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Modeling of Ferroelectric, Semiconducting and Superconducting Perovskite Oxides Using Crystalline Accommodation Law

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ABSTRACT

Perovskite oxides are very important materials for different applications because they have a variety of very interesting properties such as ferroelectric, antiferroelectric, ferromagnetic, antiferromagnetic, semiconducting and superconducting at low temperature. Since the success of crystalline accommodation law (CAL) in modeling perovskite halides, we aim in this work to use CAL for modeling perovskite oxides. Here we show that a perfect agreement with the results obtained for halides perovskite as the following: all perovskite oxides are formed at VEC = 4.8 and most of them crystallize in three systems; cubic, hexagonal and orthorhombic with the number of filled zones in the valence band $(\frac{V_F}{V_B}) = 12, 24$ and 48 respectively. It is also found that the dielectric ferroelectric perovskite oxides have the orthorhombic structure of primitive cell volume (V_P) ranges from 143.58 to 286.93 $Å^3$ corresponding to the volume of Brillouin zone (V_B , volume of quantum state) ranges from 0.86 to 1.72 $Å^{-3}$. On average, this is the smallest volume of quantum state. In the case of perovskite oxides, that can be converted into superconductor at low temperature, have cubic structure with V_P ranges from 52.73 to 68.61 $Å^3$ corresponding to V_B ranges from 3.61 to 4.70 $Å^{-3}$. On average, this is the largest volume of quantum state for example the compound $SrTiO_3$. In between it is found that the compounds which have hexagonal structure are semiconducting with V_P ranges from 108.73 to 130.43 $Å^3$ corresponding to V_B ranges from 1.90 to 2.28 $Å^{-3}$. On the average, this is intermediate between orthorhombic and cubic.

Key Words: Perovskite oxides, Brillouin zone, Valence electron concentration, Crystalline accommodation law, Volume of quantum state.

1. INTRODUCTION

Perovskite oxides (PO) are very important materials for different applications because they have a variety of very interesting properties such as ferroelectric, antiferroelectric, ferromagnetic, antiferromagnetic, semiconducting and superconducting at low temperature [1–6]. Lev Aleksevich Von Perovski, a Russian aristocrat and mineralogist, was honored with initially discovering the calcium titanium oxide ($CaTiO_3$) structure in the Ural Mountains of Russia in 1839, which gave rise to the term "perovskites" [7]. Perovskites are classified into different types and one of its important classifications is PO's. The general chemical formula for PO is ABO_3, in which O is oxygen anion that forms bonds with both A and B, two cations that are very dissimilar in size [8]. All these details are illustrated in Fig. 1, which shows the structure of

PO that is characterized by an octahedral structure. The combination of B cations lie at the center of octahedral and an oxygen anion O^{-2} at the heads of octahedron [9].

For examples the compound $BaTiO_3$ used in supercapacitors [10], $LaFeO_3$ used in gas sensors, and fuel cells [11], $PbTiO_3$ used in nonvolatile memory, infrared sensor, ultrasonic sensor and etc [12].

