

Non Inverted Isothermal Equation of state for NaCl-CsCl type Crystals

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Abstract: The Pressure-Volume-temperature(P-V-T) relation using non inverted equation of state (EOS) viz. Murnaghan EOS, Usual-Tait EOS, Vinet EOS, Born-Mayer EOS, Birch EOS, Kumar EOS, Shanker EOS, Brennan Stacey EOS, Poirier- Tarantola EOS, Universal EOS and Freund & Ingalls EOS for NaCl-CsCl type crystals has been studied. It is found that except Murnaghan EOS, Brennan-Stacey EOS and Poirier Tarantola EOS all other EOS gives close agreement with each other even at high compression ranges. Also another remarkable characteristic observed when the value of compression decreases from 0.5 the variation in value of pressure as calculated by different EOS increases.

Key words: Non inverted EOS, Bulk modulus, P-V-T relation, NaCl-CsCl type crystal

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Introduction

The exploration of matter at extreme conditions is a central theme in a broad range of scientific disciplines (e.g. material science chemistry, physics, and Earth and planetary science). The application of pressure can induces both continuous and discontinuous changes in atomic and electronic structure. Learning how atomic and electronic arrangements change under extreme conditions, provide insight into the nature of phase transformations, chemical reaction, and also evolution in micro- and nanostructural components, such as crystallite size, dislocations, voids, and grain boundaries. Once these processes are understood, it will be possible to predict responses of materials under thermo-mechanical extremes using advanced computational tools. Further, this fundamental knowledge will open new avenues for designing and synthesizing materials with unique properties. Using these thermo-mechanical extremes will allow tuning the atomic structure and the very nature of chemical bonds to produce revolutionary new materials.

The compressibility of the alkali metals is very large, and the large volume reduction with application of pressure affects significantly the otherwise free-electron like electronic structure. As a consequence, these metals undergo several pressure-induced structural transformations. These have been studied experimentally as well as by theoretical methods [1-9] and references therein).

The equation of state (EOS) of a solid (pressure–volume relation) plays an important role in

condensed matter physics, because the knowledge of the EOS is of central importance for the general understanding of the behaviour and the application of condensed matters [10]. The EOS of crystalline solids has been a long-standing topic and extensively investigated. A lot of interesting and important phenomena have been observed [10].

In the last few decades a set of equations of state for solids which can be successfully applied to the description of thermodynamic properties of minerals in wide range of temperatures and pressures have been developed. In the most known work [11] the Debye approach are used for description of quasi-harmonic part of the Helmholtz free energy and additional contributions to the Helmholtz free energy are taken into account. However, the Debye approach is true within the limits of low and high temperatures but in the intermediate field it is inter-polar. Oxides and minerals have usually a high the Debye temperature (about 500-1000 K), therefore at room temperatures the Debye approximation is not always correct. For very good description of thermodynamic functions of solids from 10 K up to melting temperature it is possible to used the Bose-Einstein approximation [12, 13] which has been successfully used at construction of equation of state for NaCl [14] and some metals [15, 16]. However in the latter case construction of equations of state needs practically full set of experimental measurements (heat capacity, thermal expansion coefficient,

adiabatic bulk modulus from ~0 K and up to melting temperature, volume depending on pressure and temperature and shock data) which in most cases are absent for minerals. Other approximations which are quite successfully applied to equations of state for solids are also known (see, for example, [17,18,]. With the development of high pressure techniques, pressure is becoming an important processing variable just like that of temperature or chemical composition for condensed phases.

In the present work, compression dependence of pressure for twelve different alkali metal halides viz. LiF, LiCl, LiBr, NaF, NaCl, NaBr, KF, KCl, KBr, RbF, RbCl, and RbBr has been calculated by using different equation of state (EOS) viz. Murnaghan EOS, Usual-Tait EOS, Vinet EOS, Born-Mayer EOS, Birch EOS, Kumar EOS, Shanker EOS, Brennan Stacey EOS, Poirier-Tarantola EOS, Universal EOS and Freund & Ingalls EOS. Also a comparative study has been made among the calculated values of pressure by using different EOS to test applicability.

Formulation of equation of state

The derivation of EOS of a thermodynamic system is based on a fundamental theorem which equates the negative of pressure to the isothermal volume derivative of a Helmholtz free energy function, F . The function F consists of two terms in the case of solids, the first of which represents the potential energy of a non vibrating lattice while the second owes its origin to the pressure of the thermal vibrations.

An extensive study of the EOS and other thermodynamic properties of solids was first made by Grüneisen [19] who used a simple power law for the potential energy expression. Murnaghan equation of state [20] is based on empirical observation that the isothermal bulk modulus is a linear function of pressure. On the basis of finite strain theory Birch modified and improved the Murnaghan EOS and gave a new EOS known as Birch Eos [21,22] which is widely used in geophysics.

