

PREDICTION OF THE UNIT CELL PARAMETERS IN MONOCLINIC $A_2BB'O_6$ PEROVSKITES BY MULTIPLE LINEAR REGRESSION AND ARTIFICIAL NEURAL NETWORKS

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Abstract: The unit cell edges (a , b , c), as well as, the volume (V) of the isomorphous series of complex perovskites of $A_2BB'O_6$ type, were expressed as a function of the ionic radii of the constituents and the oxidation state of the B-cation. For this purpose two methods for modeling were used: multiple linear regression and feed-forward artificial neural networks. In both analyses 76 compounds were included divided in two sets: calibration set (65) and test set (11). The agreement between the actual and predicted values for the dependent variables, obtained by both methods, is excellent. It could be concluded that these models can be used for prediction of the unit cell parameters of new members of this series.

Keywords: monoclinic perovskites, structural predictions, artificial neural networks, multiple linear regression.

1. INTRODUCTION

The perovskites form a large family of isotypic compounds with general formula ABX_3 (A, B – cations, X – anion). These compounds are subject of different investigations because of their interesting physical properties [1–3], that consider them as one of the most important technical materials.

Although the anion X in the perovskite structure could be O, S, H, N, CN or halogen, the most extensively studied are oxygen containing one. As a result of extensive study of oxygen containing perovskites, this group is enlarged with different series of compounds with general formulas: $(A'_x A''_{1-x})BO_3$, $A(B'_x B''_{1-x})O_3$, $(A'_{1-x} A''_x)BO_3$, $(A'_x A''_{1-x})(B'_x B''_{1-x})O_3$ etc. [1–3].

The ideal perovskite structure is composed of a three-dimensional framework of corner-sharing BX_6 octahedra. This framework forms cube-octahedral cavities which are filled with A-site cations. As a result, in the ideal perovskite structure, A-cation is surrounded with twelve equidistant oxygen atoms, thus having coordination number twelve. This kind of crystal structure was firstly ascribed to $CaTiO_3$ (perovskite), and was assumed that it has cubic structure ($Pm\bar{3}m$) [1]. Further refinement of the crystal structure of $CaTiO_3$ revealed its real structure as orthorhombic [4]. The deviation from the cubic structure is a result of the mismatch in the size of the cube-octahedral cavity and the size of the ionic radii of the Ca^{2+} ion. Namely, the ionic radii of the Ca^{2+} ion is too small for the cavities formed by the corner shearing TiO_6 octahedra, thus resulting in their tilting and reduction of symmetry from space group $Pm\bar{3}m$ to $Pnma$. Also, because of the tilting, the coordination number of Ca^{2+} ions is reduced to eight. Now it is known that different perovskites, at room temperature, can adopt different crystal structures (monoclinic, tetrahedral, hexagonal, rhombohedral), depending on the composition, the degree of tilting, etc. [1–3].

In each series of perovskites there is a large number of compounds, so having structural data available, one may try to systematize and analyze them in order to get some structural information for compounds whose structures have either not been determined so far or whose reliability is for some reason questionable. Therefore, numerous attempts have been made to correlate the structural parameters with physical variables of the constituents, that have influence on the structure [5–10].

In our previous work on structural correlations in isomorphous series, it was shown that multiple linear regression can be used to predict unit cell parameters, as well as, the whole crystal structure [11–16]. Recently, we have tried to make similar predictions in some series of perovskites by multiple linear regression and also by artificial neural networks [17, 18].

Relating to our previous work on cubic complex perovskites with $A_2BB'O_6$ formula [18], we now focus our attention on the perovskites with the same general formula but of monoclinic structure. So, here we present a simple model for prediction of the unit cell parameters and volumes of monoclinic $A_2BB'O_6$ perovskites by feed-forward neural networks (FF-ANN) and multiple linear regression (MLR).

2. DATA ANALYSIS

In this investigation 76 monoclinic compounds with general formula $A_2BB'O_6$ were included. These perovskites are usually described using non-standard setting $P2_1/n$, with in-phase tilt along c -axis. Particularity of these perovskites is different tilt angles of BO_6 and $B'O_6$ octahedra as a result of differences in size and distortion of the polyhedra [2].

The investigated compounds have divalent cation in the A-position, and two different cations in B-position. There are several possible combinations of the oxidation states of the B-cations: $A_2B^{2+}B'^{6+}O_6$, $A_2B^{3+}B'^{5+}O_6$, $A_2B^{4+}B'^{4+}O_6$ [1, 2].

