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Original Research Article

Mechanical Properties of Pervoskites Compounds and Values of Lattice Constants of Some orthorhombic ABO_3 type Perovskite Solids

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Abstract: In this present research work, structural and mechanical properties of ABO_3 type perovskite and their lattice constants have studied. This work corresponds to the extensive survey and keen interest of the literatures. This would helpful to understand the structral properties and some other physical parameters of ABO_3 type perovskite. Experimental approach, computer data, statistical approach would also very helpful in order to understand structural and mechanical properties of ABO_3 type perovskites. The theoretical approach used empirical relations and thus resolves the difference in results obtained by other approaches and can fix the actual value of the observation. In the theoretical approach, the empirical methods are basically used to predict the structural parameters and lattice constants of solids.

Keywords: Elastic constant, Lattice constant, Crystallographic Ratio. Refractive Index, Empirical relations

Introduction

In present days, the structural and mechanical properties of materials can be studied by using high speed computer technology. This technology computes and simulates data obtained by researchers instead of traditional experiments. In modern high-speed computer techniques, they allow researchers to investigate many properties like physical or structural can of materials only by computation or simulation instead of by traditional experiments. In the theoretical approach, the empirical methods are basically used to predict the structural parameters of solids. In some cases we have used theoretical approach to understand the structural and mechanical properties of ABO_3 type perovskite and to calculate lattice constants. But we note that empirical relations always do not give highly accurate results for a specific solid. On the other hand, empirical relations allow researchers to calculate useful physical parameters and useful properties which become more evident. Some empirical parameters such as valency, atomic or ionic radii, electro-negativity, plasmon energy etc are specific in use to characterize the chemical bonds and classifying many atomic/molecular properties of solids.

Generally the elastic modulus has been observed and calculated and established a relationship among various characteristics at microscopic level of different sorts of materials. Scientists and researchers are now able to calculate various physical properties of condensed matters in computational technique as experimental way of research are difficult in obtaining exact values of various physical properties. Also experimental process is not suited due to their cost. Therefore it is very obvious to calculate the solid state properties of binary and ternary compounds through density function theory (DFT) and ab-initio methods in theoretical physics. Experimental datas are not fully covering the proof and it can be difficult to interpret the accuracy of published data.

Perovskite compounds are the family of ferroelectric materials. Crystals are classified into seven systems. They may be triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, and cubic. Further these seven systems can be sub- divided into 32 crystal classes. These 32 crystals have many different structural properties. Among the 32 crystals, 11 are centrally symmetric and remaining 21 groups do not possess centre of symmetry. The centrally symmetric cystas possess polar properties while non-centrally symmetric may have one or more polar axes. 20 of the 21 are form the piezoelectric class. The pyroelectrics form a subclass of the piezoelectrics, comprising 10 of the 20. The ferroelectrics are members of the pyroelectric subclass. Out of all the polar crystals, the most widely studied and technologically important are the perovskite oxides. Pervoskite

compounds can be represents by some complex oxides and halides and some classes inorganic compounds viz. sulphides, hydrides, cyanides, oxyfluorides, oxynitrides, inter-metallic, and metal organic compounds. The excitation of some chemical elements that are responsible to form pervoskite compounds and their property to form deficient structure of cation-anion corresponds to an extremely broad range of physical properties. Pervosite type oxides also shows very significant properties including superconductivity, insulator–metal transition, ionic conduction characteristics, dielectric properties and ferroelasticity etc.

The Structural Stability and Formability of Perovskite Solids

Elastic moduli are important for theoretical understanding of material properties. It is determined by the phonon density of states and lattice anharmonicity effects or by electron-phonon interaction processes mediated via deformation potentials. In view of the still unsatisfactory and contradictory data on the mechanical properties of the compounds on the one hand and of the importance of their knowledge for a comprehensive analysis of a wide variety of material characteristics on the other hand it was the aim of the present study to critically evaluate and review related experimental and theoretical data reported in the literature so far.