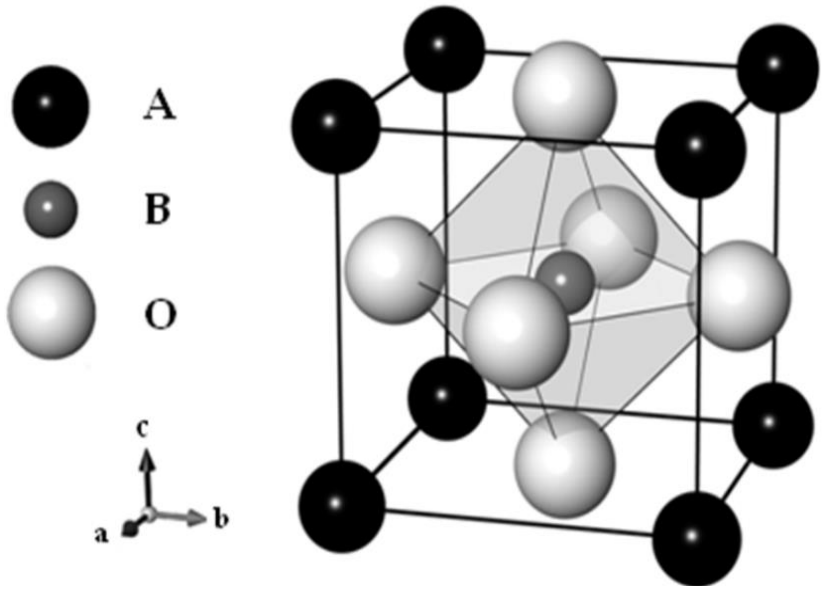

Fig. 1 : Crystal structure of perovskite oxides [13].

There are several attempts have been made to explain the structure of PO by analyzing the size ratio and the geometry of the ions distribution. Goldschmidt attempted to determine the tolerance factor t in 1927 [14] depending on the ionic radius (r) which is given by the following equation;

$$t = \frac{r_A + r_O}{\sqrt{2}(r_B + r_O)} \quad (1)$$

where r_A, r_B and r_O are ionic radii of A, B cations and O anion respectively. This model depends on three probably possible predictions of t values as following; i- the predicted structure is cubic if t equal 1. ii- if t value fall in range $0.825 < t \leq 1.059$, the structure will be either orthorhombic, tetragonal or cubic and iii- in case of t is greater than 1.059, the structure will be hexagonal. If t is lower than 0.825, it will not be crystallized in perovskite structure [14]–[17]. After 47 years exactly in 1974, Muller and Roy [18] assumed the structure of 197 perovskite compounds depending on the ionic radii of cations A and B of PO. They made a structural map between r_A and r_B of 197 PO in structural map and they found that PO where in region away from non-perovskites compounds. However, this model lack of data accuracy of some compounds. In 2001, An octahedral factor μ was proposed by Rohere [19] as given by equation 2;

$$\mu = {}^{r_B}/_{r_O} \quad (2)$$

where r_B and r_O are ionic radius of B cation and O oxygen anion atom respectively. Rohere found that the structure of PO is stable when μ value larger than 0.414 and lower than 0.732. Li et al. [20] in 2003 created a t-μ 2D structure map model, which was based on the previous two models developed by Goldschmidt and Rohere. They investigated 64 PO using the structural map. They found that 63 PO follow the structural map and only one compound not follows the structural map. This model is still limited and cannot determine the exact crystal structure of PO. L.Q. Jiange et al. [21] in 2006 tried to predict the lattice constant in the ideal cubic structures of PO using 77 PO have cubic structure. They found that the lattice parameters of all these compounds with average error not exceed 0.63% according to the following equation:

$$a = 1.8836(r_B + r_O) + 1.4898\,\frac{(r_A + r_O)}{\sqrt{2}(r_B + r_O)} - 1.2062 \quad (3)$$

where r_A , r_B and r_O are ionic radii of A and B cations and O^{-2} anion respectively. However, some numbers in this equation do not have any physical interpretation and this equation was applied only for cubic PO. Recently in 2019, a modification of t to new tolerance factor τ was applied by Christopher J. Bartel et al. [22] to predict the formation of PO. The new tolerance factor τ is given by;

$$\tau = \frac{r_O}{r_B} - n_A\left(n_A - \frac{{}^{r_A}/_{r_B}}{\ln({}^{r_A}/_{r_B})}\right) \quad (4)$$

where n_A is the oxidation state of atom A. This study increased the correction possibility of producing perovskite compounds from 83% of Goldschmidt's model to be 92% in this model.

All the previous models are geometrical empirical and have no theoretical basis. In 2017, crystalline accommodation law (CAL) was introduced by Tarek El Ashram [23] and succeeded in explanation the crystalline structure of materials. Moreover a very important model, based on CAL, was obtained by Tarek El Ashram [24] called the quantum quantitative model (CALQQM). CALQQM is succeeded in explaining the superconductivity at room temperature, energy levels, and the work functions of materials. In addition CAL is succeeded in modeling inorganic perovskite halides (PH) and determined the electronic structures of their valence bands [25]. Since the success of crystalline accommodation law in modeling PH's, we aim in this work to use CAL for modeling PO's.