The dependent variables in the analysis were the lattice parameters. Although the monoclinic unit cell is specified with 4 parameters (three cell lengths a , b , c and β angle), the angle has not been taken into consideration as a dependent variable. The numerical values for the β angles differ slightly through the series (maximal value for β is 90.335° and the minimal one is 89.802°). Therefore, the angle may be considered as a parameter which is rather insensitive to the variation of the constituent radii. Nevertheless, in order to obtain more predictable structural information, another dependent variable was included in the analysis, namely the unit cell volume.

At the beginning, only the ionic radii of the cations (A, B and B') were taken into account, as independent variables. The values for the effective ionic radii were taken from Shanon [19] for the corresponding coordination number and oxidation state of the ions. As was mentioned, due to the tilting of the BO_6 octahedra, the coordination number of A-cations is eight. The B-cations were treated as six coordinated and in their high spin state for transition metal ions.

The B-cations in these perovskites might be in different oxidation states, so an attempt was made to include the oxidation number of one of the B-cations as an independent variable. Since the sum of the oxidation numbers of the B ions is eight, only the oxidation number (z) of one of the B ions was taken into account e.g. that of lower oxidation state. This variable was shown to be statistically significant. However, enlarging the model with some other independent variables, for instance the electronegativities of B-ions, has not improved the proposed model, and the variables were shown to be insignificant.

The data, both for dependent and independent variables, taken from the literature, [20–37] are listed in Table 1.

As pointed out earlier, two methods for modeling were used: multiple linear regression and feed-forward neural networks. To validate the performances of the model the data were randomly divided in two sets: calibration set (65 compounds) and test set (11 compounds).

Tab. 1: The data for dependent and independent variables used throughout the analyses.