The study of ABO_3 compounds has a long history. Megaw accurately determined the structure of a number of doubled perovskites by examining high angle lines on X-ray powder photographs. Lattice parameter is one of the most critical parameters of the solids in materials design, especially for interface applicants. In this regard, a fast and reliable solution to predict lattice constant for a large number of unknown compounds becomes the winning edge in high technology development. Often, there are two broad methods to determine the crystal structure of unknown compounds. The first method is Traditional method of determining lattice constants (LC) is usually based on X-ray, neutron or electron diffraction techniques, and the other is by theoretical or empirical models.

The first method is usually a complicated, difficult and time-consuming. Specifically, for large number of unknown compounds, these are very slow processes. These techniques form a powerful approach and are very popular among crystallographers, and widely used for structure determination. However, it is very difficult if not impossible to prepare the form of single crystals of sufficient size and quality for conventional single-crystal X-ray diffraction studies for many important crystalline materials.

We have work out on various meachnical perameters of ABO_3 type perovskite. The bulk modulus is an important mechanical property of a material and defines its resistance to volume change when compressed. Therefore, we have presented and studied the various models and theories describing the bulk modulus (B) of these materials. The bulk modulus, elastic moduli, which are of importance in assessing the competition between the ductile and brittle failures, have been extensively investigated in relation to various microscopic characteristics of different sorts of materials, such as metals and covalently bonded crystals. Recently, the bulk modulus, elastic modulus evaluations are carried out using ab-initio method; first-principles calculations for understanding the nature of the chemical bonding and its attributes in various solid systems. But due to the long process, as well as complicated computational methods involving a series of approximations, such a method has always been complicate. Therefore it seems an urgent need to evolve some sort of correlation by simulation of ionic charge and bulk modulus of perovskite materials. We have made efforts in this regards and succeed to establish an empirical relation between these two parameters.

Result:

Lattice constants of orthorhombic Perovskites

Perovskite oxide can be defined in different systems like as $A^{+1}B^{+5}O_3$, $A^{+2}B^{+4}O_3$ and $A^{+3}B^{+3}O_3$. When we plot a graph of lattice constant of orthorhombic perovskite solids against average ionic radii r_{av} (Å), we obtained a linear relationship between them. But the plotted graph fall on different straight lines according to the ionic charge product of the compounds. We concluded that the lines of $A^{+2}B^{+4}O_3$ orthorhombic perovskite oxides are just nearly parallel to the line for $A^{+3}B^{+3}O_3$ orthorhombic perovskite oxides. It also concludes that the lattice constant trends increases with rise of average ionic radii. Similarly, lattice constants fall on straight lines related to the ionic charge product of solids.

To obtain better agreement between experimental and theoretical data for orthorhombic perovskite type crystal structure compounds, following may proceeds:

$$\text{Lattice constant (a in Å)} = 4\,(Z_1Z_2Z_3)^{0.054}\,r_{av}$$
$$\text{Lattice constant (b in Å)} = 4\,(Z_1Z_2Z_3)^{0.055}\,r_{av}$$
$$\text{Lattice constant (c in Å)} = 6\,(Z_1Z_2Z_3)^{0.04}\,r_{av}$$

Where Z_1, Z_2 and Z_3 are the ionic charge on the A, B and O_3 respectively, r_{av} is the average ionic radii of ABO_3 in Å and it can be calculated by $r_{av} = \{(r_A + r_B + r_O) / 3\}$. The value of product of ionic charge $(Z_1Z_2Z_3) = 30$ for $A^{+1}B^{+5}O_3$, $(Z_1Z_2Z_3) = 48$ for $A^{+2}B^{+4}O_3$ and $(Z_1Z_2Z_3) = 54$ for $A^{+3}B^{+3}O_3$ orthorhombic perovskites and ionic radii of oxide (r_o) is 1.35.