Shanker et.al. [23] obtained three sets of equations each for pressure, isothermal bulk modulus and its pressure derivative corresponding to three functions showing the dependence of short range force constant on volume. The first function is represented by the inverse power form which leads to the EOS given by Born-Mie [24,25]. The second function is represented by an exponential form which leads to the EOS which is identical to that obtained by Brennan and Stacey

[26,27], using thermodynamic formulation for the Grüneisen parameter. The third function is represented by a modified exponential form which leads to Shanker EOS [23]. Using relationship between binding energy and interatomic distance, Vinet proposed an EOS known as Vinet EOS [28,29]. By using an exponential function for short range overlap energy, Born-Mayer proposed a new equation of state known as Born-Mayer EOS [30]. A slight modification in Murnaghan EOS gave a new EOS known as Usual-Tait EOS [31,32]. On the basis of Modification in adjustable parameter of non inverted equation of state [33] we get universal equation of state [28,34] and further modifying in adjustable parameter we get another new equation of state known as Freund & Ingalls EOS [31]. By defining a Strain in terms of Logarithmic function, Poirier and Tarantola [35] derived a new equation of state known as Poirier & Tarantola EOS

An Equation of state can be derived from the volume derivative of lattice potential energy [24, 30] by using the relation

$$P = - \left(\frac{dW}{dV} \right)_T \quad (1)$$

where W for an ionic crystal can be written as the sum of electrostatic energy and short range overlap repulsive energy

$$W = -\alpha_M \frac{Z^2 e^2}{V^{1/3}} + \Phi(V) \quad (2)$$

By using an inverse power form for Φ such as (aV^{-n}) , we get an equation by eliminating the parameters 'a' and 'n' in terms of isothermal bulk modulus (K_0) and first derivative of isothermal bulk modulus (K'_0) at zero pressure known as Born-Mie EOS [24] which can be written as

$$P = \frac{3K_0}{3K_0 - 8} \left[\left(\frac{V}{V_0} \right)^{4/3 - K'_0} - \left(\frac{V}{V_0} \right)^{-4/3} \right] \quad (3)$$

when we use an exponential function for Φ [such as $b \exp \{-K(V/V_0)\}^{1/3}$ and eliminating b and K in terms of K_0 and K'_0 using the relationship for

potential parameter [36]] we get Born-Mayer EOS which is

$$P = \frac{3K_0}{(\eta-2)} \left[\left(\frac{V}{V_0} \right)^{-2/3} \exp \left\{ \eta \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right] \right\} - \left(\frac{V}{V_0} \right)^{-4/3} \right] \quad (4)$$

where

$$\eta = \frac{3(K'_0 - 1)}{2} + \left[\frac{9(K'_0 - 1)^2}{4} - 6K'_0 + 12 \right]^{1/2}$$

A simple EOS based on assumption according to which the isothermal bulk modulus K_T depends linearly on pressure i.e.

$$K_T = K_0 + K'_0 P$$

Murnaghan gave an equation of state known as Murnaghan EOS [20] which can be expressed as

$$P = \frac{K_0}{K'_0} \left[\left(\frac{V}{V_0} \right)^{-K'_0} - 1 \right] \quad (5)$$

A slight modification in Murnaghan EOS performed by Usual - Tait yields a new EOS known as Usual - Tait EOS [31,32], given by

$$P = \frac{K_0}{(K'_0 + 1)} \left[\left\{ \exp(K'_0 + 1) \left(1 - \frac{V}{V_0} \right) \right\} - 1 \right] \quad (6)$$

Kumar has presented a derivative of the UTE on the basis of Chopelas - Boehler approximation [37,38] and gave an EOS known as Kumar EOS

$$P = \frac{K_0}{K'_0 + 1} \left[\left\{ \exp(K'_0 + 1) \left(1 - \frac{V}{V_0} \right) \right\} - 1 \right] \quad (7)$$

which is same as Usual-Tait EOS

On the basis of finite strain theory [39] in which the expansion of Helmholtz free energy is considered as a polynomial series in terms of Eulerian Strain and taking third order

approximation Birch obtained an EOS [40] which is as follows

$$P = \frac{3K_0}{2} \left[\left(\frac{V}{V_0} \right)^{-7/3} - \left(\frac{V}{V_0} \right)^{-5/3} \right] \left[1 - \frac{3(4-K'_0)}{4} \left\{ \left(\frac{V}{V_0} \right)^{-2/3} - 1 \right\} \right] \quad (8)$$

Poirier and Tarantola [35] derived an equation similar to Birch EOS but define strain as

$\epsilon = \log(l_0/l)$ rather than Eulerian Strain $\epsilon = 1/2[(V/V_0)^{2/3} - 1]$ used by Birch and give an EOS as

$$P = K_0 \left(\frac{V_0}{V} \right) \left[\ln \left(\frac{V_0}{V} \right) + \left\{ \left(\frac{K'_0 - 2}{2} \right) \right\} \left\{ \ln \left(\frac{V_0}{V} \right)^2 \right\} \right] \quad (9)$$