Formula	$r(A)/\text{Å}$	$r(B)/\text{Å}$	$r(B')/\text{Å}$	$z(B)$	$a/\text{Å}$	$b/\text{Å}$	$c/\text{Å}$	$V/\text{Å}^3$	Ref.
<i>Calibration set</i>									
$\text{Ca}_2(\text{CoTe})\text{O}_6$	1.12	0.745	0.56	2	5.4569	5.5904	7.7399	236.11	20
$\text{Ca}_2(\text{MgW})\text{O}_6$	1.12	0.72	0.6	2	5.4243	5.54786	7.7205	232.33	21
$\text{Ca}_2(\text{MnW})\text{O}_6$	1.12	0.83	0.6	2	5.4694	5.6504	7.8122	241.43	22
$\text{Sr}_2(\text{CaMo})\text{O}_6$	1.26	1	0.59	2	5.76151	5.84449	8.18437	275.59	21
$\text{Sr}_2(\text{CaW})\text{O}_6$	1.26	1	0.6	2	5.76861	5.85008	8.19467	276.54	21
$\text{Sr}_2(\text{FeW})\text{O}_6$	1.26	0.78	0.6	2	5.65	5.61	7.94	251.67	23
$\text{Sr}_2(\text{MnRe})\text{O}_6$	1.26	0.83	0.55	2	5.66798	5.64506	7.99	255.65	24
$\text{Sr}_2(\text{MnTe})\text{O}_6$	1.26	0.83	0.56	2	5.7009	5.677	8.0334	259.99	25
$\text{Sr}_2(\text{MnW})\text{O}_6$	1.26	0.83	0.6	2	5.6803	5.6723	8.0199	258.40	22
$\text{Ba}_2(\text{DyIr})\text{O}_6$	1.42	0.912	0.57	3	5.9245	5.9186	8.3653	293.33	26
$\text{Ba}_2(\text{DyRe})\text{O}_6$	1.42	0.912	0.58	3	5.934	5.933	8.391	295.42	27
$\text{Ba}_2(\text{ErRe})\text{O}_6$	1.42	0.89	0.58	3	5.9118	5.9126	8.3701	292.57	27
$\text{Ba}_2(\text{EuIr})\text{O}_6$	1.42	0.947	0.57	3	5.9615	5.9588	8.4231	299.22	26
$\text{Ba}_2(\text{EuRe})\text{O}_6$	1.42	0.947	0.58	3	5.9756	5.9737	8.4685	302.29	27
$\text{Ba}_2(\text{EuTa})\text{O}_6$	1.42	0.947	0.64	3	6.0191	6.0152	8.4964	307.62	28
$\text{Ba}_2(\text{GdIr})\text{O}_6$	1.42	0.938	0.57	3	5.90504	5.9467	8.4108	295.35	26
$\text{Ba}_2(\text{GdRe})\text{O}_6$	1.42	0.938	0.58	3	5.9602	5.9638	8.4329	299.75	27
$\text{Ba}_2(\text{HoIr})\text{O}_6$	1.42	0.901	0.57	3	5.9319	5.9048	8.3501	292.48	26
$\text{Ba}_2(\text{HoRe})\text{O}_6$	1.42	0.901	0.58	3	5.921	5.921	8.3748	293.60	27
$\text{Ba}_2(\text{LaIr})\text{O}_6$	1.42	1.032	0.57	3	6.051	6.0603	8.5737	314.40	26
$\text{Ba}_2(\text{LaTa})\text{O}_6$	1.42	1.032	0.64	3	6.1453	6.0946	8.6091	322.43	28
$\text{Ba}_2(\text{LuIr})\text{O}_6$	1.42	0.861	0.57	3	5.8689	5.8608	8.2885	285.09	26
$\text{Ba}_2(\text{LuRe})\text{O}_6$	1.42	0.861	0.58	3	5.88	5.88	8.3171	287.56	27
$\text{Ba}_2(\text{NdRe})\text{O}_6$	1.42	0.983	0.58	3	6.0064	6.0067	8.5229	307.49	27
$\text{Ba}_2(\text{NdTa})\text{O}_6$	1.42	0.983	0.64	3	6.0808	6.0476	8.5425	314.14	28
$\text{Ba}_2(\text{PrTa})\text{O}_6$	1.42	0.99	0.64	3	6.0919	6.0561	8.5545	315.60	28
$\text{Ba}_2(\text{SmIr})\text{O}_6$	1.42	0.958	0.57	3	5.9731	5.9718	8.4468	301.30	26
$\text{Ba}_2(\text{SmRe})\text{O}_6$	1.42	0.958	0.58	3	5.9847	5.9868	8.4685	303.42	27
$\text{Ba}_2(\text{SmTa})\text{O}_6$	1.42	0.958	0.64	3	6.0468	6.0225	8.5107	309.93	28
$\text{Ba}_2(\text{TbRe})\text{O}_6$	1.42	0.923	0.58	3	5.944	5.946	8.4075	297.15	27
$\text{Ba}_2(\text{TbTa})\text{O}_6$	1.42	0.923	0.64	3	5.993	5.993	8.4651	304.03	28
$\text{Ba}_2(\text{TmIr})\text{O}_6$	1.42	0.88	0.57	3	5.8916	5.8799	8.3148	288.04	26
$\text{Ba}_2(\text{TmRe})\text{O}_6$	1.42	0.88	0.58	3	5.898	5.898	8.3417	290.18	27
$\text{Ba}_2(\text{YRe})\text{O}_6$	1.42	0.9	0.58	3	5.9205	5.9202	8.375	293.55	27
$\text{Ba}_2(\text{YbIr})\text{O}_6$	1.42	0.868	0.57	3	5.8793	5.8682	8.301	286.39	26
$\text{Ca}_2(\text{CrNb})\text{O}_6$	1.12	0.615	0.64	3	5.4195	5.4907	7.7073	229.34	29
$\text{Ca}_2(\text{CrTa})\text{O}_6$	1.12	0.615	0.64	3	5.4287	5.50201	7.72254	230.66	30
$\text{Ca}_2(\text{CrW})\text{O}_6$	1.12	0.615	0.62	3	5.39	5.45	7.66	225.02	23
$\text{Ca}_2(\text{FeMo})\text{O}_6$	1.12	0.645	0.61	3	5.41	5.52	7.71	230.24	23
$\text{Ca}_2(\text{FeNb})\text{O}_6$	1.12	0.645	0.64	3	5.448	5.5517	7.7612	234.74	31
$\text{Ca}_2(\text{FeRe})\text{O}_6$	1.12	0.645	0.58	3	5.4	5.52	7.68	228.92	23
$\text{Ca}_2(\text{GaTa})\text{O}_6$	1.12	0.62	0.64	3	5.43228	5.51024	7.72365	231.19	30
$\text{Ca}_2(\text{InTa})\text{O}_6$	1.12	0.8	0.64	3	5.52884	5.70805	7.92248	250.02	30