Table 1. Values of lattice constant (a in Å) for orthorhombic perovskite solids.

Solids	r_A(Å) [20]	r_B(Å) [20]	a (Å) [12]	a (Å) [this work]	% error
NaUO3	1.39	0.76	5.775	5.607	2.9
NaTaO3	1.39	0.64	5.494	5.415	1.4
NaNbO3	1.39	0.64	5.51	5.415	1.7
NaPaO3	1.39	0.78	5.82	5.639	3.1
CaMnO3	1.34	0.53	5.27	5.292	0.4
CaCrO3	1.34	0.55	5.287	5.324	0.7
CaVO3	1.34	0.58	5.326	5.374	0.9
CaTiO3	1.34	0.605	5.381	5.415	0.6
CaRuO3	1.34	0.68	5.36	5.538	3.3
CaMoO3	1.34	0.65	5.45	5.489	0.7
CaNbO3	1.34	0.68	5.56	5.538	0.4
CaSnO3	1.34	0.69	5.519	5.554	0.6
CaHfO3	1.34	0.71	5.568	5.587	0.3
CaZrO3	1.34	0.72	5.587	5.604	0.3
CaUO3	1.34	0.89	5.78	5.883	1.8
BaPbO3	1.61	0.775	6.024	6.138	1.9
SrRuO3	1.44	0.68	5.53, 5.567 [5]	5.702	3.1
SrUO3	1.44	0.89	6.01	6.047	0.6
SrIrO3	1.44	0.625	5.58	5.612	0.6
SrHfO3	1.44	0.71	5.785	5.752	0.6
SrZrO3	1.44	0.72	5.792, 5.796 [4]	5.768	0.4
SrPbO3	1.44	0.775	5.86	5.858	0
SrCeO3	1.44	0.87	5.986	6.015	0.5
LaCrO3	1.36	0.615	5.515	5.498	0.3
LaGaO3	1.36	0.62	5.526, 5.527 [1]	5.507	0.3
LaFeO3	1.36	0.645	5.556	5.548	0.1
LaVO3	1.36	0.64	5.54	5.54	0
LaMnO3	1.36	0.645	5.529, 5.582 [1]	5.548	0.3
LaRhO3	1.36	0.665	5.524	5.581	1
LaTiO3	1.36	0.67	5.546	5.589	0.8
LaScO3	1.36	0.745	5.678	5.713	0.6
LaInO3	1.36	0.8	5.723	5.804	1.4
LaYO3	1.36	0.645	5.877, 6.086 [1]	5.548	5.6
CeCrO3	1.34	0.615	5.475	5.465	0.2
CeFeO3	1.34	0.645	5.519	5.515	0.1
CeVO3	1.34	0.64	5.486	5.507	0.4
CeMnO3	1.3	0.645	5.532	5.449	1.5
CeTiO3	1.34	0.67	5.513	5.556	0.8
PrCrO3	1.3	0.615	5.484	5.399	1.5
PrGaO3	1.3	0.62	5.458	5.407	0.9
PrFeO3	1.3	0.645	5.495	5.449	0.8
PrVO3	1.3	0.64	5.487	5.441	0.8
PrMnO3	1.3	0.645	5.545	5.449	1.7
PrRhO3	1.3	0.665	5.414	5.482	1.3
PrTiO3	1.3	0.67	5.499	5.49	0.2
PrCoO3	1.3	0.545	5.331	5.283	0.9
PrScO3	1.3	0.745	5.615	5.614	0
PrAlO3	1.3	0.535	5.347	5.267	1.5
NdCrO3	1.27	0.615	5.425	5.35	1.4
NdGaO3	1.27	0.62	5.431	5.358	1.3
NdFeO3	1.27	0.645	5.441	5.399	0.8
NdVO3	1.27	0.64	5.451	5.391	1.1

