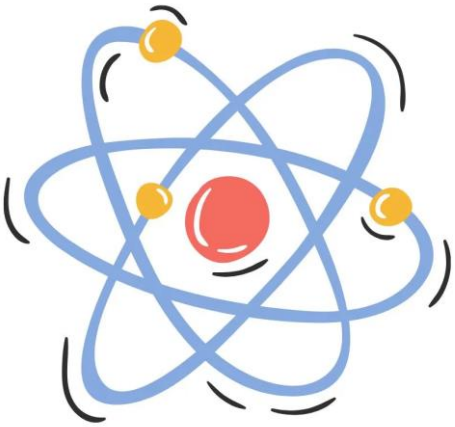

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Abstract: *In the present study, we have derived a well-known Usual-Tait equation of state using a simple fitting parameter method and primary boundary conditions of the equation of state. The accuracy of Usual-Tait EOS is very high compared to other equations of state taken in the study, and for better clarity, we compare with available experimental data. The most straightforward equation quickly transforms into an inverted equation of state without neglecting any term or approximation; therefore, the accuracy of calculated values of other properties becomes very high. Usual-Tait also deviates at high compression regions; behind this is a fundamental principle considered during derivation. An atom's binding energy contains attractive and repulsive terms, but all the equations of state are considered attractive terms. This study also suggests developing a new state equation that includes beautiful and vile terms, is simple, and contains minimum terms.*

Keywords: *Equation of state, Usual-Tait EOS, Compression, Compression-dependent pressure.*

Introduction:

The equation of state (EOS) is essential in various fields such as physics, material science, condensed matter physics, and planetary science. It provides a fundamental link between thermodynamic parameters like pressure, volume, and temperature. Accurate models are crucial for predicting compression behaviour, pressure, thermal expansion coefficient, Gruneisen parameter, and Debye temperature under extreme conditions in planetary interiors, condensed matter systems, and material science. There are several derived equations, with the Murnaghan EOS being the simplest one. However, its deviation from experimental results increases with higher compression [1-3]. The formulation of the pressure derivative of bulk modulus also remains constant concerning compression, but experimentally, the first-order pressure derivative of bulk modulus decreases with increasing compression [4].

Recently, Srivastava et al. derived a new equation of state by considering higher-order compression terms, which modifies the Shanker EOS. They found that increasing the order of compression improves the accuracy of the equation of state but also makes the equation more complex. Birch-Murnaghan also derived third and fourth-order equations of state with increasing accuracy, but the equations became more complex. When such equations of state are converted into an inverted type, neglecting higher term deviation leads to compression value inaccuracies [5-6]. In recent years, there has been growing interest in developing EOS models that balance simplicity and precision. This paper introduces a novel equation of state characterised by a minimal number of terms yet delivering exceptional accuracy across a broad range of materials and conditions. The development of this EOS is inspired by the need for a model that reduces computational overhead and retains predictive power comparable to more elaborate formulations. Traditionally, these equations have become increasingly complex, incorporating numerous parameters to achieve higher accuracy. However, this complexity often limits their practical use, especially in computational applications where simplicity and efficiency are paramount [7-8].

We have been developing a new equation of state on the principle of fitting parameters and conditions of the equation of state that satisfied the Stacey criterion. The proposed model is a streamlined approach that enhances the EOS's applicability without compromising performance. It can easily be converted into an inverted type of equation of state without neglecting any term of the equation of state. This property enhanced its application in condensed matter physics [9-10].

The derivation of the equation is grounded on a fundamental thermodynamical property of the equation of state [6], that is, at $V = V_0$, $P = 0$, $K_T = K_0$, and $K_T' = K_0'$. This EOS is tested against experimental and computational data, showing excellent agreement with real-world measurement and simulation across various phases and pressure ranges.

This paper presents the proposed equation's names as Usual-Tait equation with theoretical foundation, demonstrates its versatility in predicting material properties, and compares its performance with well-established EOS models such as Murnaghan EOS, the Universal equation of state named Vinet EOS, Kholiya EOS, Murnaghan EOS, Birch-Murnaghan EOS, Usual-Tait EOS, Shanker EOS, Modified Lennard-Jones EOS (mL-J EOS), Brennan-Stacey EOS, Born-Mie EOS, and compared with experimental data [11-19].