Using the free volume formula [41] for the Grüneisen parameter γ and assuming that the Grüneisen parameter γ is proportional to volume, Brennan and Stacey obtained an EOS [28] which is given as

$$P = \frac{3K_0 \left(\frac{V}{V_0} \right)^{-4/3}}{(3K'_0 - 5)} \left[\exp \left\{ \frac{(3K'_0 - 5) \left(1 - \frac{V}{V_0} \right)}{3} \right\} - 1 \right] \quad (10)$$

Vinet proposed a new EOS on account of relating binding energy with inter atomic distances known as Vinet EOS [29] which may be expressed as

$$P = 3K_0 (1 - X) X^{-2} \exp[\eta(1 - X)] \quad (11)$$

where

$$\eta = \frac{3(K'_0 - 1)}{2}$$

and

$$X = \left(\frac{V}{V_0} \right)^{1/3}$$

On the basis of Born lattice theory [42] taking the volume derivative of short range force constant,

Shanker obtained a equation of state known as Shanker EOS [23, 43] which are as

$$P = \frac{\left[K_0 \left(\frac{V}{V_0} \right)^{-4/3} \right]}{t} \left[\left(1 - \frac{1}{t} + \frac{2}{t^2} \right) \{ \exp(ty) - 1 \} + y \left(1 + y - \frac{2}{t} \right) \exp(ty) \right] \quad (12)$$

where

$$y = 1 - \frac{V}{V_0} \quad \text{and} \quad t = \left(K_0' - \frac{8}{3} \right)$$

K_0 is isothermal bulk modulus and K_0' is the first derivative of isothermal bulk modulus at zero pressure.

The modification in the basic assumption of Kumari et al [33] EOS can be written as

$$P = \frac{K_0}{(K_0' + \alpha)} \frac{\exp\{-(K_0' + \alpha)\}}{\alpha} \left[\left\{ \left(\frac{V}{V_0} \right)^\alpha - 1 \right\} - 1 \right] \quad (13)$$

This equation can also be written as

$$\frac{V}{V_0} = \left[1 - \frac{\alpha}{[K_0' + \alpha]} \ln \left\{ 1 + \frac{K_0' + \alpha}{K_0} P \right\} \right]^{1/\alpha} \quad (14)$$

where α , K_0 & K_0' are adjustable parameters.

By Substituting the adjustable parameter $\alpha=1/3$ Freund and Ingalls introduced a new EOS known as Freund & Ingalls EOS [31] given by

$$P = \frac{K_0}{(K_0' + 1/3)} \frac{\exp\{-(K_0' + 1/3)\}}{1/3} \left[\left\{ \left(\frac{V}{V_0} \right)^{1/3} - 1 \right\} - 1 \right] \quad (15)$$

Further improving the adjustable parameter and putting $\alpha=2/3$ in equation (13) we obtained a new EOS known as Universal EOS [28,34] written as

$$P = \frac{3K_0}{(K_0' + 2/3)} \frac{\exp\{-(K_0' + 2/3)\}}{2} \left[\left\{ \left(\frac{V}{V_0} \right)^{2/3} - 1 \right\} - 1 \right] \quad (16)$$

Result and discussion:

- The pressure have been calculated at different compression ranges (from $V/V_0=1.0$ to 0.1) for twelve different alkali metal halides viz. LiF, LiCl, LiBr, NaF, NaCl, NaBr, KF, KCl, KBr, RbF, RbCl, and RbBr using twelve different isothermal equation of state viz. Murnaghan EOS, Usual –Tait EOS, Vinet EOS, Born Mayer EOS, Birch EOS, Kumar EOS, Shanker EOS, Brennan Stacey EOS, Poirier Tarantola EOS, Universal EOS and Freund Ingalls EOS from equation (3-12, 15 and 16). The calculated values are displayed in table (2 to13). The input values of isothermal bulk modulus (K_0) and its first pressure derivative (K_0') at zero pressure has been taken from the literature [37] displayed in table (1). The logarithmic values of calculated pressure obtained by using different isothermal EOS have been plotted against the logarithmic values of unit cell volume ratio (V/V_0), displayed graphically in figure (1-12).