2. COMPUTATIONAL METHODOLOGY

The computational methodology was based on CAL. The parameters of CAL are *VEC*, *n*, V_F and V_B. These parameters were calculated from the crystal structure data obtained from ICDD cards [26] shown in Table 1 as the following;

1- ***VEC*** *is given by;*

$$\text{VEC} = \frac{\text{VEC of A}+\text{VEC of B}+\text{VEC of O}}{5} \quad (5)$$

The PO molecule consists of five atoms, 2 cations A and B and 3 anions O. According to the charge neutrality of the molecule, the charge on cations must equal to the charge on the anions. The charge on the cations varies in three different forms as the following; $A^{+3}B^{+3}O_3$ such as $GdGaO_3$, $A^{+2}B^{+4}O_3$ such as $CaTiO_3$ and $A^{+1}B^{+5}O_3$ such as $KTaO_3$. For examples;

For $GdGaO_3$ VEC = $\frac{1*3+1*3+3*6}{5}$= 4.8, $CaTiO_3$ VEC = $\frac{1*2+1*4+3*6}{5}$= 4.8 and for $KTaO_3$

VEC= $\frac{1*1+1*5+3*6}{5}$= 4.8. Actually it was found that all PO and PH are formed at VEC = 4.8.

2- ***n*** is the number of atoms per lattice point calculated from diffraction data shown on Table 1.

3- $\mathbf{V_F}$ is the volume of Fermi sphere and determined by;

$$V_F = \frac{4}{3}\pi K_F^3 \quad (6)$$

where $\boldsymbol{K_F}$ is the Fermi electron wave vector given by;

$$K_F^3 = \frac{3\pi^2(0.6022)n\,VEC\,Dx}{Mwt} \quad (7)$$

where *Mwt* is the molecular weight and *Dx* is the calculated density from X-ray diffraction data

4- $\boldsymbol{V_B}$ is the volume of Brillouin zone (BZ) which is the volume of quantum state and is given by;

$$V_B = \frac{8\pi^3}{V_P} \quad (8)$$

where V_P is the primitive cell volume.

The calculations were carried out on the PO, which are stable in normal conditions of temperature and pressure as shown in Table 1.

3. RESULTS AND DISCUSSION

The parameters of CAL for PO's were calculated as given in Table 2. It is evident that all of PO's are formed at the same VEC = 4.8 in agreement with the results obtained for PH's [25]. It also found that PO's crystallize in three main systems, cubic, hexagonal and orthorhombic. For cubic system it was found that the number of filled zones in the valence band $(\frac{V_F}{V_B}) = 12$. For the hexagonal system it was found that the number of filled zones in the valence band $(\frac{V_F}{V_B}) = 24$. For the orthorhombic system it was found the number of filled zones in the valence band $(\frac{V_F}{V_B}) = 48$ in agreement with the results obtained for PH's [25].