Our findings suggest that this simple yet powerful equation of state holds promise for various scientific and engineering applications, from studying planetary interiors to designing advanced materials. I hope this equation of state provides valuable scientific insights into condensed matter physics and material science.

Methodology:

The compression-dependent pressure is given by

$$P = -\frac{dW}{dV} \tag{1}$$

Now consider an empirical formula of pressure that is based on the fitting parameter in simple form:

$$P = A\left(e^{2B\left(1-\frac{V}{V_0}\right)} - 2 \right) \tag{2}$$

Where A and B are fitting parameters.

Taking partial differentiation of equation (1) concerning V then we get:

$$\frac{\partial P}{\partial V} = -2AB\left[\frac{1}{V_0} e^{2B\left(1-\frac{V}{V_0}\right)} \right] \tag{3}$$

According to the definition of bulk modulus:

$$K_T = -V\frac{\partial P}{\partial V} \tag{4}$$

$$K_T = 2AB\left(\frac{V}{V_0}\right) e^{2B\left(1-\frac{V}{V_0}\right)} \tag{5}$$

Now

$$\frac{\partial K_T}{\partial V} = 2AB\left[\left(\frac{V}{V_0}\right) e^{2B\left(1-\frac{V}{V_0}\right)} \left(-\frac{2B}{V_0}\right) + e^{2B\left(1-\frac{V}{V_0}\right)} \frac{1}{V_0} \right] \tag{6}$$

The pressure derivative of the bulk modulus is given by:

$$\frac{\partial K_T}{\partial P} = \frac{\partial K_T}{\partial V} \times \frac{\partial V}{\partial P}$$

$$\frac{\partial K_T}{\partial P} = 2B\left(\frac{V}{V_0}\right) - 1 \tag{7}$$

$$K_T^{'} = 2B\left(\frac{V}{V_0}\right) - 1 \tag{8}$$

Applying the condition at $V = V_0$, then $K_T = K_0$ and $K_T^{'} = K_0^{'}$ Then from equation (5) and (8) we get:

$$2AB = K_0 \tag{9}$$

$$B = K_0^{'} + 2$$

And

$$A = \frac{K_0}{2(K_0^{'} + 2)} \tag{10}$$

Substituting the value of A and B In equations (2), (5), and (8), we get the expressions for compression-dependent pressure, bulk modulus, and the first pressure derivative of bulk modulus, represented by equations (11), (12), and (13).

$$P = \frac{K_0}{2(K_0^{'} + 2)}\left[e^{2\left(K_0^{'}+1\right)\left(1-\frac{V}{V_0}\right)} - 2\right] \tag{11}$$

$$K_T = 2K_0\left(\frac{V}{V_0}\right)e^{2(K_0^{'}+1)\left(1-\frac{V}{V_0}\right)} \tag{12}$$

$$K_T^{'} = \left[\left(K_0^{'} + 2\right)\frac{V}{V_0} - 2\right] \tag{13}$$

The Vinet EOS, Kholiya EOS, Murnaghan EOS, Birch-Murnaghan EOS, Usual-Tait EOS, Shanker EOS, Modified Lennard-Jones EOS (mL-J EOS), Brennan-Stacey EOS, Born-Mie EOS are expressed as:

(1) Vinet equation of state:

The Vinet equation of state, also known as the Universal Equation of State, is a phenomenological model used to describe the pressure-volume relationship of solids, particularly under high pressure. It is instrumental in geophysics and material science for studying the behaviour of materials under extreme conditions. The Vinet equation is derived from the material's interatomic potential and compressibility assumptions.

The Vinet equation of state is a powerful tool for modelling the pressure-volume relationship of materials under high pressure. Based on an interatomic potential, its universal form accurately fits experimental data, making it valuable in geophysics and material science. However, its empirical nature and reliance on accurate parameters are important considerations when applying it to specific materials and conditions [18].

$$P = 3K_0 x^{-2}(1-x)\exp\{\eta(1-x)\} \tag{14}$$

where, $x = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and $\eta = \frac{3}{2}\left(K_0^{'} - 1\right)$

(2) Kholiya equation of state:

The Kholiya equation of state describes the relationship between pressure, volume, and temperature for various high-pressure materials. This equation is handy in predicting metals' melting temperatures and nanomaterials' compression behaviour. The Kholiya equation has been compared with other state equations, such as the Murnaghan and Usual-Tait equations. It has been shown to provide closer agreement with experimental data for certain materials, especially those where the bulk modulus decreases continuously with pressure. This makes it valuable in high-pressure physics and material science applications [19].