Fig. 1

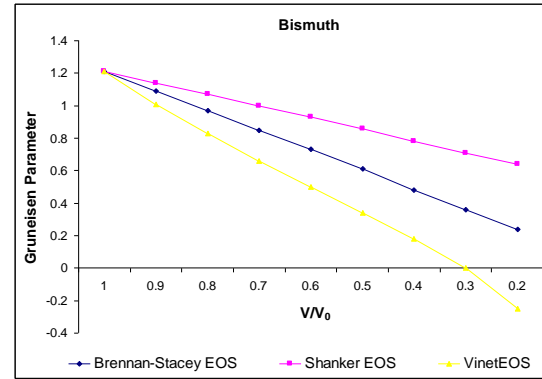


Fig. 2

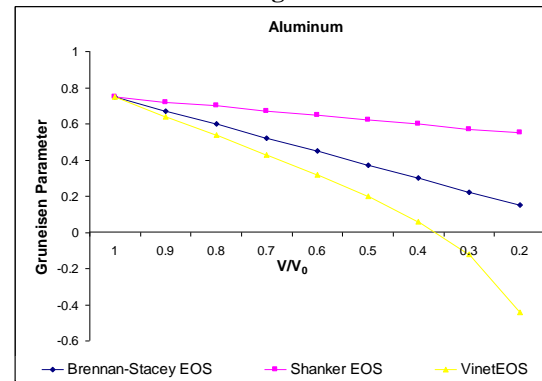


Fig. 3

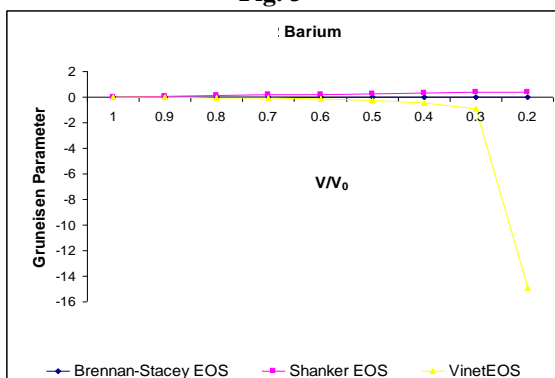


Fig. 4

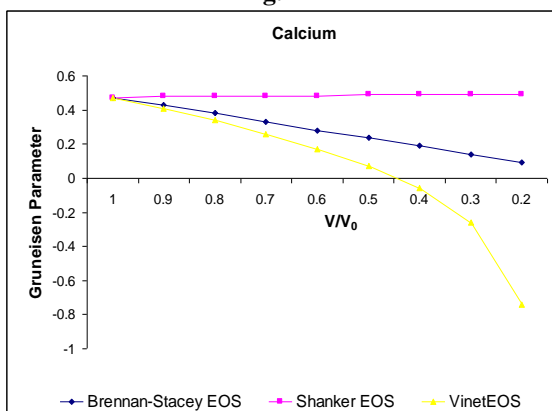


Fig. 5

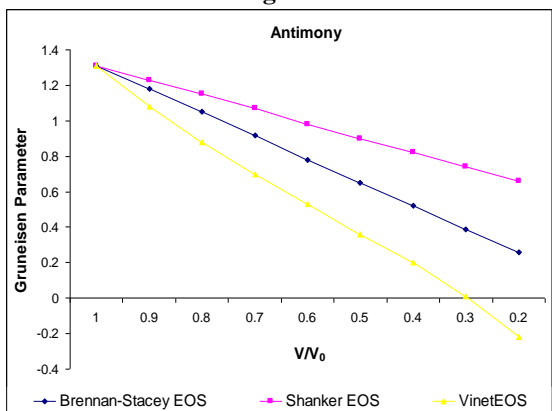


Fig. 6

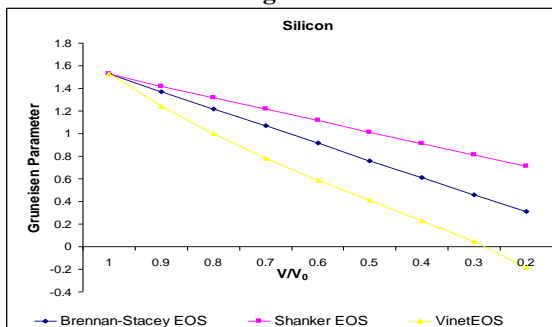


Fig. 7

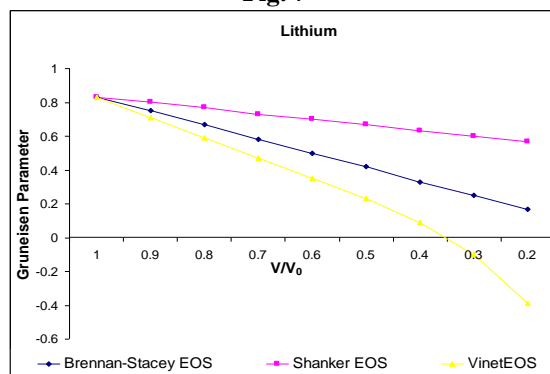


Fig. 8

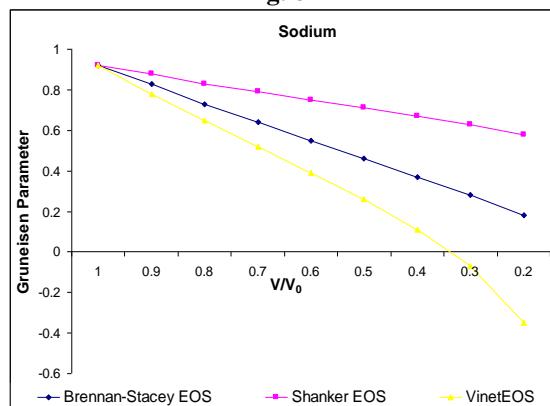


Fig. 9

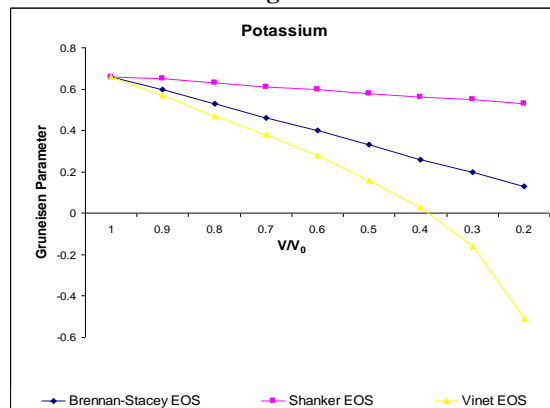


Fig. 10

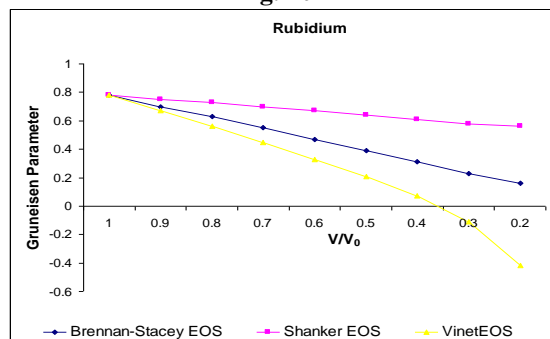


Fig. – (1-10) : The variation of Barton-Stacey Gruneisen Parameter γ_{ba-s} versus V/V_0 by using Brennan-Stacey EOS, Shanker EOS and Vinet EOS for (1) Bi (Rhom.), (2) Al (fcc) (3) Ba (bcc) (4) Ca (fcc) (5) Sb (Rhom.) (6) Si (complex) (7) Li (bcc) (8) Na (bcc) (9) K (bcc) (10) Rb (bcc)

The result thus obtained shows very interesting pattern i.e. the graph plotted between logarithmic value of pressure vs logarithmic value of unit cell volume ratio (V/V_0) appears linear characteristic [fig. (1 - 12)]. Another remarkable characteristic

is observed that the variation in value of pressure from compression range $V/V_0 = 1.0$ to 0.5 are minimum but as the compression increases the variation in the values of pressure also increases. From fig. (1-12) it is crystal clear that the Pressure (P) vs. unit cell volume ratio (V/V_0) relation for all the twelve alkali metal halides are almost same with slight variation upto $V/V_0 = 0.5$ but as the compression increases variation in pressure gradually increases and after $V/V_0 = 0.3$ it increases abruptly.

Table 1: Input value of Bulk modulus and its first pressure derivative (K'_0) for different elements at zero pressure

S.No.	Elements	K_0	K'_0
1	Bismuth	30.97	4.09
2	Aluminium	78.89	3.17
3	Barium	9.46	1.73
4	Calcium	18.26	2.62
5	Antimony	40.43	4.28
6	Silicon	100.75	4.72
7	Lithium	11.80	3.33
8	Sodium	6.20	3.50
9	Potassium	3.40	2.99
10	Rubidium	2.66	3.23