Ca ₂ (ScNb)O ₆	1.12	0.745	0.64	3	5.51222	5.63333	7.8688	244.34	30
Ca ₂ (YNb)O ₆	1.12	0.9	0.64	3	5.58148	5.80933	8.05178	261.08	30
Sr ₂ (DySb)O ₆	1.26	0.912	0.6	3	5.8224	5.8538	8.2507	281.21	32
Sr ₂ (DyTa)O ₆	1.26	0.912	0.64	3	5.8209	5.8793	8.2624	282.76	33
Sr ₂ (EuTa)O ₆	1.26	0.947	0.64	3	5.845	5.9284	8.3106	287.97	33
Sr ₂ (FeSb)O ₆	1.26	0.645	0.6	3	5.6135	5.5933	7.8956	247.91	30
Sr ₂ (GdTa)O ₆	1.26	0.938	0.64	3	5.838	5.9165	8.2989	286.65	33
Sr ₂ (HoRu)O ₆	1.26	0.901	0.565	3	5.771	5.7801	8.164	272.32	34
Sr ₂ (HoSb)O ₆	1.26	0.901	0.6	3	5.8141	5.84	8.2361	279.65	32
Sr ₂ (HoTa)O ₆	1.26	0.901	0.64	3	5.8123	5.8664	8.2479	281.23	33
Sr ₂ (InNb)O ₆	1.26	0.8	0.64	3	5.73273	5.73838	8.107	266.69	30
Sr ₂ (InTa)O ₆	1.26	0.8	0.64	3	5.73307	5.74041	8.10826	266.84	30
Sr ₂ (LuTa)O ₆	1.26	0.861	0.64	3	5.7862	5.8152	8.1972	275.82	33
Sr ₂ (NdTa)O ₆	1.26	0.983	0.64	3	5.8656	5.9797	8.3587	293.17	33
Sr ₂ (ScSb)O ₆	1.26	0.745	0.6	3	5.6945	5.6784	8.024	259.46	30
Sr ₂ (SmTa)O ₆	1.26	0.958	0.64	3	5.8528	5.9425	8.3254	289.56	33
Sr ₂ (TmRu)O ₆	1.26	0.88	0.565	3	5.7553	5.7542	8.1332	269.35	35
Sr ₂ (TmTa)O ₆	1.26	0.88	0.64	3	5.7982	5.835	8.2182	278.04	33
Sr ₂ (YSb)O ₆	1.26	0.9	0.6	3	5.8119	5.8382	8.2387	279.55	36
Sr ₂ (YbNb)O ₆	1.26	0.868	0.64	3	5.79095	5.8221	8.20358	276.59	37
Sr ₂ (YbTa)O ₆	1.26	0.868	0.64	3	5.7901	5.825	8.2054	276.74	33
Ba ₂ (CeIr)O ₆	1.42	0.87	0.625	4	5.9663	5.9567	8.4266	299.48	26
<i>Test set</i>									
Sr ₂ (CoTe)O ₆	1.26	0.745	0.56	2	5.6417	5.6063	7.9234	250.61	20
Ba ₂ (ErIr)O ₆	1.42	0.89	0.57	3	5.8988	5.8899	8.3319	289.48	26
Ba ₂ (GdTa)O ₆	1.42	0.938	0.64	3	6.015	6.013	8.4852	306.89	28
Ba ₂ (NdIr)O ₆	1.42	0.983	0.57	3	6.0008	5.9999	8.4843	305.47	26
Ba ₂ (TbIr)O ₆	1.42	0.923	0.57	3	5.9319	5.9227	8.3866	294.65	26
Ba ₂ (YbRe)O ₆	1.42	0.868	0.58	3	5.89	5.89	8.3	287.94	27
Ca ₂ (FeTa)O ₆	1.12	0.645	0.64	3	5.4498	5.5482	7.7591	234.61	31
Sr ₂ (ErTa)O ₆	1.26	0.89	0.64	3	5.8054	5.8528	8.2346	279.79	33
Sr ₂ (InSb)O ₆	1.26	0.8	0.6	3	5.7301	5.7306	8.0963	265.86	36
Sr ₂ (TbTa)O ₆	1.26	0.923	0.64	3	5.8291	5.8934	8.2773	284.35	33
Ba ₂ (PrIr)O ₆	1.42	0.85	0.625	4	5.9443	5.9379	8.3984	296.44	26

The multiple linear regression was performed using the program package *Statgraphics Plus Ver. 3.0* [38]. The unit cell parameters were expressed as a linear function of four independent variables (radii of the constituents and the oxidation number of B-ions):

$$(1) \quad p = q + s \cdot r(A)/\text{\AA} + t \cdot r(B)/\text{\AA} + u \cdot r(B')/\text{\AA} + w \cdot z(B)$$

where: p – designation for the numerical value of depended variable; q – intercept of the regression surface; s , t , u and w – slopes of the regression surface with respect to each variable.