NdMnO3	1.27	0.645	5.38	5.399	0.4
NdRhO3	1.27	0.665	5.378	5.432	1
NdTiO3	1.27	0.67	5.487	5.441	0.8
NdCoO3	1.27	0.545	5.336	5.234	1.9
NdScO3	1.27	0.745	5.574	5.565	0.2
NdInO3	1.27	0.8	5.627	5.656	0.5
PmCrO3	1.25	0.615	5.4	5.317	1.5
PmScO3	1.25	0.745	5.56	5.532	0.5
PmInO3	1.25	0.8	5.7	5.622	1.4
SmAlO3	1.24	0.535	5.285, 5.286 [3]	5.168	2.2
SmCrO3	1.24	0.615	5.367	5.3	1.2
SmGaO3	1.24	0.62	5.369	5.308	1.1
SmFeO3	1.24	0.645	5.394	5.35	0.8
SmVO3	1.24	0.64	5.393	5.341	1
SmMnO3	1.24	0.645	5.359	5.35	0.2
SmRhO3	1.24	0.665	5.321	5.383	1.2
SmTiO3	1.24	0.67	5.468	5.391	1.4
SmCoO3	1.24	0.545	5.289	5.184	2
SmScO3	1.24	0.745	5.53	5.515	0.3
SmInO3	1.24	0.8	5.589	5.606	0.3
EuAlO3	1.23	0.535	5.271 [6]	5.151	2.3
EuCrO3	1.23	0.615	5.34	5.283	1.1
EuGaO3	1.23	0.62	5.351	5.292	1.1
EuFeO3	1.23	0.645	5.371	5.333	0.7
EuMnO3	1.23	0.645	5.338	5.333	0.1
EuRhO3	1.23	0.665	5.298	5.366	1.3
EuScO3	1.23	0.745	5.51	5.498	0.2
EuInO3	1.23	0.8	5.567	5.589	0.4
GdAlO3	1.22	0.535	5.247, 5.253 [2]	5.135	2.1
GdCrO3	1.22	0.615	5.312	5.267	0.8
GdGaO3	1.22	0.62	5.322	5.275	0.9
GdFeO3	1.22	0.645	5.346, 5.351 [2]	5.317	0.6
GdVO3	1.22	0.64	5.343	5.308	0.7
GdMnO3	1.22	0.645	5.313	5.317	0.1
GdRhO3	1.22	0.665	5.277	5.35	1.4
GdTiO3	1.22	0.67	5.407	5.358	0.9
GdCoO3	1.22	0.545	5.228	5.151	1.5
GdScO3	1.22	0.745	5.487	5.482	0.1
GdInO3	1.22	0.8	5.548	5.573	0.4
TbAlO3	1.2	0.535	5.22	5.102	2.3
TbCrO3	1.2	0.615	5.291	5.234	1.1
TbGaO3	1.2	0.62	5.307	5.242	1.2
TbFeO3	1.2	0.645	5.326	5.283	0.8
TbMnO3	1.2	0.645	5.297	5.283	0.3
TbRhO3	1.2	0.665	5.254	5.317	1.2
TbTiO3	1.2	0.67	5.388	5.325	1.2
DyAlO3	1.19	0.535	5.21	5.085	2.4
DyCrO3	1.19	0.615	5.263	5.217	0.9
DyGaO3	1.19	0.62	5.282	5.226	1.1
DyFeO3	1.19	0.645	5.302	5.267	0.7
DyVO3	1.19	0.64	5.302	5.259	0.8
DyMnO3	1.19	0.645	5.275	5.267	0.2
DyRhO3	1.19	0.665	5.245	5.3	1
DyTiO3	1.19	0.67	5.361	5.308	1
DyScO3	1.19	0.745	5.43	5.432	0
DyInO3	1.19	0.8	5.519	5.523	0.1

