
247747	(La _{0.21} Pb _{0.79}) (Fe _{0.18} Ti _{0.82}) O ₃	3.9283	3.9302	0.05	3.9899	4.0330	1.08
247748	(La _{0.12} Pb _{0.88}) (Fe _{0.10} Ti _{0.90}) O ₃	3.9115	3.9095	0.05	4.0675	4.0979	0.75
247782	Pb (Zr _{0.35} Ti _{0.65}) O ₃	3.9979	3.9634	0.86	4.1557	4.2204	1.56
248396	(Ba _{0.96} Nd _{0.04}) Ti O ₃ x=0.02	3.9889	4.0352	1.16	4.0098	4.0195	0.24

249001	(Ce _{0.016} Sr _{0.984}) (Fe O ₃)	3.8642	3.8681	0.10	3.8544	3.8724	0.47
290401	(Bi _{0.65} Pb _{0.35}) (Fe _{0.65} Ti _{0.35}) O ₃	3.9468	3.8275	3.02	4.1011	4.0023	2.41
290951	(Bi _{0.8} Ba _{0.2}) (Fe _{0.97} Co _{0.03}) O ₃	3.9700	3.8551	2.89	4.0400	3.9479	2.28
291165	(Pb _{0.05} Ba _{0.95}) (Ti O ₃)	3.9890	4.0218	0.82	4.0380	4.0390	0.03
Ganguly ³	(Ba _{0.9} La _{0.066667}) (Ti O ₃) x=0.033333	3.9950	4.0280	0.83	3.9950	4.0102	0.38
Ganguly ³	(Ba _{0.94} La _{0.04}) (Ti O ₃) x=0.02	3.9986	4.0274	0.72	3.9986	4.0186	0.50
Ganguly ³	(Ba _{0.96} La _{0.0267}) (Ti O ₃) x=0.013333	3.9953	4.0280	0.82	4.0073	4.0211	0.34
This Work	Ba (Ti O ₃) x=0	3.9957	4.0250	0.73	4.0256	4.0342	0.21
This Work	(Ba _{0.88} La _{0.08}) (Ti O ₃) x=0.04	3.9940	4.0274	0.84	3.9947	4.0076	0.32
This Work	(Ba _{0.91} La _{0.06}) (Ti O ₃) x=0.03	3.9906	4.0368	1.16	3.9750	3.9945	0.49
This Work	(Ba _{0.94} La _{0.04}) (Ti O ₃) x=0.02	3.9985	4.0266	0.70	4.0016	4.0203	0.47
This Work	(Ba _{0.97} La _{0.02}) (Ti O ₃) x=0.01	3.9990	4.0246	0.64	4.0140	4.0296	0.39
This Work	(Pb _{0.22} Ba _{0.66} La _{0.08}) (Ti O ₃) x=0.04	3.9774	4.0145	0.93	4.0001	4.0173	0.43
This Work	(Pb _{0.235} Ba _{0.705} La _{0.04}) (Ti O ₃) x=0.02	3.9844	4.0063	0.55	4.0332	4.0541	0.52
This Work	(Pb _{0.25} Ba _{0.75}) (Ti O ₃) x=0	3.9729	4.0148	1.06	4.0516	4.0579	0.16
This Work	(Pb _{0.455} Ba _{0.455} La _{0.06}) (Ti O ₃) x=0.03	3.9560	3.9842	0.71	4.0202	4.0274	0.18
This Work	(Pb _{0.485} Ba _{0.485} La _{0.02}) (Ti O ₃) x=0.01	3.9571	3.9868	0.75	4.0489	4.0642	0.38
This Work	(Pb _{0.5867} Ba _{0.2933} La _{0.08}) (Ti O ₃) x=0.04	3.9416	3.9729	0.79	4.0161	4.0286	0.31
This Work	(Pb _{0.6067} Ba _{0.3033} La _{0.06}) (Ti O ₃) x=0.03	3.9416	3.9707	0.74	4.0319	4.0460	0.35
This Work	(Pb _{0.6267} Ba _{0.3133} La _{0.04}) (Ti O ₃) x=0.02	3.9424	3.9725	0.76	4.0366	4.0558	0.47
This Work	(Pb _{0.6375} Ba _{0.2125} La _{0.1}) (Ti O ₃) x=0.05	3.9346	3.9628	0.72	4.0078	4.0171	0.23
This Work	(Pb _{0.6467} Ba _{0.3233} La _{0.02}) (Ti O ₃) x=0.01	3.9431	3.9668	0.60	4.0609	4.0817	0.51

