Modeling of Bulk Modulus of $A_2BX_6$ cubic crystals $(A = K, Cs, Rb, TI, NH_4; B = \text{tetravalent cation}; X = F, Cl, Br, I)$ using semi-empirical Model

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Abstract
In this work, a semi-empirical relation is elaborated in terms of lattice constant ($a_0$) and product of ionic charges ($Z_a Z_b Z_c$) for the calculation of bulk moduli (in GPa) of $A_2BX_6$ ($A$: large cation, $B$: transition metal and $X$: halide anions) structured materials. $Z_a Z_b Z_c$ and $a_0$ were related through bulk modulus through linear regression. These two parameters yield a straight regression line, when plotted but fall on different positions due the variation in bulk modulus values. The calculated values of bulk moduli reflecting elastic characteristics are in close agreement with other available values. As, these values are only differ by average of 3% from values of literature. Moreover, the regression resulted in a good values of correlation coefficient ($R=0.77$) and Probability ($P=0.001$). These all show the accuracy and
reliability of the current work. The technique adopted in this work will be helpful to material scientists for finding new materials with preferred elastic characteristics among structurally similar materials, also the calculated data will act as reference for upcoming investigation of the studied compounds.

**Keywords:** semi-empirical relation; bulk moduli; linear regression; correlation coefficient; elastic characteristics

**1. Introduction**

Perovskite structured materials have the potential to be used in ferroelectric, semiconducting, superconducting, catalytic, and thermoelectric applications [1-6]. Magnetic perovskites possess half metallic nature with high Curie temperature, quantized magnetic moment and zero maximum spin polarizibility [7]. They have wide range of applications in diverse fields of optoelectronics, spintronic and thermo-electronics industry [8-10]. Beside these, perovskite family has been a promising candidate of many devices such as multiferroic devices, high-temperature solid oxide fuel cells, solar cells, high Tc superconductors, and thermocouple [11-17]. Magnetic character compounds of this class are much suitable for industrial based spin filters, spin valves, magnetic sensors and magnetic memories [18, 19]. The key property through which these compounds have many characteristics and applications is the ideal cubic structures as shown in **Figure 1**. This can be altered through replacing its atoms. In such a way, perovskite structure can accommodate hundreds of elements from the periodic table, thus making
huge class of halide ABX₃, oxides ABO₃ and anti-fluorites A₂BX₆, and double perovskites A₂BB’M₆.

Since last decade, a lot of experimental and theoretical works have been dedicated for the investigation of various physical properties of these materials [20-24]. Specially, Anti-fluorites have recently attracted the interest because of their stunning properties mentioned above. These compounds belongs to the cubic Fm3m space group in which alkali and alkaline earth metal occupy A site, transition element occupy B site while the X site is occupied by an element from halogen (F, Cl, Br) [20]. A and B site cations have Wyckoff’s sites 8e (1/4, 1/4, 1/4) and 4b (0, 0, 0), respectively, while X site anion occupy 24a (u, 0, 0) site. u is an anion displacement parameter having different value for each compound. Some physical properties such as electronic, elastic, optical, thermoelectric and stability under applied stimulus make anti-fluorite compounds more attractive than other perovskite compounds [25, 26].

Elastic moduli demonstrate various aspects of compounds i.e. chemical bonding nature, retention of maximum stress etc. Generally, these parameters can be calculated via first principle calculations [25]. But complex and lengthy computations along with the use of approximation makes this very complicated [27, 28]. On the other hand, empirical calculation based on concepts like valence, ionic radii, lattice constant and plasmon energy are useful and easy [29, 30]. There are a number of works reporting the mechanical properties of solids [31, 32] by applying of
empirical formulism. Cohen [33] found a semi-empirical expression for the
bulk modulus of covalent solids as:

\[
B \text{(GPa)} = \frac{N_c (1972 - 220 \lambda)}{4d^{3.5}}
\]

(1)

\(N_c\) and \(d\) represents bulk coordination number and bond length, whereas \(\lambda\) is
an empirical ionicity parameter having the values of 0, 1, and 2 respectively
for semiconductors of IV, III–V and II–VI group. Anderson and Nafe [34]
suggested an empirical correlation between bulk modulus at normal pressure
and volume (\(V_0\)) as \(B - V_0^{-x}\).

Verma et.al [35, 36] had improved the expression by introducing product of
ionic charge as ad hoc empirical ionicity parameter for the calculation of bulk
modulus of \(\text{ABX}_3\) and \(\text{ABO}_3\) compounds.