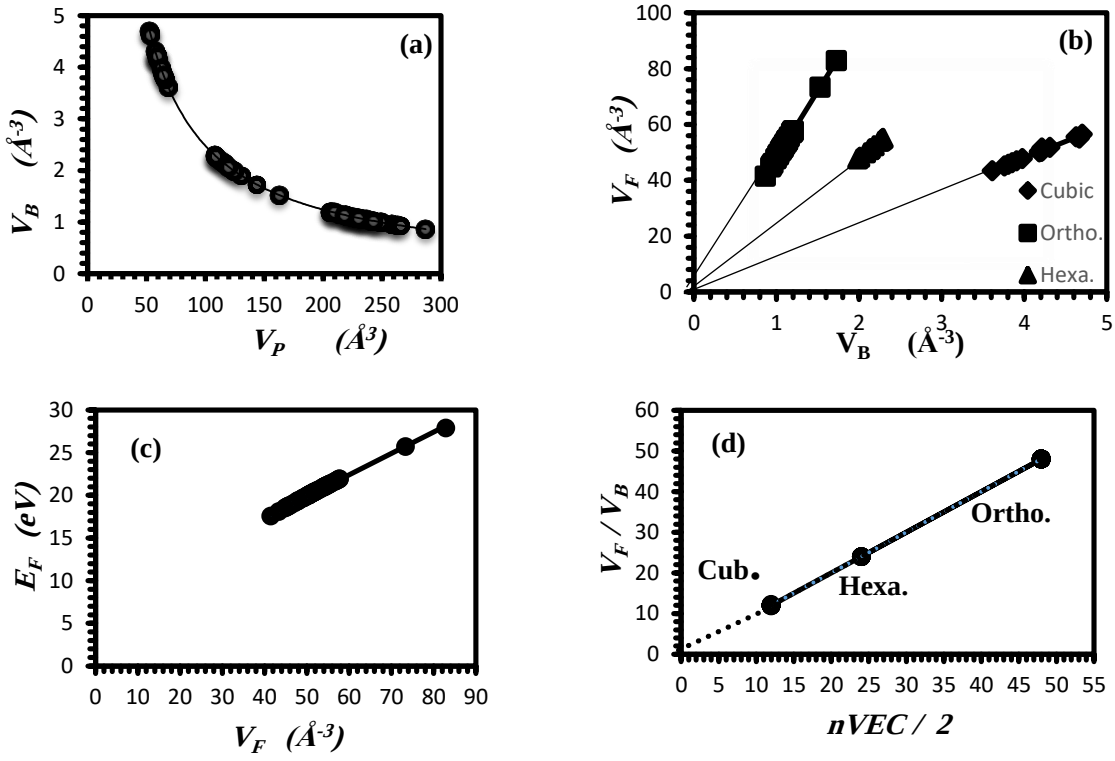

Fig. 2: (a) Variation of BZ volume with the primitive cell volume. (b) Variation of Fermi sphere volume with BZ volume. (c) Variation of Fermi energy with Fermi sphere volume. (d) Verification of CAL for PO's.

Fig. 2a. shows the variation of V_B with V_P. It shows that V_B decreases by increasing V_P as predicted by equation (8). This means that the volume of quantum state decreases by incresing V_P. The maximum volume of quantum state was found to be V_B = 4.70767 $Å^{-3}$ for $SmCoO_3$ and the minimum volume of quantum state was found to be V_B = 0.864487 $Å^{-3}$ for $PrLuO_3$. This result indicates that $SmCoO_3$ can be converted into superconductor at low temperature while $PrLuO_3$ is dielectric [6]. It was also found that for PO's, that have the orthorhombic structure, V_P ranges from 143.5876 to 286.9334 Å^3 corresponding to V_B ranges from 0.864487 to 1.72751 Å^{-3}. On the average, this is the smallest volume of quantum state. In case of PO's with cubic structure, V_P ranges from 52.73438 to 68.61886 Å^3 corresponding to the volume V_B ranges from 3.614898 to 4.703767 Å^{-3}. On the average, this is the largest volume of quantum state. In

between we found that PO's, that have hexagonal structure, have V_P ranges from 108.7328 to 130.4333 $Å^3$ corresponding to V_B ranges from 1.90174 to 2.281282 $Å^{-3}$.

Fig. 2b. shows the variation of V_F with V_B. It shows that V_F increases linearly with V_B according to CAL for the three crystalline systems (cubic, hexagonal and orthorhmbic). The maximum V_F was found for orthorhmbic system V_F = 82.9195 $Å^{-3}$ for $PbZrO_3$, and the minimum was found for distorted cubic system V_F = 34.59461 $Å^{-3}$ for $BaBiO_3$. Fig. 2c shows the variation of E_F with V_F. It shows that E_F increases by increasing V_F from 15.567 eV up to maximum value 27.8807 eV for $PbZrO_3$ orthorhombic compound. The minimum value of E_F was found to be 15.567 eV for $BaBiO_3$ distorted cubic. On the average E_F is greater for orthorhmbic system than hexagonal system and is small for cubic system.