In aim to check proposed relationship and also to find even better model capable of modeling some nonlinearities, artificial neural networks were applied. The ANNs have been proven as efficient tool for analysis of chemical data [39]. Until now they have been widely used for modeling [17, 18] as well as for classification purposes [39].

In this work three layered feed-forward ANN with sigmoid transfer function in the hidden layer and linear transfer function in the output layer was used. The optimal network architecture was searched by changing the number of neurons in the hidden

layer. The number of input neurons was 4, while the number of output neurons was determined of the number of dependent variables which in this case is 4.

The ANNs were created and optimized by implementation of Matlab programming package [40]. The weights and biases were initialized by Nguyen-Widrow algorithm. The networks were trained using Levenberg-Marquardt algorithm for back-propagation of error. The generalization performances of the networks during the training were controlled by use of early stopping procedure which was also implemented in our previous work [17, 18].

3. RESULTS AND DISCUSSION

The regression equations obtained taking into account the calibration set, as well as, the coefficients of determination R_{adj}^2 are given below.

$$\begin{aligned}
 (2) \quad a/\text{\AA} &= 3.00393 + 1.14778 \cdot r(A)/\text{\AA} + 0.767592 \cdot r(B)/\text{\AA} + \\
 &\quad 0.87165 \cdot r(B')/\text{\AA} + 0.0356547 \cdot z(B) \\
 &\quad R_{adj}^2 = 98.23 \% \\
 (3) \quad b/\text{\AA} &= 3.67172 + 0.513105 \cdot r(A)/\text{\AA} + 1.04107 \cdot r(B)/\text{\AA} + \\
 &\quad 0.634758 \cdot r(B')/\text{\AA} + 0.0693267 \cdot z(B) \\
 &\quad R_{adj}^2 = 98.54 \% \\
 (4) \quad c/\text{\AA} &= 4.71596 + 1.18801 \cdot r(A)/\text{\AA} + 1.295 \cdot r(B)/\text{\AA} + \\
 &\quad 0.90688 \cdot r(B')/\text{\AA} + 0.0943646 \cdot z(B) \\
 &\quad R_{adj}^2 = 99.36 \% \\
 (5) \quad V/\text{\AA}^3 &= -74.2989 + 120.282 \cdot r(A)/\text{\AA} + 124.111 \cdot r(B)/\text{\AA} + \\
 &\quad 107.363 \cdot r(B')/\text{\AA} + 7.95801 \cdot z(B) \\
 &\quad R_{adj}^2 = 99.05 \%
 \end{aligned}$$

As can be seen, the predictive strength of the proposed model is very high. A measure for the *goodness of fit* is the value of the R_{adj}^2 which is very high for each dependent variable. In order to obtain even better picture of the predictable performances of the models, the regression equations were used to predict the unit cell parameters of the compounds in the test set.

Also, using the same data set, the unit cell parameters were predicted by FF-ANN. Prior to training of the FF-ANN the data set was autoscaled. After several trials, by changing number of hidden neurons, the optimal architecture of ANNs was found. The ANN with best performances had four neurons in hidden layer.

The results obtained by both methods (MLR and FF-ANN) are presented in Table 2. It could be notice that the agreement between actual and predicted values for the lattice parameters of the compounds in test set is excellent. Also, the predicted values for lattice cell parameters by MLR and FF-ANN are close to each other.

Tab. 2: The results of the analyses. Comparison between the actual and the predicted values for the lattice parameters of the compounds of test set as well as the relative error in percents.