**Theoretical details;**

At the equilibrium state, 2nd derivative of the total energy (E) as a function
of the fitting deformation parameter (\(\Omega, \gamma\)) can give elastic moduli such as
bulk (\(B\)) and shear (\(G\)) moduli as by the relations [33]:

\[
B = \left| \Omega \frac{\partial^2 E}{\partial \Omega^2} \right|_{\Omega=\Omega}, \quad G = \left| \frac{1}{\Omega} \frac{\partial^2 E}{\partial \gamma^2} \right|_{\gamma=\gamma},
\]

(2)

Where, \(\Omega\) and \(\gamma\) symbolize volume and dimensionless deformation
parameter, respectively. First phase is to estimate the derivatives of
energies in terms of chemical bonding parameters to set up the formulae for
\(B\) and \(G\), as can be judged from eq. 2. Low energy perturbation under elastic
deformation do not effect core electrons, because of their tight-binding
nature [37]. The valence electrons being not tight can be affected by such perturbation. In result, the core electrons do not take part in elastic deformation while the valence electrons have a significant contribution in the distortion process. Therefore, the variation of total energy of core electrons with respect to deformation parameter is insignificant. Only the second derivative of the total energy of valence electrons can be approximated within elastic system. Valance bond strength inside covalent bonded materials, resulting from ionic contributions of the atoms can be estimated from band gap energy (E\text{g}) as follow [30]:

\[
E_g = \sqrt{E_h^2 + E_c^2}
\]  

(3)

Here, \(E_h\) corresponds to covalent involvement in the bonding, while \(E_c\) refers to the ionic contribution to the bonds. In pure covalent compounds, \(E_g\) is equal to \(E_h\). From the discussion, it is clear that \(E_h\) dominates the intrinsic properties of covalent materials and the strength of the covalent bond as well. \(E_h\) can be written in terms of \(d\) (nearest neighbor distance) as follows [30]:

\[
E_h = \frac{39.74}{d^{2.5}}
\]  

(4)

\(E_h\) and \(d\) are measured in eV and Å, respectively. For small deformation, the second derivative of total energy as a function of strain parameter has a linear relation with \(d\), from eq. 4, it follows that:

\[
\frac{\partial^2 E}{\partial \delta^2} \propto \frac{1}{d^{4.5}}
\]  

(5)
As \[ \Omega = 4 \pi d \left| a^B \right|^2 \] and can be employed in eq. 2, since it encompasses huge numbers of electrons [33] so eqs. 2–5 yield

\[ B \propto \frac{1}{d^{3.5}} \]  

(6)

Most of the properties of solids depend upon loosely bonded valence electrons; in term of ionic charge is the property of valence electrons. So, there must be a relationship between ionic charge and the properties of materials. Goldschmidt confirmed this statement by indicating that valence number of anions and cations can be considered for a direct estimation of hardness of a material [38].

Linear regression analysis has been performed for the bulk modulus as a function of \[ \frac{(Z_a Z_b Z_c)^{0.35}}{a^{3.5}} \], which gave in expression of the form:

\[ B = 0.7504 + 30100.3450 \times \frac{(Z_a Z_b Z_c)^{0.35}}{a^{3.5}} \]

(7)

Where \( Z_a, Z_b \) and \( Z_c \) are the ionic charges residing on A, B and X atoms, respectively. \( a_0 \) refers to lattice constant taken in Å. The constant values 0.7504 and 30100.3450 are intercept (S) and slope (V) of the line which depends on the crystal structure. Table 1 tabulates the values of S and V along with correlation coefficient R and probability P (significance of the regression).