Fig. 2d shows the relation between V_F/V_B and nVEC/2. It shows that a linear relation as predicted by CAL. That means verification of CAL for PO's.

The PO's that can be converted into superconductors at low temperature have cubic structure with the largest volume of quantum state as $SrTiO_3$. This compound is the most famous compound to have superconducting properties [27]. The dielectric PO's have the orthorhombic structure with the smallest volume of quantum state. It is found that the PO's with hexagonal structure are semiconducting and have intermediate volume of quantum state such as $BaCoO_3$. It is clear from the above results that the electrical properties of PO's depend on the volume of quantum states. The connection between the electrical properties and the volume of quantum state is in a good agreement with CALQQM results [24].

Table 1 : Crystal structure data obtained from ICDD cards [26] for PO's used in this study.

compound	card no.	System	*S.G*	*Z*	*VEC*	*n*	*Dx* (gm/cm^3)	*Mwt* (*gm / mol*)	*a* (Å)	*b* (Å)	*c* (Å)
$CeCrO_3$	750289	Cub.	$Pm3^-m$	1	4.8	5	6.774	240.11	3.89		
$PrCoO_3$	750280	Cub	$Pm3^-m$	1	4.8	5	7.62	247.84	3.76		
$SmCoO_3$	750282	Cub	$Pm3^-m$	1	4.8	5	8.103	257.33	3.75		
$SrNbO_3$	790625	Cub	$Pm3^-m$	1	4.8	5	5.824	228.52	4.024		
$KTaO_3$	770918	Cub	$Pm3^-m$	1	4.8	5	7.016	268.04	3.9883		
$NdCoO_3$	750281	Cub	$Pm3^-m$	1	4.8	5	7.784	251.17	3.77		
$SrTiO_3$	840443	Cub	$Pm3^-m$	1	4.8	5	5.145	183.52	3.898		
$SrZrO_3$	760167	Cub	$Pm3^-m$	1	4.8	5	5.489	226.84	4.094		
$CeVO_3$	750284	Cub	$Pm3^-m$	1	4.8	5	6.692	239.06	3.9		
$NdVO_3$	750286	Cub	$Pm3^-m$	1	4.8	5	6.86	243.18	3.89		
$PrCrO_3$	750290	Cub	$Pm3^-m$	1	4.8	5	6.796	240.9	3.89		
$PrVO_3$	750285	Cub	$Pm3^-m$	1	4.8	5	6.766	239.85	3.89		
$SmCrO_3$	750292	Cub	$Pm3^-m$	1	4.8	5	7.23	250.39	3.86		
$SmVO_3$	750287	Cub	$Pm3^-m$	1	4.8	5	7.034	244.34	3.89		
$SrMoO_3$	810640	Cub	$Pm3^-m$	1	4.8	5	6.168	231.56	3.9651		
$BaMoO_3$	893139	Cub	$Pm3^-m$	1	4.8	5	7.081	281.27	4.0404		
$BaTiO_3$	831880	Distorted cub.	P4mm	1	4.8	5	6.018	233.23	3.9945		4.0335
BaBiO3	700602	Distorted cub.	$P4^-2m$	1	4.8	5	7.61	394.31	4.364		4.518