This Work	(Pb _{0.66} Ba _{0.22} La _{0.08}) (Ti O ₃) x=0.04	3.9344	3.9618	0.69	4.0199	4.0316	0.29
This Work	(Pb _{0.667} Ba _{0.333}) (Ti O ₃) x=0	3.9340	3.9669	0.84	4.0914	4.0960	0.11
This Work	(Pb _{0.6825} Ba _{0.2275} La _{0.06}) (Ti O ₃) x=0.03	3.9359	3.9588	0.58	4.0337	4.0506	0.42
This Work	(Pb _{0.705} Ba _{0.235} La _{0.04}) (Ti O ₃) x=0.02	3.9367	3.9577	0.54	4.0449	4.0663	0.53
This Work	(Pb _{0.7275} Ba _{0.2425} La _{0.02}) (Ti O ₃) x=0.01	3.9295	3.9559	0.67	4.0748	4.0843	0.23
This Work	(Pb _{0.75} Ba _{0.25}) (Ti O ₃) x=0	3.9247	3.9529	0.72	4.1035	4.1055	0.05
This Work	(Pb _{0.82} La _{0.12}) (Ti O ₃) x=0.06	3.9174	3.9193	0.05	4.0194	4.0296	0.25
Mean Relative Errors %				0.92			0.92

Table 4. Tetragonalities and polarizations of 43 $P4mm$ tetragonal perovskites.

ICSD#	Data Type	Compound	c/a Exptl.	c/a Calc.	Error%	Polarizaiton, $\mu\text{C}/\text{cm}^2$ Exptl.	Polarizaiton, $\mu\text{C}/\text{cm}^2$ Calc.	Error%
183213	Neutron	PbTiO ₃	1.0645	1.0692	0.44	60.6395	59.3921	2.06
164352	Neutron	Pb _{0.85} La _{0.1} TiO ₃	1.0291	1.0337	0.44	39.8023	37.5841	5.57
165498	Neutron	PbTiO ₃	1.0619	1.0668	0.46	60.3676	58.2479	3.51
73644	Neutron	BaTiO ₃	1.0111	1.0095	0.15	18.1446	18.1824	0.21
185407	Neutron	Ba (Ti O ₃)	1.0098	1.0099	0.00	16.8794	16.5401	2.01
71368	Neutron	(Ba _{0.88} Ca _{0.12}) (Ti O ₃)	1.0097	1.0060	0.37	21.9164	16.3317	25.48
280137	Neutron	Pb ((Hf _{0.4} Ti _{0.6}) O ₃)	1.0219	1.0984	7.48	24.6827	30.7691	24.66
90472	Neutron	Pb (Zr _{0.2} Ti _{0.8}) O ₃	1.0496	1.0892	3.78	50.3498	52.0693	3.41
90473	Neutron	Pb (Zr _{0.3} Ti _{0.7}) O ₃	1.0429	1.0997	5.45	48.6938	48.0465	1.33
90474	Neutron	Pb (Zr _{0.4} Ti _{0.6}) O ₃	1.0363	1.1109	7.20	37.1466	43.4206	16.89
90475	Neutron	Pb (Zr _{0.5} Ti _{0.5}) O ₃	1.0284	1.1174	8.66	36.3525	36.9834	1.74
90478	Neutron	Pb (Zr _{0.52} Ti _{0.48}) O ₃	1.0135	1.1223	10.74	27.4355	21.2328	22.61
93451	Neutron	Pb (Hf _{0.2} Ti _{0.8}) O ₃	1.0414	0.9752	6.36	55.9190	47.0687	15.83
98057	Neutron	K _{0.5} Bi _{0.5} (Ti O ₃)	1.0057	0.9886	1.70	20.6315	10.7519	47.89
152424	Neutron	Pb (Hf _{0.1} Ti _{0.9}) O ₃	1.0524	1.0717	1.83	53.0715	53.6450	1.08
152426	Neutron	Pb (Hf _{0.2} Ti _{0.8}) O ₃	1.0440	1.0786	3.32	52.5066	48.7158	7.22
152428	Neutron	Pb (Hf _{0.3} Ti _{0.7}) O ₃	1.0357	1.0860	4.86	47.1210	42.9511	8.85
152430	Neutron	Pb (Hf _{0.4} Ti _{0.6}) O ₃	1.0287	1.0946	6.41	29.1294	37.2108	27.74
156987	Neutron	(Pb _{0.97} Cd _{0.03}) (Ti O ₃)	1.0673	1.0720	0.44	57.4231	60.5267	5.40
156988	Neutron	(Pb _{0.94} Cd _{0.06}) (Ti O ₃)	1.0681	1.0887	1.93	56.5607	60.8432	7.57
187081	Neutron	(Ba _{0.91} Ca _{0.11}) (Ti O ₃)	1.0041	1.0092	0.50	8.0088	8.4251	5.20
152277	Neutron	Pb (V O ₃)	1.2295	1.1837	3.72	100.6168	100.9659	0.35
187635	Neutron	Pb (V O ₃)	1.2210	1.1791	3.43	100.2324	99.7261	0.51