When we consider about the success of equation of state derived from certain scientists, we have observed that nine EOS show very good agreement with each other except Murnaghan, Brennan-Stacey and Poirier tarantola EOS. Murnaghan EOS agreement with other EOS only upto $V/V_0 = 0.7$ holds good and after that it deviate sharply and shows higher pressure values, but Brennan-Stacey EOS and Poirier Tarantola EOS shows abrupt deviation. It is observed that It is observed that one equation of state shows deviation in upward direction, where as other shows a linear type projection. Now the question arises, why both these equations of state show a variation of marked difference.

Brennan-Stacey EOS is based on assumption that Grüneisen parameter is proportional to volume and equation is obtained on account of free volume formula. The metallic crystals have a packed arrangement, where as BMGs have random close packing with the existence of free volume. Due to this reason Brennan EOS in case of bulk metallic glasses fails hopelessly.

The Poirier-Tarantola proposed a equation of state derived using Hencky logarithmic strain [25] equivalent to the Eulerian strain for small strain and better behaved for large strain. The reference strain is neither the initial nor the final configuration, but the instantaneous configuration of the body being deformed. In uniaxial deformation as the instantaneous volume (V) of the body is increased by an infinitesimally small increment dV , the ratio (dV/V) is considered as an increment of the current state of strain $dE=(dV/V)$ When the solid goes from volume V_0 to V the total finite strain or normal strain also called the Hencky measure of strain.

$$E_H = (1/3) \log (V/V_0)$$

It has been observed that Hencky strain is as a function of the ratio (V_0/V) and in this way what we find that as the compression increases this potential deviates from other potential and successively it shows a pseudo linear characteristic. The conclusion is very interesting and it requires a critical and comprehensive study for further research work.