PbTiO3	780299	Distorted cub.	P4mm	1	4.8	5	7.98	303.1	3.94		4.063
$CdTiO_3$	781015	ortho	Pbn21	4	4.8	20	6.315	208.31	5.3063	5.4215	7.6176
$NdGaO_3$	812294	ortho	Pbn21	4	4.8	20	7.571	261.96	5.4243	5.5014	7.7016
$CaZrO_3$	762401	ortho	Pcmn	4	4.8	20	4.611	179.3	5.5912	8.0171	5.7616
$NdCrO_3$	880472	ortho	Pnma	4	4.8	20	7.098	244.23	5.4798	7.6918	5.4221
$NdFeO_3$	886644	ortho	Pnma	4	4.8	20	6.971	248.09	5.5887	7.7619	5.4489
$CaVO_3$	860358	ortho	Pnma	4	4.8	20	4.312	139.02	5.3171	7.5418	5.3396
$SrRuO_3$	895713	ortho	Pnma	4	4.8	20	6.488	236.69	5.5368	7.8523	5.5731
$LaCrO_3$	831327	ortho	Pnma	4	4.8	20	6.782	238.9	5.476	7.752	5.512
$PrLuO_3$	894507	ortho	Pnma	4	4.8	20	8.423	363.87	5.9868	8.3202	5.7604
$LaTiO_3$	841089	ortho	Pbnm	4	4.8	20	6.246	234.8	5.6247	5.6071	7.9175
$CaSnO_3$	771797	ortho	Pbnm	4	4.8	20	5.527	206.77	5.532	5.681	7.906
$CaTiO_3$	820232	ortho	Pbnm	4	4.8	20	3.876	135.98	5.475	5.4863	7.7579
$CaGeO_3$	751764	ortho	Pbnm	4	4.8	20	5.171	160.67	5.2607	5.2688	7.4452
$DyCoO_3$	731197	ortho	Pbnm	4	4.8	20	8.678	269.43	5.162	5.4	7.398
$HoCoO_3$	731198	ortho	Pbnm	4	4.8	20	8.719	271.86	5.157	5.429	7.397
$TbCoO_3$	731196	ortho	Pbnm	4	4.8	20	8.484	265.86	5.2	5.394	7.421
$LaVO_3$	782305	ortho	Pbnm	4	4.8	20	6.558	237.85	5.543	5.543	7.84
$MgSiO_3$	841289	ortho	Pbnm	4	4.8	20	4.107	100.39	4.7754	4.9292	6.8969
$YFeO_3$	892609	ortho	Pbnm	4	4.8	20	5.696	192.75	5.2819	5.5956	7.6046
$SrSnO_3$	771798	ortho	Pbnm	4	4.8	20	6.431	254.31	5.707	5.707	8.064
$GdGaO_3$	700238	ortho	Pbnm	4	4.8	20	8.098	274.97	5.334	5.548	7.621
$TbMnO_3$	720379	ortho	Pbnm	4	4.8	20	7.607	261.86	5.297	5.831	7.403
$PrRhO_3$	231388	ortho	Pbnm	4	4.8	20	7.983	291.81	5.4143	5.7473	7.8026
$SmAlO_3$	711597	ortho	Pbnm	4	4.8	20	7.155	225.38	5.2912	5.2904	7.474
$SmFeO_3$	741474	ortho	Pbnm	4	4.8	20	7.246	254.25	5.4	5.597	7.711
$SmInO_3$	251106	ortho	Pbnm	4	4.8	20	7.825	313.22	5.587	5.875	8.1
$SmNiO_3$	801948	ortho	Pbnm	4	4.8	20	7.789	257.1	5.3283	5.4374	7.5675
$TbCrO_3$	251072	ortho	Pbnm	4	4.8	20	7.803	258.92	5.288	5.506	7.57
$NdNiO_3$	801947	ortho	Pbnm	4	4.8	20	7.546	250.94	5.3888	5.3845	7.6127