formula	$a(ac)/\text{\AA}$	MLR		FF-ANN		$b(ac)/\text{\AA}$	MLR		FF-ANN	
		$a(pr)/\text{\AA}$	$E/\%$	$a(pr)/\text{\AA}$	$E/\%$		$b(pr)/\text{\AA}$	$E/\%$	$b(pr)/\text{\AA}$	$E/\%$
$\text{Sr}_2(\text{CoTe})\text{O}_6$	5.6417	5.5814	1.07	5.6282	0.24	5.6063	5.5879	0.33	5.5949	0.20
$\text{Ba}_2(\text{ErIr})\text{O}_6$	5.8988	5.9207	0.37	5.8962	0.04	5.8899	5.8967	0.12	5.8974	0.13
$\text{Ba}_2(\text{GdT a})\text{O}_6$	6.015	6.019	0.07	6.0156	0.02	6.013	5.991	0.37	6.002	0.18
$\text{Ba}_2(\text{NdIr})\text{O}_6$	6.0008	5.9921	0.14	6.0144	0.23	5.9999	5.9935	0.11	5.9969	0.05
$\text{Ba}_2(\text{TbIr})\text{O}_6$	5.9319	5.9461	0.24	5.9351	0.05	5.9227	5.9310	0.14	5.9312	0.14
$\text{Ba}_2(\text{YbRe})\text{O}_6$	5.890	5.913	0.39	5.885	0.09	5.890	5.880	0.17	5.890	0.00
$\text{Ca}_2(\text{FeTa})\text{O}_6$	5.4498	5.4494	0.01	5.4284	0.39	5.5482	5.5321	0.29	5.5496	0.03
$\text{Sr}_2(\text{ErTa})\text{O}_6$	5.8054	5.7981	0.13	5.8047	0.01	5.8528	5.8590	0.11	5.8431	0.17
$\text{Sr}_2(\text{InSb})\text{O}_6$	5.7301	5.6942	0.63	5.7253	0.08	5.7306	5.7399	0.16	5.7294	0.02
$\text{Sr}_2(\text{TbTa})\text{O}_6$	5.8291	5.8234	0.10	5.8275	0.03	5.8934	5.8934	0.00	5.8876	0.10
$\text{Ba}_2(\text{PrIr})\text{O}_6$	5.9443	5.9736	0.49	5.9402	0.07	5.9379	5.9593	0.36	5.9334	0.08

formula	$c(ac)/\text{\AA}$	MLR		FF-ANN		$V(ac)/\text{\AA}^3$	MLR		FF-ANN	
		$c(pr)/\text{\AA}$	$E/\%$	$c(pr)/\text{\AA}$	$E/\%$		$V(pr)/\text{\AA}^3$	$E/\%$	$V(pr)/\text{\AA}^3$	$E/\%$
$\text{Sr}_2(\text{CoTe})\text{O}_6$	7.9234	7.8742	0.62	7.9118	0.15	250.61	245.76	1.94	249.70	0.36
$\text{Ba}_2(\text{ErIr})\text{O}_6$	8.3319	8.3555	0.28	8.3370	0.06	289.48	292.03	0.88	289.55	0.02
$\text{Ba}_2(\text{GdT a})\text{O}_6$	8.4852	8.4811	0.05	8.4832	0.02	306.89	305.50	0.45	306.31	0.19
$\text{Ba}_2(\text{NdIr})\text{O}_6$	8.4843	8.4759	0.10	8.4743	0.12	305.47	303.57	0.62	305.54	0.02
$\text{Ba}_2(\text{TbIr})\text{O}_6$	8.3866	8.3982	0.14	8.3837	0.03	294.65	296.13	0.50	294.85	0.07
$\text{Ba}_2(\text{YbRe})\text{O}_6$	8.300	8.336	0.43	8.327	0.33	287.94	290.37	0.84	288.17	0.08
$\text{Ca}_2(\text{FeTa})\text{O}_6$	7.7591	7.7453	0.18	7.7362	0.30	234.61	233.05	0.66	232.74	0.80
$\text{Sr}_2(\text{ErTa})\text{O}_6$	8.2346	8.2289	0.07	8.2366	0.02	279.79	280.30	0.18	279.50	0.10
$\text{Sr}_2(\text{InSb})\text{O}_6$	8.0963	8.0761	0.25	8.0996	0.04	265.86	264.84	0.38	265.84	0.01
$\text{Sr}_2(\text{TbTa})\text{O}_6$	8.2773	8.2716	0.07	8.2781	0.01	284.35	284.40	0.02	284.24	0.04
$\text{Ba}_2(\text{PrIr})\text{O}_6$	8.3984	8.4479	0.59	8.3883	0.12	296.44	300.93	1.51	296.05	0.13

The relative error is less than 1 % except for the a - parameter and V for $\text{Sr}_2(\text{CoTe})\text{O}_6$ obtained by MLR. The possible explanation for larger discrepancies for this compound might be the observed distortion of BO_6 octahedra ($B = \text{Co}$ and Te) [20].

Bearing all these results in mind, it could be concluded that the model proposed by both MLR and FF-ANN show very good results and can be used for prediction of the lattice parameters of new perovskites of this series. The proposed relationships give a possibility by varying the composition (A , B and B' ions) to obtain a compound of desired structural characteristics. It is also possible to use these models to check the experimental values for the unit cell parameters of this perovskite series.

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