$$P = \frac{K_0}{2}\left[\left(K_0^{'} - 3\right) - 2\left(K_0^{'} - 2\right)\left(\frac{V}{V_0}\right)^{-1} + \left(K_0^{'} - 1\right)\left(\frac{V}{V_0}\right)^{-2}\right] \quad (15)$$

(3) Murnaghan equation of state:

The Murnaghan equation of state is a foundational model for understanding the compressibility of solids. It is instrumental in geophysics and material science. Its simplicity makes it a practical choice, although more complex models like the Vinet equation may offer improved accuracy for extreme conditions [18].

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

(4) Birch-Murnaghan equation of state:

The Birch-Murnaghan equation of state is a robust and widely accepted model for describing the compressibility of solids under high pressure. Its derivation from finite strain theory and inclusion of higher-order terms gives a more accurate representation of material behaviour, making it invaluable in geophysics and material science [19].

$$P = \frac{3}{2}K_0[x^{-7} - x^{-5}]\left[1 + \frac{3}{4}\left(K_0^{'} - 4\right)\left(x^{-2} - 1\right)\right] \quad (17)$$

Where $x = \left(V / V_0\right)^{1/3}$.

(5) Singh and Kao equation of state:

The Singh and Kao equation of state is a valuable tool in studying high-pressure material behaviour. Incorporating the bulk modulus and its pressure derivative provides a means to accurately describe the compressibility of materials under extreme conditions. Its applicability to nanomaterials and metals makes it a versatile choice in material science and high-pressure physics research [19].

$$P = K_0\left(1 - \frac{V}{V_0}\right) + \left\{\frac{K_0(K_0^{'} + 1)}{2}\right\}\left(1 - \frac{V}{V_0}\right)^2 \quad (18)$$

(7) Shanker equation of state:

The Shanker equation of state (EOS) is a model used to describe the behaviour of solids under high pressure, particularly nanomaterials. It is derived using the Grüneisen theory of thermal expansion and is particularly useful for high-pressure physics. The Shanker EOS incorporates principles from the Grüneisen theory, which relates to thermal properties and their changes under pressure. In some

contexts, the Shanker EOS is modified to include higher order terms, resulting in the Higher Order Shanker (HOS) EOS, which improves its accuracy for specific materials [19].

$$P = \frac{3K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{\left(3K_0^{'}-8\right)}\left[\left\{\left(1-\frac{1}{t}+\frac{2}{t^2}\right)\left(\exp ty-1\right)\right\}+\left\{y\left(1+y-\frac{2}{t}\right)\exp ty\right\}\right] \tag{19}$$

Where $y = 1-\frac{V}{V_0}$ and $t = K_0^{'}-\frac{8}{3}$

(8) Modified Lennard-Jones equation of state:

The Modified Lennard-Jones (LJ) equation of state extends the classic Lennard-Jones potential and is designed better to model the thermodynamic properties of fluids and solids. The original Lennard-Jones potential describes the interaction between a pair of neutral atoms or molecules using two parameters: a well depth indicating the strength of attraction and a finite distance, where the interparticle potential is zero [19].

$$P = \frac{3K_0}{K_0^{'}}\left(\frac{V}{V_0}\right)^{-K_0^{'}/3}\left[\left(\frac{V}{V_0}\right)^{-K_0^{'}/3}-1\right] \tag{20}$$

(9) Brennan-Stacey equation of state:

The Brennan-Stacey equation of state is a model used in thermodynamics to describe the behaviour of fluids, particularly gases. It is named after its developers, R.E. Brennan and F.D. Stacey, who introduced it in 1962. This equation describes the properties of gases at high pressures and temperatures, where ideal gas behaviour breaks down. Unlike the perfect gas law, which assumes that gas particles have no volume and do not interact with each other, the Brennan-Stacey equation of state accounts for both molecular volume and intermolecular forces [19].

$$P = \frac{3K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{\left(3K_0^{'}-5\right)}\left[\left\{\exp\left(\frac{3K_0^{'}-5}{3}\right)\left(1-\frac{V}{V_0}\right)\right\}-1\right] \tag{21}$$

(10) Born-Mie equation of state:

The Born-Mie equation of state, sometimes referred to as the Born-Mayer equation, is a model used in thermodynamics to describe the properties of simple molecular fluids, particularly gases and liquids. It's named after Max Born and Maria Goeppert-Mayer, who developed it in the early 20th century. The Born-Mie equation of state describes the intermolecular potential energy between particles in a fluid. It considers both the repulsive and attractive forces between molecules [19].

$$P = \frac{3K_0}{3K_0^{'}-8}\left[\left(\frac{V}{V_0}\right)^{\frac{4}{3}-K_0^{'}}-\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}\right] \tag{22}$$

Result and Discussion:

In the present study, we have derived the Usual-Tait equation of state by using fitting parameters and boundary conditions of the equation of state. The Murnaghan equation of state is a straightforward equation of state and contains a very minimum term. Second, the equation of state, which includes a very minimum term, is the Usual-Tait equation of state. By using equations (11), (14), (15), (16), (17), (18), (19), (20), (21), and (22) we calculate compression-dependent pressure by using Vinet EOS, Kholiya EOS, Murnaghan EOS, Birch-Murnaghan EOS, Usual-Tait EOS, Shanker EOS, Modified Lennard-Jones EOS (mL-J EOS), Brennan-Stacey EOS, Born-Mie EOS and calculated values are compared with available experimental data listed in table 1. It is clear from the table that the result obtained by Usual-Tait EOS is similar to the experimental data.

This study suggests the requirement of a simple and minimal term-dependent equation of state that gives the exact calculation of compression-dependent pressure resembling the experimental values. Fitting parameters becomes a better tool for deriving the equation of state.

The equation of state, which contains minimal terms, is better than the complex equation of state, and its conversion into an inverted type of equation of state is straightforward. Therefore, establishing a formula for other thermophysical properties becomes very easy.

Conclusion:

In conclusion, the Usual-Tait equation of state, derived using fitting parameters, proves to be a simple yet accurate tool for calculating compression-dependent pressure. Its minimal-term structure provides results that closely match experimental data, making it efficient for deriving other thermophysical properties and practical for various thermophysical applications.

Table 1: Input values of B_0 and B_0', utilised in the calculation based on experimental data [4,9, 17].

Materials	B_0 (GPa)	B_0'
Mo	266	3.99
K	3.177	3.98
Xe	36.5	8.87
NaF	46.5	5.28

Table 2. Calculated values of pressure (P) at different compression (V/V_0) By using (A) Vinet EOS, (B) Kholiya EOS, (C) Murnaghan EOS, (D) Birch-Murnaghan EOS, (E) Usual-Tait EOS, (F) Shanker EOS, (G) Modified Lennard-Jones EOS (mL-J EOS), (H) Brennan-Stacey EOS, (I) Born-Mie EOS, and (J) experimental [4, 9, 18].

Element	V/V_0	(A)	(B)	(C)	(D)	(E)	(F)	(G)	(H)	(I)	(J)
Mo	1.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	0.974	7.40	7.40	7.40	7.40	7.40	7.40	7.40	7.40	7.40	7.40
	0.966	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00
	0.958	12.60	12.60	12.60	12.60	12.60	12.60	12.60	12.60	12.60	12.60
	0.943	17.70	17.70	17.70	17.70	17.70	17.70	17.70	17.70	17.70	17.70
	0.936	20.20	20.20	20.20	20.20	20.20	20.20	20.20	20.20	20.20	20.10
	0.918	27.10	27.00	27.20	27.10	27.00	27.00	27.10	27.00	27.10	27.00