$PrNiO_3$	801946	ortho	Pbnm	4	4.8	20	7.415	247.61	5.4154	5.3755	7.6192
$YCrO_3$	340365	ortho	Pnma	4	4.8	20	5.751	188.9	5.5237	7.5343	5.2427
$GdFeO_3$	780451	ortho	Pnma	4	4.8	20	7.533	261.1	5.616	7.668	5.346
$PbZrO_3$	770856	ortho	Pbma	4	4.8	20	16.025	346.42	5.89	5.897	4.134
YBO_3	880356	Hexa	P63/m	2	4.8	10	4.512	147.71	3.776		8.806
$YAlO_3$	741334	Hexa	P63/mmc	2	4.8	10	4.411	163.89	3.68		10.52
$InFeO_3$	852306	Hexa	P63/mmc	2	4.8	10	6.222	218.67	3.327		12.175
$BaCoO_3$	740902	Hexa	P63/mmc	2	4.8	10	6.219	244.26	5.59		4.82
$DyBO_3$	741933	Hexa	P63/mmc	2	4.8	10	6.668	221.31	3.793		8.847
$ErBO_3$	741935	Hexa	P63/mmc	2	4.8	10	6.937	226.07	3.767		8.807
$GdBO_3$	741932	Hexa	P63/mmc	2	4.8	10	6.312	216.06	3.839		8.906
$HoBO_3$	741934	Hexa	P63/mmc	2	4.8	10	6.782	223.74	3.784		8.836
$SmBO_3$	741930	Hexa	P63/mmc	2	4.8	10	5.991	209.21	3.862		8.978
$BiFeO_3$	712494	Roh-Hex	R3c	6	4.8	10	8.313	312.83	5.5876		13.867
$LaAlO_3$	851071	Roh-Hex	$R\bar{3}m$	6	4.8	10	6.52	213.89	5.3651		13.11199
$LaCoO_3$	861665	Roh-Hex	$R\bar{3}m$	6	4.8	10	6.838	245.84	5.5397		13.47863

Table 2: Results of CAL parameters for PO's.

Compound	*System*	V_P ($Å^3$)	V_B ($Å^{-3}$)	E_F(eV)	V_F ($Å^{-3}$)	nVEC/2	V_F/V_B
$CeCrO_3$	Cub	58.86387	4.213964	20.05073	50.57042	12	12.00068
$PrCoO_3$	Cub	53.15738	4.666337	21.23388	55.11187	12	11.81052
$SmCoO_3$	Cub	52.73438	4.703767	21.57466	56.4439	12	11.99972
$SrNbO_3$	Cub	65.15893	3.806849	18.73722	45.68344	12	12.00033
$KTaO_3$	Cub	63.44004	3.909995	19.07364	46.91931	12	11.99984
$NdCoO_3$	Cub	53.58263	4.629302	21.34668	55.55161	12	12
$SrTiO_3$	Cub	59.22779	4.188072	19.96679	50.25318	12	11.99912
$SrZrO_3$	Cub	68.61886	3.614898	18.10045	43.37457	12	11.99884
$CeVO_3$	Cub	59.319	4.181632	19.94679	50.17768	12	11.99955
$NdVO_3$	Cub	58.86387	4.213964	20.04954	50.56591	12	11.99961
$PrCrO_3$	Cub	58.86387	4.213964	20.05017	50.56828	12	12.00017
$PrVO_3$	Cub	58.86387	4.213964	20.04942	50.56545	12	11.9995
$SmCrO_3$	Cub	57.51246	4.312982	20.3636	51.75865	12	12.00066
$SmVO_3$	Cub	58.86387	4.213964	20.32258	51.60234	12	12.24556
$SrMoO_3$	Cub	62.33937	3.97903	19.2972	47.7466	12	11.99956
$BaMoO_3$	Cub	65.95885	3.760681	18.58465	45.12662	12	11.99959
$BaTiO_3$	Distorted cub.	64.3587	3.854186	18.89233	46.25188	12	12.00043
BaBiO3	Distorted cub.	86.043	2.882862	15.567	34.59461	12	12.00009
PbTiO3	Distorted cub.	63.0724	3.932786	19.14777	47.19311	12	11.99992
$CdTiO_3$	ortho	219.1439	1.131906	21.03532	54.34065	48	48.00812
$NdGaO_3$	ortho	229.8253	1.079299	20.37601	51.80598	48	47.99966
$CaZrO_3$	ortho	258.2649	0.960449	18.85024	46.0974	48	47.99569
$NdCrO_3$	ortho	228.5389	1.085374	20.4518	52.09531	48	47.99756
$NdFeO_3$	ortho	236.3675	1.049426	19.99697	50.36716	48	47.99495
$CaVO_3$	ortho	214.1207	1.15846	21.35869	55.5985	48	47.99346
$SrRuO_3$	ortho	242.2995	1.023734	19.66954	49.13518	48	47.99605
$LaCrO_3$	ortho	233.9841	1.060116	20.13422	50.88658	48	48.00097
$PrLuO_3$	ortho	286.9334	0.864487	17.57333	41.4937	48	47.99806
$LaTiO_3$	ortho	249.7041	0.993376	19.28011	47.68321	48	48.00115