Table - 2

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Bismuth using
(a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	K_T' (a)= δ_T	K_T' (b)= δ_T	K_T' (c)= δ_T	γ_{ba-s} (a)	γ_{ba-s} (b)	γ_{ba-s} (c)
1.00	0.00	0.00	0.00	30.97	30.97	30.97	4.09	4.09	4.09	1.21	1.21	1.21
0.90	4.03	4.04	4.04	46.26	46.48	46.36	3.56	3.64	3.41	1.09	1.14	1.01
0.80	10.73	10.80	10.77	68.48	69.84	69.15	3.13	3.30	2.91	0.97	1.07	0.83
0.70	21.98	22.26	22.21	101.48	106.06	103.93	2.78	3.01	2.51	0.85	1.00	0.66
0.60	41.32	42.22	42.25	151.91	164.44	159.11	2.47	2.77	2.19	0.73	0.93	0.50
0.50	75.98	78.37	79.17	232.39	263.51	251.39	2.20	2.57	1.92	0.61	0.86	0.34
0.40	142.25	148.23	152.57	369.59	444.51	417.77	1.97	2.39	1.69	0.48	0.78	0.18
0.30	283.45	298.37	317.22	630.28	815.51	753.72	1.76	2.23	1.48	0.36	0.71	0.00
0.20	650.14	690.85	772.88	1234.92	1748.04	1576.43	1.58	2.10	1.28	0.24	0.64	-0.25

Table – 3

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Aluminum using
(a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	K_T' (a)= δ_T	K_T' (b)= δ_T	K_T' (c)= δ_T	γ_{ba-s} (a)	γ_{ba-s} (b)	γ_{ba-s} (c)
1.00	0.00	0.00	0.00	78.88	78.88	78.88	3.17	3.17	3.17	0.75	0.75	0.75
0.90	9.79	9.81	9.80	107.96	108.49	108.16	2.81	2.90	2.75	0.67	0.72	0.64
0.80	24.77	24.91	24.84	147.68	150.56	148.76	2.52	2.68	2.42	0.60	0.70	0.54
0.70	48.07	48.66	48.42	203.34	212.25	206.66	2.28	2.50	2.15	0.52	0.67	0.43
0.60	85.40	87.12	86.59	284.15	306.40	292.29	2.07	2.35	1.92	0.45	0.65	0.32
0.50	147.94	152.23	151.43	407.46	457.98	425.26	1.89	2.21	1.72	0.37	0.62	0.20
0.40	260.27	270.27	269.68	610.08	721.26	646.53	1.74	2.10	1.53	0.30	0.60	0.06
0.30	486.07	509.27	510.67	984.41	1235.72	1055.23	1.60	2.00	1.36	0.22	0.57	-0.12
0.20	1042.28	1101.28	1106.33	1836.92	2473.10	1957.34	1.49	1.92	1.20	0.15	0.55	-0.44

Table - 4

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K'_T), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for **Barium** using
(a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	$K'_T(a)=\delta_T$	$K'_T(b)=\delta_T$	$K'_T(c)=\delta_T$	$\gamma_{ba-s}(a)$	$\gamma_{ba-s}(b)$	$\gamma_{ba-s}(c)$
1.00	0.00	0.00	0.00	9.46	9.46	9.46	1.73	1.73	1.73	0.03	0.03	0.03
0.90	1.09	1.09	1.09	11.31	11.37	11.28	1.67	1.76	1.62	0.03	0.08	0.00
0.80	2.56	2.58	2.55	13.73	13.99	13.58	1.62	1.77	1.52	0.02	0.12	-0.04
0.70	4.61	4.66	4.56	16.99	17.69	16.55	1.57	1.77	1.43	0.02	0.17	-0.09
0.60	7.57	7.70	7.41	21.57	23.10	20.50	1.53	1.76	1.34	0.02	0.22	-0.16
0.50	12.10	12.40	11.63	28.40	31.42	26.02	1.49	1.74	1.26	0.01	0.26	-0.26
0.40	19.60	20.24	18.32	39.44	45.23	34.21	1.45	1.72	1.18	0.01	0.31	-0.44
0.30	33.66	35.00	30.00	59.61	71.03	47.53	1.42	1.69	1.10	0.01	0.36	-0.91
0.20	66.25	69.32	54.13	105.29	130.52	72.97	1.39	1.67	1.01	0.01	0.41	-14.90