HoAlO3	1.18	0.535	5.18	5.068	2.2
HoCrO3	1.18	0.615	5.243	5.201	0.8
HoGaO3	1.18	0.62	5.251	5.209	0.8
HoFeO3	1.18	0.645	5.278	5.25	0.5
HoMnO3	1.18	0.645	5.255	5.25	0.1
HoRhO3	1.18	0.665	5.23	5.283	1
HoTiO3	1.18	0.67	5.339	5.292	0.9
HoScO3	1.18	0.745	5.42	5.416	0.1
ErAlO3	1.17	0.535	5.16	5.052	2.1
ErCrO3	1.17	0.615	5.223	5.184	0.7
ErGaO3	1.17	0.62	5.239	5.193	0.9
ErFeO3	1.17	0.645	5.263	5.234	0.6
ErVO3	1.17	0.64	5.262	5.226	0.7
ErMnO3	1.17	0.645	5.24	5.234	0.1
ErRhO3	1.17	0.665	5.216	5.267	1
ErTiO3	1.17	0.67	5.318	5.275	0.8
TmAlO3	1.16	0.535	5.15	5.035	2.2
TmCrO3	1.16	0.615	5.209	5.168	0.8
TmGaO3	1.16	0.62	5.224	5.176	0.9
TmFeO3	1.16	0.645	5.251	5.217	0.6
TmMnO3	1.16	0.645	5.23	5.217	0.2
TmRhO3	1.16	0.665	5.203	5.25	0.9
TmTiO3	1.16	0.67	5.306	5.259	0.9
YbAlO3	1.15	0.535	5.12	5.019	2
YbCrO3	1.15	0.615	5.195	5.151	0.8
YbGaO3	1.15	0.62	5.208	5.159	0.9
YbFeO3	1.15	0.645	5.233	5.201	0.6
YbMnO3	1.15	0.645	5.22	5.201	0.4
YbTiO3	1.15	0.67	5.293	5.242	1
LuCrO3	1.14	0.615	5.176	5.135	0.8
LuGaO3	1.14	0.62	5.188	5.143	0.9
LuFeO3	1.14	0.645	5.213	5.184	0.6
LuMnO3	1.14	0.645	5.205	5.184	0.4
LuRhO3	1.14	0.665	5.186	5.217	0.6
LuTiO3	1.14	0.67	5.274	5.226	0.9
YAlO3	1.2	0.535	5.179	5.102	1.5
YCrO3	1.2	0.615	5.241	5.234	0.1
YGaO3	1.2	0.62	5.257	5.242	0.3
YFeO3	1.2	0.645	5.283	5.283	0
YVO3	1.2	0.64	5.284	5.275	0.2
YMnO3	1.2	0.645	5.26	5.283	0.4
YTiO3	1.2	0.67	5.34	5.325	0.3
YScO3	1.2	0.745	5.431	5.449	0.3
YInO3	1.2	0.8	5.5	5.54	0.7

Table 2. Values of lattice constants (b and c in Å) for orthorhombic perovskite solids.

Solids	b (Å) [12]	c (Å) [12]	b (Å) [this work]	c (Å) [this work]	% error of b	% error of c
NaUO3	5.905	8.25	5.627	8.02	4.7	2.8
NaTaO3	5.513	7.751	5.434	7.745	1.4	0.1
NaNbO3	5.57	7.77	5.434	7.745	2.4	0.3
NaPaO3	5.92	8.36	5.659	8.065	4.4	3.5
CaMnO3	5.275	7.464	5.312	7.519	0.7	0.7
CaCrO3	5.316	7.486	5.345	7.565	0.5	1.1
CaVO3	5.352	7.547	5.394	7.635	0.8	1.2
CaTiO3	5.443	7.645	5.436	7.694	0.1	0.6