2. Results and Discussion
Bulk moduli (B) are vital to understand many basic properties, calculated theoretically via interceding deformation potentials in phonon density of states and electron-phonon interaction processes. Moreover, B is an important parameter for calculation of mechanical parameters such as Young modulus, Pugh’s ration, Poisson’s ratio, mechanical hardness [39, 40]. Mechanical properties are very important in the exploration of materials industrial based application. Additionally, these properties are also can be used in broad analysis of wide characteristics of materials. Unfortunately, the data obtained so far is still insufficient and inconsistent. So, following eq. 7, the bulk moduli of A$_2$BX$_6$ compounds were calculated from the summation of intercept (S) and slope (V) of the line times of ionic charge product/lattice constant. Using the linear regression analysis of previous calculated bulk moduli of compounds of this family, the regression line is plotted in Figure 2 (b). The S and V values obtained from regression analysis are given in Table 1. We observe that in the Figure 2 (b) that the B shows linear relation with ionic charge product and lattice parameter but lie on different point due to the variation in B values. Elastic moduli adopt a decreasing trend with increasing lattice constant [33]. Another investigation also confirmed this statement of inverse relation between lattice parameter and elastic moduli [41]. So, based on eq. 6, the current compounds also follow the same statement as shown in Figure 2 (a). Furthermore, we noted from the figures that the B depends explicitly on lattice parameter and ionic charge. Table 2 list the calculated values of B for compounds under study along with
available data evaluated by other researchers [18, 21, 42-45] for the sake of comparison. It can be seen that our results through proposed relation agrees well with previous calculated data. The previous calculated and predicted values of B are plotted in Figure 3. The values for bulk moduli differ from previous calculated by 0.5% (K$_2$SnI$_6$), 6% (K$_2$SnCl$_6$) and 8% (Cs$_2$NbI$_6$) in the current work. As a result, the reliability and accuracy of proposed formula is well verified. Since the noted difference between current and previous calculated measurements arise errors but the present study reveal that analogous relation also exists for the estimation the bulk moduli from their lattice parameter and ionic charges. In addition, it should be noted that experimental results are unavailable for B for A$_2$BX$_6$ perovskites. Therefore we are still confident about our calculations.

3. Conclusions

There are a number of techniques available from experimental to theoretical calculations of elastic properties of materials, but the accuracy of the resulted data always has been impulsive by the reason of negligible change in the dimension of unit cell. From the relation of elastic parameters with ionic charges and lattice parameter as discussed in section 2, we got the conclusion that there must be a way of finding elastic parameters from lattice parameters. So, through linear regression analysis based on the already calculated data, a semi-empirical relation in term of lattice constant and product of ionic charge is achieved. Through the proposed empirical relation, bulk moduli of broad class of compounds exhibiting A$_x$BX$_y$ structures
can be calculated. The bulk moduli of $A_2BX_6$ (X=F, Cl, Br, I) is evaluated in this work in which the bulk moduli exhibit a linear relationship when plotted against lattice parameter but lie on different straight lines according to the bulk moduli of the compounds. From these, it is quite obvious that the bulk moduli can be expressed in terms of ionic charge product and lattice parameter of these compounds. Author’s calculated values in this work and pre-reported values calculated by other researchers are in good agreement. We hope that the adopted method and the data calculated in this work will serve as a reference for future project on the studied compounds.

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**Figures Caption**

**Figure 1.** Unit cell structure of $A_2BX_6$ in polyhedral presentation

**Figure 2.** Regression Plot of (a) Bulk modulus $B$ (GPa) versus lattice constant (in Å) for $A_2BX_6$ compounds. (b) Bulk modulus $B$ (GPa) as a function of $(Z_aZ_bZ_c)^{0.35}/a^{3.5}$

**Figure 3.** Cross-plot between previous and predicted values of Bulk moduli of $A_2BX_6$ compounds
Table 1. Obtained data from linear regression analysis for A_2BX_6 (X=F, Cl, Br, I) compounds.

| Material      | Parameter       | S       | V       | R       | P       |
|---------------|-----------------|---------|---------|---------|---------|
| A_2BX_6 (X=F, Cl, Br, I) | Bulk Modulus | 0.7504±6. | 30100±712 | 0.7772 | 0.001  |

Table 2. Calculated values of bulk modulus (B in GPa) for A_2BX_6, (X = F, Cl, Br, I) compoundsthrough Equation 7. The value of product of ionic charges (Z_aZ_bZ_c) is 48.