	0.892	38.40	38.20	38.70	38.30	38.20	38.20	38.40	38.20	38.40	38.20
	0.856	56.80	56.30	57.60	56.70	56.30	56.40	56.80	56.20	56.80	56.30
	0.821	77.90	76.80	79.70	77.70	76.90	77.10	77.90	76.70	77.90	76.90
	0.809	86.10	84.80	88.40	85.90	84.70	85.10	86.10	84.60	86.10	84.70
	0.795	96.80	95.00	99.80	96.50	95.00	95.40	96.80	94.80	96.80	95.00
K	1.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	0.881	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50
	0.807	1.00	1.00	1.10	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	0.755	1.60	1.50	1.60	1.60	1.50	1.50	1.60	1.50	1.60	1.50
	0.713	2.10	2.00	2.30	2.10	2.00	2.10	2.10	2.00	2.10	2.00
Xe	1.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	0.956	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20
	0.926	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40
	0.903	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60
	0.884	0.80	0.70	0.80	0.80	0.80	0.80	0.80	0.80	0.80	0.80
	0.868	1.00	0.90	1.00	0.90	1.00	1.00	1.00	1.00	1.00	1.00
	0.854	1.20	1.00	1.30	1.10	1.20	1.20	1.20	1.20	1.20	1.20
	0.842	1.40	1.20	1.50	1.30	1.40	1.40	1.40	1.40	1.40	1.40
	0.831	1.60	1.30	1.70	1.40	1.60	1.60	1.60	1.50	1.60	1.60
NaF	1.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	0.983	0.80	0.80	0.80	0.80	0.80	0.80	0.80	0.80	0.80	1.00
	0.962	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
	0.946	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
	0.932	4.00	3.90	4.00	4.00	4.00	3.90	4.00	3.90	4.00	4.00
	0.868	9.60	9.40	9.80	9.60	9.60	9.50	9.60	9.50	9.60	9.40
	0.832	14.00	13.40	14.50	13.90	13.90	13.80	14.00	13.70	14.00	14.00
	0.804	18.30	17.20	19.10	18.10	18.00	17.80	18.20	17.70	18.30	18.00
	0.782	22.30	20.70	23.50	21.90	21.70	21.60	22.10	21.40	22.30	21.00
	0.778	23.10	21.40	24.30	22.70	22.40	22.30	22.80	22.10	23.10	22.40

Ethical Approval:

The authors confirm that the manuscript is their original work and has not been published anywhere else before.

Competing interests:

The individuals who authored this paper state that they do not possess any known financial interests or personal relationships that could have potentially influenced the work presented in this report.

Author's Contribution:

All authors participated in creating the research outline. Abhay P. Srivastava completed all calculations and the initial manuscript draft. Professor B. K. Pandey and Dr. Anjani K. Pandey provided resources and guidance throughout the project.

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References:

[1] A. P. Srivastava. B. K. Pandey, A. K. Gupta, A. K. Pandey, *Natl. Acad. Sci. Lett. (2024). https://doi.org/10.1007/s40009-024-01409-0.*

[2] A. P. Srivastava. B. K. Pandey, A. K. Gupta, A. K. Pandey, *J Math Chem* **62**, 2253–2264 (2024). https://doi.org/10.1007/s10910-024-01647-z.

[3] P. Singh, B. K. Pandey, S. Mishra, A. P. Srivastava, *Computational Condensed Matter*, **35**, e00807, (2023).

[4] A.P. Srivastava, B.K. Pandey, A.K. Gupta, M. Upadhyay, *Iran J Sci* **48**, 1067–1074 (2024). https://doi.org/10.1007/s40995-024-01657-1.

[5] O L. Anderson, *Equation of State of Solids for Geophysics and Ceramic Science*. Oxford Univ. Press, Oxford (1995).

[6] F. D. Stacey and P. M. Davis, Phys. Earth Planet. Inter., **142,** 137 (2004).

[7] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices*. Oxford University Press, New York, (1954).

[8] J. Shanker and S. Dixit, Phys. Status Solidi (a) **123**, 17 (1991).

[9] J. Shanker, S. S. Kushwah, and P. Kumar, *Phys. B*, **239**, 337, (1997).

[10] O. L. Anderson, *J. Geophys. Res.*, **75**, 2719, (1970)

[11] B. J. Brennan, F.D. Stacey, J. Geophys. Res, **84**, 5535, (1979).

[12] P. Vinet, J. H. Rose, J. Ferrante, and J. R. Smith, *J. Phys. Condens. Matter*, **1**, 1941, (1989).

[13] F. D. Murnaghan, *Proc. Acad. Sci.*, **30**, 244, (1944).

[14] W. B. Holzapfel, Rep. Prog. Phys. **59**, 29 (1996).

[15] F. Birch, *J. Geophys. Res.*, **57**, 227, (1952).

[16] P. K. Singh, *Indian J. Pure Appl. Phys.*, **48**, 403, (2010).

[17] M Kumar, Physica B, **217**, 143, (1996).

[18] A. P. Srivastava, B. K. Pandey, M. Upadhyay, East European Journal of Physics, **37(3),** 333-339, (2024).

[19] A. P. Srivastava, B. K. Pandy. Journal of Dynamics and Control, **8 (9),** 2024, 152 – 170, (2024).