CaRuO3	5.53	7.67	5.559	7.869	0.5	2.6
CaMoO3	5.58	7.8	5.51	7.799	1.3	0
CaNbO3	5.77	8.016	5.559	7.869	3.7	1.8
CaSnO3	5.668	7.885	5.576	7.892	1.6	0.1
CaHfO3	5.732	7.984	5.609	7.939	2.1	0.6
CaZrO3	5.758	8.008	5.625	7.962	2.3	0.6
CaUO3	5.97	8.29	5.906	8.359	1.1	0.8
BaPbO3	6.065	8.506	6.162	8.721	1.6	2.5
SrRuO3	5.57,5.53[5]	7.847,7.85 [5]	5.724	8.102	2.8	3.3
SrUO3	6.17	8.6	6.071	8.593	1.6	0.1
SrIrO3	5.6	7.89	5.634	7.974	0.6	1.1
SrHfO3	5.786	8.182	5.774	8.173	0.2	0.1
SrZrO3	5.814,5.82 [4]	8.196,8.205 [4]	5.79	8.196	0.4	0
SrPbO3	5.958	8.331	5.881	8.324	1.3	0.1
SrCeO3	6.125	8.531	6.038	8.546	1.4	0.2
LaCrO3	5.479	7.753	5.521	7.794	0.8	0.5
LaGaO3	5.473,5.5 [1]	7.767,7.781 [1]	5.529	7.806	1	0.5
LaFeO3	5.565	7.862	5.57	7.864	0.1	0
LaVO3	5.54	7.83	5.562	7.852	0.4	0.3
LaMnO3	5.662,5.58 [1]	7.715,7.89 [1]	5.57	7.864	1.6	
LaRhO3	5.629	7.9	5.604	7.911	0.5	0.1
LaTiO3	5.753	7.832	5.612	7.923	2.5	1.2
LaScO3	5.787	8.098	5.736	8.099	0.9	0
LaInO3	5.914	8.207	5.828	8.227	1.5	0.2
LaYO3	6.087,5.89 [1]	8.493,8.511 [1]	5.57	7.864	8.5	7.4
CeCrO3	5.475	7.74	5.487	7.747	0.2	0.1
CeFeO3	5.536	7.819	5.537	7.817	0	0
CeVO3	5.486	7.74	5.529	7.806	0.8	0.8
CeMnO3	5.557	7.812	5.471	7.723	1.6	1.1
CeTiO3	5.757	7.801	5.579	7.876	3.1	1
PrCrO3	5.479	7.718	5.421	7.653	1.1	0.8
PrGaO3	5.49	7.733	5.429	7.665	1.1	0.9
PrFeO3	5.578	7.81	5.471	7.723	1.9	1.1
PrVO3	5.562	7.751	5.462	7.712	1.8	0.5
PrMnO3	5.787	7.575	5.471	7.723	5.5	2
PrRhO3	5.747	7.803	5.504	7.77	4.2	0.4
PrTiO3	5.724	7.798	5.512	7.782	3.7	0.2
PrCoO3	5.373	7.587	5.305	7.489	1.3	1.3
PrScO3	5.776	8.027	5.637	7.958	2.4	0.9
PrAlO3	5.322	7.481	5.288	7.466	0.6	0.2
NdCrO3	5.478	7.694	5.371	7.583	2	1.4
NdGaO3	5.499	7.71	5.379	7.595	2.2	1.5
NdFeO3	5.573	7.753	5.421	7.653	2.7	1.3
NdVO3	5.579	7.734	5.413	7.641	3	1.2
NdMnO3	5.854	7.557	5.421	7.653	7.4	1.3
NdRhO3	5.755	7.775	5.454	7.7	5.2	1
NdTiO3	5.707	7.765	5.462	7.712	4.3	0.7
NdCoO3	5.336	7.547	5.255	7.419	1.5	1.7
NdScO3	5.771	7.998	5.587	7.888	3.2	1.4
NdInO3	5.891	8.121	5.678	8.016	3.6	1.3
PmCrO3	5.49	7.69	5.338	7.536	2.8	2
PmScO3	5.79	7.94	5.554	7.841	4.1	1.3
PmInO3	5.9	8.2	5.645	7.97	4.3	2.8
SmAlO3	5.29,5.28 [3]	7.473,7.46 [3]	5.189	7.325	1.9	2
SmCrO3	5.508	7.643	5.321	7.513	3.4	1.7
SmGaO3	5.52	7.65	5.33	7.524	3.4	1.6