| Material | a_0 (A) [21,42] | B (GP a) | B (This Work) (GPa) | Material | a_0 (A) [21,42] | B (GP a) | B (This Work) (GPa) |
|----------|-----------------|----------|---------------------|----------|-----------------|----------|---------------------|
| Cs_2GeF_6 | 8.99            | 52.35    | 64.95               | Rb_2SiF_6 | 8.44            | 61.51    | 33.57               |
| Cs_2MnF_6 | 8.97            | 52.71    | 33.78               | Cs_2GeCl_6 | 10.23          | 33.00    | 34.19               |
| Rb_2CoF_6 | 8.91            | 53.90    | 34.01               | Cs_2GeCl_6 | 10.23          | 33.00    | 34.19               |
| Cs_2NiF_6 | 8.93            | 53.41    | 33.78               | Cs_2IrCl_6 | 10.21          | 33.00    | 34.19               |
| Cs_2PdF_6 | 9.00            | 52.15    | 33.78               | Cs_2MoCl_6 | 10.21          | 33.00    | 34.19               |
| Cs_2SiF_6 | 8.89            | 54.41    | 31.57               | Cs_2PbCl_6 | 10.41          | 31.57    | 34.01               |
| Rb_2CrF_6 | 8.52            | 62.94    | 31.57               | Cs_2PtCl_6 | 10.19          | 34.01    | 34.99               |
| Rb_2GeF_6 | 8.58            | 61.44    | 33.30               | Cs_2ReCl_6 | 10.25          | 33.30    | 34.99               |
| K_2HfF_6  | 9.01            | 51.95    | 37.73               | Tl_2TeCl_6 | 10.10          | 37.73    | 34.99               |
| K_2MnF_6  | 8.22            | 71.31    | 38.63               | (NH_4)_2MnCl_6 | 9.82          | 38.63    | 34.99               |
| K_2NiF_6  | 8.10            | 74.78    | 38.63               | (NH_4)_2VCl_6 | 9.85          | 38.23    | 34.99               |
| K_2SiF_6  | 8.14            | 73.74    | 38.63               | (NH_4)_2SeC l_6 | 9.93          | 37.12    | 34.99               |
| (NH_4)_2SiF_6 | 8.39   | 66.32    | 38.36               | (NH_4)_2PdCl_6 | 9.84          | 38.36    | 34.99               |
| (NH_4)_2GeF_6 | 8.46   | 64.28    | 38.44               | (NH_4)_2PtCl_6 | 9.83          | 38.44    | 34.99               |
| (NH_4)_2PtF_6 | 8.45   | 64.81    | 38.44               | (NH_4)_2PtCl_6 | 9.83          | 38.44    | 34.99               |
| Cs_2SeCl_6 | 10.26          | 33.24    | 37.96               | (NH_4)_2IrCl_6 | 9.87          | 37.96    | 34.99               |
| Compound         | Unit Cell Dimension | Density (g/cm³) | Phase | Temperature Range (°C) | Additional Information |
|------------------|---------------------|-----------------|-------|------------------------|------------------------|
| Cs₂SnCl₆         | 10.3 5              | 32.21           | (NH₄)₂ReCl₆ | 9.93 | 37.18 |
| Cs₂TaCl₆         | 10.2 7              | 33.12           | (NH₄)₂TcCl₆ | 9.91 | 37.44 |
| Cs₂TeCl₆         | 10.4 4              | 31.27           | (NH₄)₂SnCl₆ | 10.03 | 35.83 |
| Cs₂TiCl₆         | 10.2 1              | 33.70           | (NH₄)₂TeCl₆ | 10.17 | 34.17 |
| Cs₂WCl₆          | 10.2 4              | 33.41           | (NH₄)₂PbCl₆ | 10.15 | 34.43 |
| Cs₂ZrCl₆         | 10.4 2              | 31.44           | Cs₂NpBr₆   | 11.08 | 25.56 |
| K₂MnCl₆          | 9.64                | 41.10           | Cs₂PoBr₆   | 10.99 | 26.29 |