Table – 5

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K'_T), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for **Calcium** using
(a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	$K'_T(a)=\delta_T$	$K'_T(b)=\delta_T$	$K'_T(c)=\delta_T$	$\gamma_{ba-s}(a)$	$\gamma_{ba-s}(b)$	$\gamma_{ba-s}(c)$
1.00	0.00	0.00	0.00	18.26	18.26	18.26	2.62	2.62	2.62	0.47	0.47	0.47
0.90	2.20	2.21	2.21	23.74	23.86	23.76	2.37	2.46	2.34	0.43	0.48	0.41
0.80	5.42	5.45	5.42	31.01	31.61	31.09	2.17	2.33	2.11	0.38	0.48	0.34
0.70	10.20	10.32	10.22	40.94	42.70	41.14	2.00	2.21	1.90	0.33	0.48	0.26
0.60	17.56	17.90	17.62	55.07	59.23	55.41	1.85	2.11	1.73	0.28	0.48	0.17
0.50	29.45	30.26	29.58	76.25	85.21	76.63	1.73	2.02	1.57	0.24	0.49	0.07
0.40	50.10	51.91	50.27	110.61	129.33	110.36	1.62	1.94	1.42	0.19	0.49	-0.06
0.30	90.39	94.43	90.06	173.54	213.67	169.55	1.52	1.87	1.28	0.14	0.49	-0.26
0.20	187.04	196.91	181.98	316.12	412.49	292.74	1.44	1.81	1.14	0.09	0.49	-0.74

Table - 6

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K'_T), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Antimony using
(a) Brennan Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	$K'_T(a)=\delta_T$	$K'_T(b)=\delta_T$	$K'_T(c)=\delta_T$	$\gamma_{ba-s}(a)$	$\gamma_{ba-s}(b)$	$\gamma_{ba-s}(c)$
1.00	0.00	0.00	0.00	40.43	40.43	40.43	4.28	4.28	4.28	1.31	1.31	1.31
0.90	5.32	5.33	5.32	61.48	61.79	61.61	3.71	3.80	3.54	1.18	1.23	1.08
0.80	14.30	14.39	14.36	92.55	94.39	93.43	3.26	3.43	3.00	1.05	1.15	0.88
0.70	29.64	30.02	29.95	139.30	145.64	142.67	2.88	3.12	2.58	0.92	1.07	0.70
0.60	56.41	57.65	57.70	211.67	229.31	221.94	2.56	2.86	2.24	0.78	0.98	0.53
0.50	105.08	108.45	109.67	328.45	373.07	356.60	2.27	2.64	1.96	0.65	0.90	0.36
0.40	199.47	208.00	214.84	529.49	638.92	603.46	2.02	2.45	1.72	0.52	0.82	0.20
0.30	403.23	424.83	455.44	914.41	1190.10	1111.39	1.79	2.29	1.50	0.39	0.74	0.01
0.20	938.85	998.71	1137.00	1812.01	2590.21	2382.96	1.60	2.14	1.29	0.26	0.66	-0.22

Table - 7

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K'_T), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Silicon using
(a) Brennan Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	$K'_T(a)=\delta_T$	$K'_T(b)=\delta_T$	$K'_T(c)=\delta_T$	$\gamma_{ba-s}(a)$	$\gamma_{ba-s}(b)$	$\gamma_{ba-s}(c)$
1.00	0.00	0.00	0.00	100.75	100.75	100.75	4.72	4.72	4.72	1.53	1.53	1.53
0.90	13.56	13.58	13.57	159.69	160.48	159.92	4.07	4.16	3.83	1.37	1.42	1.24
0.80	37.40	37.63	37.51	249.74	254.73	251.67	3.56	3.72	3.20	1.22	1.32	1.00
0.70	79.60	80.67	80.33	389.72	407.68	398.31	3.13	3.37	2.72	1.07	1.22	0.78
0.60	155.95	159.48	159.36	613.08	665.27	642.41	2.76	3.08	2.35	0.92	1.12	0.59
0.50	299.56	309.50	312.96	983.68	1121.42	1072.01	2.44	2.82	2.04	0.76	1.01	0.41
0.40	587.38	613.48	636.43	1637.29	1989.85	1890.37	2.14	2.60	1.77	0.61	0.91	0.23
0.30	1228.45	1296.85	1410.25	2913.70	3840.89	3648.10	1.88	2.41	1.54	0.46	0.81	0.05
0.20	2963.28	3159.66	3721.96	5932.89	8665.40	8277.27	1.65	2.23	1.32	0.31	0.71	-0.18

Table - 8

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Lithium using
(a) Brennan- Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	$K_T'(a)=\delta_T$	$K_T'(b)=\delta_T$	$K_T'(c)=\delta_T$	$\gamma_{ba-s}(a)$	$\gamma_{ba-s}(b)$	$\gamma_{ba-s}(c)$
1.00	0.00	0.00	0.00	11.80	11.80	11.80	3.33	3.33	3.33	0.83	0.83	0.83
0.90	1.48	1.48	1.48	16.40	16.48	16.44	2.94	3.03	2.88	0.75	0.80	0.71
0.80	3.77	3.79	3.78	22.75	23.20	22.94	2.63	2.79	2.52	0.67	0.77	0.59
0.70	7.39	7.48	7.45	31.74	33.13	32.33	2.37	2.59	2.22	0.58	0.73	0.47
0.60	13.25	13.52	13.47	44.88	48.43	46.39	2.14	2.42	1.97	0.50	0.70	0.35
0.50	23.19	23.87	23.84	65.07	73.26	68.51	1.94	2.27	1.76	0.42	0.67	0.23
0.40	41.23	42.84	43.06	98.42	116.73	105.85	1.77	2.15	1.56	0.33	0.63	0.09
0.30	77.85	81.63	82.91	160.27	202.32	175.90	1.63	2.04	1.39	0.25	0.60	-0.10
0.20	168.84	178.58	183.42	301.46	409.63	333.36	1.50	1.95	1.21	0.17	0.57	-0.39