SmFeO3	5.592	7.711	5.371	7.583	3.9	1.7
SmVO3	5.588	7.672	5.363	7.571	4	1.3
SmMnO3	5.843	7.482	5.371	7.583	8.1	1.3
SmRhO3	5.761	7.708	5.404	7.63	6.2	1
SmTiO3	5.665	7.737	5.413	7.641	4.5	1.2
SmCoO3	5.354	7.541	5.205	7.348	2.8	2.6
SmScO3	5.76	7.95	5.537	7.817	3.9	1.7
SmInO3	5.886	8.082	5.629	7.946	4.4	1.7
EuAlO3	5.292 [6]	7.458 [6]	5.172	7.302	2.3	2.1
EuCrO3	5.515	7.622	5.305	7.489	3.8	1.7
EuGaO3	5.528	7.628	5.313	7.501	3.9	1.7
EuFeO3	5.611	7.686	5.355	7.559	4.6	1.6
EuMnO3	5.842	7.453	5.355	7.559	8.3	1.4
EuRhO3	5.761	7.68	5.388	7.606	6.5	1
EuScO3	5.76	7.94	5.521	7.794	4.2	1.8
EuInO3	5.835	8.078	5.612	7.923	3.8	1.9
GdAlO3	5.304,5.30 [2]	7.447,7.44 [2]	5.155	7.278	2.8	2.3
GdCrO3	5.525	7.606	5.288	7.466	4.3	1.8
GdGaO3	5.537	7.606	5.296	7.477	4.3	1.7
GdFeO3	5.616,5.61 [2]	7.668,7.67 [2]	5.338	7.536	5	1.7
GdVO3	5.614	7.637	5.33	7.524	5.1	1.5
GdMnO3	5.853	7.432	5.338	7.536	8.8	1.4
GdRhO3	5.761	7.658	5.371	7.583	6.8	1
GdTiO3	5.667	7.692	5.379	7.595	5.1	1.3
GdCoO3	5.404	7.436	5.172	7.302	4.3	1.8
GdScO3	5.756	7.925	5.504	7.77	4.4	2
GdInO3	5.842	8.071	5.595	7.899	4.2	2.1
TbAlO3	5.28	7.41	5.122	7.231	3	2.4
TbCrO3	5.518	7.576	5.255	7.419	4.8	2.1
TbGaO3	5.531	7.578	5.263	7.43	4.8	1.9
TbFeO3	5.602	7.635	5.305	7.489	5.3	1.9
TbMnO3	5.831	7.403	5.305	7.489	9	1.2
TbRhO3	5.749	7.623	5.338	7.536	7.1	1.1
TbTiO3	5.648	7.676	5.346	7.548	5.3	1.7
DyAlO3	5.31	7.38	5.106	7.208	3.9	2.3
DyCrO3	5.2	7.552	5.238	7.395	0.7	2.1
DyGaO3	5.534	7.556	5.247	7.407	5.2	2
DyFeO3	5.598	7.623	5.288	7.466	5.5	2.1
DyVO3	5.602	7.601	5.28	7.454	5.8	1.9
DyMnO3	5.828	7.375	5.288	7.466	9.3	1.2
DyRhO3	5.731	7.6	5.321	7.513	7.1	1.2
DyTiO3	5.659	7.647	5.33	7.524	5.8	1.6
DyScO3	5.71	7.89	5.454	7.7	4.5	2.4
DyInO3	5.751	8.041	5.546	7.829	3.6	2.6
HoAlO3	5.33	7.36	5.089	7.184	4.5	2.4
HoCrO3	5.519	7.538	5.222	7.372	5.4	2.2
HoGaO3	5.531	7.536	5.23	7.384	5.4	2
HoFeO3	5.591	7.602	5.272	7.442	5.7	2.1
HoMnO3	5.831	7.354	5.272	7.442	9.6	1.2
HoRhO3	5.726	7.582	5.305	7.489	7.4	1.2
HoTiO3	5.665	7.626	5.313	7.501	6.2	1.6
HoScO3	5.71	7.87	5.438	7.677	4.8	2.5
ErAlO3	5.32	7.33	5.072	7.161	4.7	2.3
ErCrO3	5.516	7.519	5.205	7.348	5.6	2.3
ErGaO3	5.527	7.522	5.213	7.36	5.7	2.2
ErFeO3	5.582	7.591	5.255	7.419	5.9	2.3