169589	Neutron	(Bi _{0.6} Pb _{0.4}) ((Fe _{0.6} Ti _{0.4}) O ₃)	1.1624	1.1623	0.01	86.8166	87.3904	0.66
169590	Neutron	(Bi _{0.5} Pb _{0.5}) ((Fe _{0.5} Ti _{0.5}) O ₃)	1.1352	1.1407	0.49	80.4405	80.4774	0.05
169591	Neutron	(Bi _{0.4} Pb _{0.6}) ((Fe _{0.4} Ti _{0.6}) O ₃)	1.1167	1.1218	0.45	76.9254	75.7234	1.56
169592	Neutron	(Bi _{0.3} Pb _{0.7}) ((Fe _{0.3} Ti _{0.7}) O ₃)	1.0963	1.1054	0.82	70.2720	70.2110	0.09
169593	Neutron	(Bi _{0.2} Pb _{0.8}) ((Fe _{0.2} Ti _{0.8}) O ₃)	1.0821	1.0907	0.80	66.3100	65.8954	0.63
169594	Neutron	(Bi _{0.1} Pb _{0.9}) ((Fe _{0.1} Ti _{0.9}) O ₃)	1.0709	1.0777	0.63	62.4753	61.9738	0.80
188784	Neutron	(Ba _{0.95} Sr _{0.05}) (Ti O ₃)	1.0093	1.0085	0.08	8.8597	15.7734	78.04
188785	Neutron	(Ba _{0.9} Sr _{0.1}) (Ti O ₃)	1.0080	1.0070	0.10	8.6757	14.0620	62.08
188786	Neutron	(Ba _{0.85} Sr _{0.15}) (Ti O ₃)	1.0068	1.0052	0.16	12.7429	12.3027	3.45
245945	Synchrotron	BaTiO ₃	1.0082	1.0105	0.22	6.4205	14.3440	123.41
150086	XRD	(Pb _{0.85} La _{0.1}) (Ti O ₃)	1.0306	1.0322	0.15	48.0853	38.8828	19.14
90693	XRD	PbTiO ₃	1.0591	1.0646	0.52	63.8469	56.9976	10.73
189383	XRD	(Ba _{0.94} La _{0.04}) (Ti O ₃)	1.0000	1.0047	0.47	0.0000	-	0.00
189384	XRD	(Ba _{0.9} La _{0.067}) (Ti O ₃)	1.0000	1.0023	0.23	0.0000	-	0.00
161710	XRD	(Pb _{0.95} Bi _{0.05}) (Ti O ₃)	1.0556	1.0604	0.46	63.0335	55.2667	12.32
161711	XRD	(Pb _{0.9} Bi _{0.1}) (Ti O ₃)	1.0517	1.0556	0.37	67.4114	53.2604	20.99
150087	XRD	(Pb _{0.775} La _{0.15}) (Ti O ₃)	1.0204	1.0243	0.39	40.9570	29.1703	28.78
150088	XRD	(Pb _{0.7} La _{0.2}) (Ti O ₃)	1.0120	1.0161	0.41	37.1237	19.3274	47.94
150089	XRD	(Pb _{0.625} La _{0.25}) (Ti O ₃)	1.0049	1.0082	0.33	25.8963	9.4963	63.33
150085	XRD	Pb _{0.925} La _{0.05} TiO ₃	1.0413	1.0441	0.27	53.1718	46.9430	11.71

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9