Table - 9

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Sodium using
(a) Brennan- Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	$K_T'(a)=\delta_T$	$K_T'(b)=\delta_T$	$K_T'(c)=\delta_T$	$\gamma_{ba-s}(a)$	$\gamma_{ba-s}(b)$	$\gamma_{ba-s}(c)$
1.00	0.00	0.00	0.00	6.20	6.20	6.20	3.50	3.50	3.50	0.92	0.92	0.92
0.90	0.78	0.78	0.78	8.76	8.80	8.78	3.08	3.17	3.00	0.83	0.88	0.78
0.80	2.02	2.03	2.02	12.33	12.57	12.44	2.74	2.90	2.61	0.73	0.83	0.65
0.70	3.99	4.04	4.03	17.42	18.19	17.78	2.46	2.68	2.29	0.64	0.79	0.52
0.60	7.23	7.38	7.36	24.95	26.94	25.90	2.21	2.50	2.02	0.55	0.75	0.39
0.50	12.79	13.17	13.20	36.59	41.26	38.83	2.00	2.34	1.80	0.46	0.71	0.26
0.40	23.00	23.91	24.19	55.94	66.56	60.99	1.82	2.20	1.59	0.37	0.67	0.11
0.30	43.93	46.10	47.39	91.99	116.79	103.25	1.65	2.08	1.41	0.28	0.63	-0.07
0.20	96.42	102.10	107.14	174.52	239.38	200.04	1.52	1.98	1.23	0.18	0.58	-0.35

Table - 10

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K'_T), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for **Potassium** using
(a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	$K'_T(a)=\delta_T$	$K'_T(b)=\delta_T$	$K'_T(c)=\delta_T$	$\gamma_{ba-s}(a)$	$\gamma_{ba-s}(b)$	$\gamma_{ba-s}(c)$
1.00	0.00	0.00	0.00	3.40	3.40	3.40	2.99	2.99	2.99	0.66	0.66	0.66
0.90	0.42	0.42	0.42	4.58	4.60	4.58	2.67	2.76	2.62	0.60	0.65	0.57
0.80	1.05	1.05	1.05	6.17	6.29	6.21	2.41	2.57	2.33	0.53	0.63	0.47
0.70	2.01	2.04	2.03	8.38	8.75	8.49	2.19	2.41	2.08	0.46	0.61	0.38
0.60	3.54	3.61	3.58	11.57	12.46	11.83	2.00	2.27	1.86	0.40	0.60	0.28
0.50	6.07	6.25	6.18	16.40	18.40	16.94	1.84	2.15	1.67	0.33	0.58	0.16
0.40	10.57	10.97	10.85	24.30	28.63	25.31	1.70	2.05	1.50	0.26	0.56	0.03
0.30	19.51	20.43	20.18	38.84	48.46	40.52	1.57	1.96	1.34	0.20	0.55	-0.16
0.20	41.35	43.64	42.76	71.90	95.84	73.47	1.47	1.88	1.18	0.13	0.53	-0.51

Table – 11

Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K'_T), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for **Rubidium** using
(a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	$K_T(a)$	$K_T(b)$	$K_T(c)$	$K'_T(a)=\delta_T$	$K'_T(b)=\delta_T$	$K'_T(c)=\delta_T$	$\gamma_{ba-s}(a)$	$\gamma_{ba-s}(b)$	$\gamma_{ba-s}(c)$
1.00	0.00	0.00	0.00	2.66	2.66	2.66	3.23	3.23	3.23	0.78	0.78	0.78
0.90	0.33	0.33	0.33	3.66	3.68	3.67	2.86	2.95	2.80	0.70	0.75	0.67
0.80	0.84	0.85	0.84	5.04	5.14	5.08	2.56	2.73	2.46	0.63	0.73	0.56
0.70	1.64	1.66	1.65	6.97	7.28	7.09	2.31	2.54	2.18	0.55	0.70	0.45
0.60	2.92	2.98	2.97	9.79	10.56	10.09	2.10	2.38	1.94	0.47	0.67	0.33
0.50	5.08	5.23	5.21	14.10	15.86	14.77	1.91	2.24	1.73	0.39	0.64	0.21
0.40	8.98	9.32	9.33	21.19	25.09	22.59	1.75	2.12	1.55	0.31	0.61	0.07
0.30	16.84	17.65	17.79	34.32	43.18	37.14	1.61	2.02	1.37	0.23	0.58	-0.11
0.20	36.26	38.33	38.85	64.24	86.80	69.47	1.49	1.93	1.20	0.16	0.56	-0.42

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