ErVO3	5.604	7.578	5.247	7.407	6.4	2.3
ErMnO3	5.82	7.335	5.255	7.419	9.7	1.1
ErRhO3	5.712	7.561	5.288	7.466	7.4	1.3
ErTiO3	5.657	7.613	5.296	7.477	6.4	1.8
TmAlO3	5.33	7.29	5.056	7.137	5.1	2.1
TmCrO3	5.508	7.5	5.189	7.325	5.8	2.3
TmGaO3	5.515	7.505	5.197	7.337	5.8	2.2
TmFeO3	5.576	7.584	5.238	7.395	6.1	2.5
TmMnO3	5.81	7.32	5.238	7.395	9.8	1
TmRhO3	5.697	7.543	5.272	7.442	7.5	1.3
TmTiO3	5.647	7.607	5.28	7.454	6.5	2
YbAlO3	5.33	7.31	5.039	7.114	5.5	2.7
YbCrO3	5.51	7.49	5.172	7.302	6.1	2.5
YbGaO3	5.51	7.49	5.18	7.313	6	2.4
YbFeO3	5.557	7.57	5.222	7.372	6	2.6
YbMnO3	5.8	7.3	5.222	7.372	10	1
YbTiO3	5.633	7.598	5.263	7.43	6.6	2.2
LuCrO3	5.497	7.475	5.155	7.278	6.2	2.6
LuGaO3	5.505	7.484	5.164	7.29	6.2	2.6
LuFeO3	5.547	7.565	5.205	7.348	6.2	2.9
LuMnO3	5.79	7.31	5.205	7.348	10	0.5
LuRhO3	5.67	7.512	5.238	7.395	7.6	1.6
LuTiO3	5.633	7.58	5.247	7.407	6.9	2.3
YAlO3	5.329	7.37	5.122	7.231	3.9	1.9
YCrO3	5.521	7.532	5.255	7.419	4.8	1.5
YGaO3	5.536	7.533	5.263	7.43	4.9	1.4
YFeO3	5.592	7.603	5.305	7.489	5.1	1.5
YVO3	5.605	7.587	5.296	7.477	5.5	1.4
YMnO3	5.83	7.36	5.305	7.489	9	1.8
YTiO3	5.665	7.624	5.346	7.548	5.6	1
YScO3	5.712	7.894	5.471	7.723	4.2	2.2
YInO3	5.787	8.053	5.562	7.852	3.9	2.5

Conclusion:

I predicted a simple prediction for the calculation of lattice constant of orthorhombic perovskite solids. From the proposed relation, it is clear that the lattice constants of pervoskite can be expressed as the product of ionic charge and average ionic radii of the perovskites solids.

The values evaluated are presented in tables 1 and table 2. It is also to be noteworthy that proposed empirical relation is simpler, widely applicable and values obtained are in better agreement with experiment data as compared to the empirical relations proposed by different scholars. The method presented in this work will be helpful to the material scientists for finding new materials with desired structural parameters among series of similar perovskite materials.

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