| K₂MoCl₆          | 9.85                | 38.23           | Cs₂PtBr₆   | 10.67 | 29.08 |
| Rb₂MnF₆          | 8.53                | 62.74           | Cs₂SnBr₆   | 10.77 | 24.9 [43] 28.17 |
| Rb₂CoF₆          | 8.46 28             | 64.50           | Cs₂TeBr₆   | 10.87 | 27.27 |
| Rb₂NiF₆          | 8.46                | 64.52           | Cs₂UBr₆    | 11.07 | 25.65 |
| Rb₂PdF₆          | 8.57                | 61.75           | Cs₂WBr₆    | 10.73 | 28.50 |
| K₂OsCl₆          | 9.72 49.9 [18]      | 39.88           | K₂SeBr₆    | 10.42 | 31.50 |
| K₂PdCl₆          | 9.70                | 40.16           | K₂SnBr₆    | 10.48 | 27.80 [43] 30.91 |
| K₂PtCl₆          | 9.75                | 39.57           | K₂TeBr₆    | 10.78 | 28.08 |
| K₂ReCl₆          | 9.84                | 38.36           | Rb₂PdBr₆   | 10.02 | 36.05 |
| K₂RuCl₆          | 9.77                | 39.77           | Rb₂SnBr₆   | 10.58 | 26.27 [43] 29.93 |
| K₂SnCl₆          | 9.98 34.12 [43]     | 36.45           | Rb₂TeBr₆   | 10.71 | 28.68 |
| K₂TaCl₆          | 9.99                | 36.38           | Rb₂TaBr₆   | 10.73 | 34.95 [45] 28.53 |
| K₂TcCl₆          | 9.83                | 38.49           | Rb₂UBr₆    | 10.94 | 26.70 |
| K₂TiCl₆          | 9.79                | 39.01           | Rb₂WBr₆    | 10.48 | 30.82 |
| K₂WCl₆           | 9.82                | 38.60           | (NH₄)₂SeBr₆ | 10.46 | 31.12 |
| Rb₂MnCl₆         | 9.83                | 38.39           | (NH₄)₂TiBr₆ | 10.43 | 31.42 |
| Compound | R | a (Å) | c (Å) | r<sub>6</sub> (Å) | Δ (Å) | Δa (Å) |
|----------|---|-------|------|--------|------|--------|
| Tl<sub>2</sub>MoCl<sub>6</sub> | 9.86 | 38.05 | (NH<sub>4</sub>)<sub>2</sub>NbB<sub>6</sub> | 10.55 | 30.19 |
| Rb<sub>2</sub>NbCl<sub>6</sub> | 9.98 | 36.43 | (NH<sub>4</sub>)<sub>2</sub>SnB<sub>6</sub> | 10.57 | 30.02 |
| Rb<sub>2</sub>PbCl<sub>6</sub> | 10.19 | 33.97 | (NH<sub>4</sub>)<sub>2</sub>TeB<sub>6</sub> | 10.72 | 28.54 |
| Rb<sub>2</sub>PdCl<sub>6</sub> | 9.99 | 36.42 | K<sub>2</sub>SnI<sub>6</sub> | 11.95 | 19.91 [43] |
| Rb<sub>2</sub>TaCl<sub>6</sub> | 10.21 [44] | 38.17 | Rb<sub>2</sub>PdI<sub>6</sub> | 11.18 | 19.80 |
| Rb<sub>2</sub>PtCl<sub>6</sub> | 9.88 | 37.78 | Rb<sub>2</sub>PtI<sub>6</sub> | 11.21 | 24.77 |
| Tl<sub>2</sub>PtCl<sub>6</sub> | 9.75 | 39.52 | Rb<sub>2</sub>SnI<sub>6</sub> | 11.62 | 20.29 [43] |
| Rb<sub>2</sub>TiCl<sub>6</sub> | 9.92 | 37.28 | Cs<sub>2</sub>NbI<sub>6</sub> | 11.54 | 24.72 [45] |
| Rb<sub>2</sub>WCl<sub>6</sub> | 9.95 | 36.83 | Rb<sub>2</sub>SeCl<sub>6</sub> | 9.97 | 36.57 |
| Rb<sub>2</sub>ZrCl<sub>6</sub> | 10.17 | 34.17 | Cs<sub>2</sub>PdI<sub>6</sub> | 11.33 | 23.69 |
| Tl<sub>2</sub>SnCl<sub>6</sub> | 9.97 | 36.67 | Rb<sub>2</sub>SnCl<sub>6</sub> | 10.17 | 32.50 [43] |
| Cs<sub>2</sub>HfI<sub>6</sub> | 11.60 | 21.83 | Cs<sub>2</sub>PoI<sub>6</sub> | 11.79 | 20.72 |
| Rb<sub>2</sub>TeCl<sub>6</sub> | 10.23 | 33.54 | Cs<sub>2</sub>PtI<sub>6</sub> | 11.15 | 24.97 |
| K<sub>2</sub>OsBr<sub>6</sub> | 10.30 [18] | 41.25 | Cs<sub>2</sub>SnI<sub>6</sub> | 11.65 | 19.59 [43] |
| K<sub>2</sub>PtBr<sub>6</sub> | 10.29 | 32.88 | Cs<sub>2</sub>TeI<sub>6</sub> | 11.70 | 21.27 |
| K<sub>2</sub>ReBr<sub>6</sub> | 10.38 | 31.89 | | | |