$CaSnO_3$	ortho	248.4642	0.998334	19.34231	47.91412	48	47.99408
$CaTiO_3$	ortho	233.0279	1.064466	20.18891	51.09405	48	47.99971
$CaGeO_3$	ortho	206.3629	1.20201	21.89106	57.69011	48	47.99471
$DyCoO_3$	ortho	206.2178	1.202856	21.90229	57.73449	48	47.99785
$HoCoO_3$	ortho	207.0964	1.197752	21.8401	57.48876	48	47.99721
$TbCoO_3$	ortho	208.1501	1.191689	21.76734	57.20174	48	48.00057
$LaVO_3$	ortho	240.8828	1.029755	19.7463	49.42309	48	47.99501
$MgSiO_3$	ortho	162.3455	1.527916	25.68797	73.33239	48	47.99504
$YFeO_3$	ortho	224.757	1.103637	20.68033	52.97088	48	47.99664
$SrSnO_3$	ortho	262.6433	0.944438	18.64019	45.32906	48	47.99581
$GdGaO_3$	ortho	225.5285	1.099862	20.6333	52.79029	48	47.9972
$TbMnO_3$	ortho	228.655	1.084823	20.44575	52.07219	48	48.00064
$PrRhO_3$	ortho	242.7982	1.021631	19.64344	49.03741	48	47.99914
$SmAlO_3$	ortho	209.2164	1.185615	21.69218	56.90571	48	47.99677
$SmFeO_3$	ortho	233.0557	1.064339	20.18669	51.08566	48	47.99756
$SmInO_3$	ortho	265.8714	0.932971	18.48971	44.78128	48	47.99858
$SmNiO_3$	ortho	219.2464	1.131377	21.02616	54.30518	48	47.9992
$TbCrO_3$	ortho	220.4061	1.125424	20.95259	54.02038	48	48.00003
$NdNiO_3$	ortho	220.8901	1.122958	20.92208	53.90245	48	48.00042
$PrNiO_3$	ortho	221.7986	1.118358	20.86423	53.67902	48	47.99807
$YCrO_3$	ortho	218.1866	1.136872	21.09508	54.57239	48	48.00223
$GdFeO_3$	ortho	230.2174	1.077461	20.35234	51.71573	48	47.99779
$PbZrO_3$	ortho	143.5876	1.727519	27.8807	82.9195	48	47.9992
YBO_3	Hexa	108.7328	2.281282	21.14202	54.75462	24	24.00169
$YAlO_3$	Hexa	123.3756	2.010529	19.43107	48.24432	24	23.99584
$InFeO_3$	Hexa	116.7058	2.125432	20.16512	51.00378	24	23.99691
$BaCoO_3$	Hexa	130.4333	1.90174	18.72488	45.63834	24	23.9982
$DyBO_3$	Hexa	110.2249	2.250401	20.94932	54.00776	24	23.99917
$ErBO_3$	Hexa	108.2274	2.291936	21.20604	55.0035	24	23.99871
$GdBO_3$	Hexa	113.6676	2.182241	20.52274	52.36658	24	23.99669
$HoBO_3$	Hexa	109.566	2.263934	21.03374	54.33451	24	24.00004
$SmBO_3$	Hexa	115.9637	2.139033	20.25124	51.33085	24	23.99722
$BiFeO_3$	Roh-Hex	124.9806	1.98471	19.26667	47.63333	24	24.00015
$LaAlO_3$	Roh-Hex	108.9514	2.276705	21.11276	54.64101	24	24.00004
$LaCoO_3$	Roh-Hex	119.4153	2.077207	19.86208	49.85838	24	24.00261

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