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ANTICIPATING PRESSURE CHANGES IN HALIDES UNDER COMPRESSION

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A new equation of state (NEOS) for Halides has been developed using the theory of lattice potential and the concept of volume dependence of the short-range force constant. The derivation of this equation of state involved the use of the third-order approximation of the lattice potential. A comparative analysis was conducted between the isothermal equations of state, including Vinet EOS, Murnaghan EOS, Holzapfel EOS, Born-Mie EOS, Birch-Murnaghan EOS, and the newly derived NEOS. The NEOS was used to analyze the compression behavior of Halides, and it was found that Vinet EOS and NEOS agreed with the experimental data for Halides up to high compression. However, Murnaghan EOS, Born-Mie EOS, Holzapfel EOS, and Birch-Murnaghan EOS are usually less sensitive to calculating pressure at high compression. It was also observed that for some Halides, such as NaBr and NaI, Vinet EOS could not produce results consistent with experimental findings. In contrast, NEOS consistently produced results that matched the experimental findings for all Halides samples, unequivocally demonstrating its reliability and accuracy.

Keywords: *Equation of state (EOS); Vinet EOS; Murnaghan EOS; Holzapfel EOS; Born-Mie EOS; Birch-Murnaghan EOS; New EOS (NEOS); Halides*
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1. INTRODUCTION

Studying ionic and mixed crystals under non-ambient conditions is a crucial aspect of materials science. Owing to their unique properties, ionic crystals and halides, in particular, are scientifically and technologically significant. Researchers have focused on these materials to better understand their behavior under different conditions [1-3].

Understanding the compression behavior of materials is essential to their application in various fields. The equation of state (EOS) is crucial to understanding this. Several potentials and equations of state have been developed to estimate the compression behavior of solids and their thermoelastic properties. These properties are essential in condensed matter physics, geophysics, and ceramic sciences [4-7].

The EOS formulations are based on three thermodynamic parameters: pressure (P), volume (V), and temperature (T). In this research, we have tested the validity of different equations of state, including Vinet EOS, Murnaghan EOS, Holzapfel EOS, Born-Mie EOS, Birch-Murnaghan EOS, and a newly developed isothermal equation of state (NEOS), to calculate the pressure at different compressions [7-10].

Our research aims to provide a comprehensive understanding of the compression behavior of materials under different conditions. We hope our findings will contribute to developing more accurate equations of state and potentials for predicting the behavior of materials under non-ambient conditions [11, 12].

2. METHOD OF ANALYSIS

According to the essential thermodynamics relation [13], the compression-dependent pressure and bulk modulus B_T are expressed as

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

And

$$B_T = -V\frac{dP}{dV} = V\frac{d^2W}{dV^2} \tag{2}$$

where B_T is the bulk modulus at constant temperature and W is the crystal lattice potential energy, which can be expressed as a function of the unit cell volume V. The volume of the unit cell in terms of interatomic separation r is given by

$$V = kr^3 \tag{3}$$

where k is the geometrical factor depending on the structure of the solid. Using equation (3) in the equation (1) and second, we get

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$$\frac{dW}{dV}=\frac{dW}{dr}\times\frac{dr}{dV}=\frac{1}{3kr^2}\frac{dW}{dr} \tag{4}$$

and

$$V\frac{d^2W}{dV^2}=\frac{1}{9kr}\left[\frac{d^2W}{dr^2}-\frac{2}{r}\frac{dW}{dr}\right] \tag{5}$$

Using equation (1) and (4) in equation (5) then we get

$$V\frac{d^2W}{dV^2}=\frac{1}{9kr}\left(\frac{d^2W}{dr^2}+\frac{2}{r}\frac{dW}{dr}\right)+\frac{4P}{3} \tag{6}$$

Using the standard definition of the short-range force constant A in terms of the Laplacian operator can be given by Born and Huang [14],

$$A=\frac{1}{3}\left[\frac{d^2W}{dr^2}+\frac{2}{r}\frac{dW}{dr}\right] \tag{7}$$

Then equation (6) can be written as

$$V\frac{d^2W}{dV^2}=\frac{A}{3kr}+\frac{4P}{3} \tag{8}$$

The short-range force constant can be expressed as a function of the interatomic separation and lattice volume, and the volume derivative of A have been used in studies on the pressure dependence of the dielectric properties [15]. Using equation (3) and (8), equation (2) can be written as

$$B_T=\frac{A}{3k^{2/3}V^{1/3}}+\frac{4P}{3} \tag{9}$$

Where B_T is the bulk modulus at temperature T.

The pressure derivative of B_T represented by $B_T^{'}=\frac{dB_T}{dP}$ obtained from equation (9) given below

$$B_T^{'}=\left(\frac{4}{3}\frac{P}{B_T}-1\right)\left(\frac{V}{A}\frac{dA}{dV}-\frac{5}{3}\right)+\frac{16P}{9B_T} \tag{10}$$

To find the volume dependence of A we consider

$$A=A_0f \tag{11}$$

Where A_0 is volume independent constant and f is a function of V/V_0. Now at $P=0, V=V_0$ we have from equations (9) and (11)

$$\frac{A_0}{3k^{2/3}}=\frac{B_0V_0^{1/3}}{f_0} \tag{12}$$

Where B_0 is the value of the isothermal bulk modulus at $P=0$ and f_0 is the value of f at $V=V_0$. Using the definition of B_T and using equation (12) in equation (9), we get

$$-V\left(\frac{dP}{dV}\right)_T=\frac{B_0}{f_0}\left(\frac{V}{V_0}\right)^{-1/3}\times f+\frac{4}{3}P \tag{13}$$

On integrating equation (13), we get

$$P\left(\frac{V}{V_0}\right)^{4/3}=-\frac{B_0}{f_0V_0}\int_{V_0}^{V}f\ dV \tag{14}$$

Equation (14) is the basic equation that leads to the derivation of an EOS. [16]Shanker et al. have shown that the above formulation is valid for all EOS for different types of solid material [17] that equation (14) yields the Born-Mie EOS [18, 19-26] and the Brenan-Stacey EOS [27].

The equation of state can be derived by taking the short-range potential function as inverse or exponential form. In the case of the exponential function, the range force remains finite to the limit of substantial compression (i.e. $V/V_0 \rightarrow 0$) but inverse power function gives infinitely large force. Here, we consider the exponential function $f\left(V/V_0\right)$ as

$$f = \frac{V}{V_0}\exp\alpha\left(1-\frac{V}{V_0}\right) \tag{15}$$

Let $y = 1-\frac{V}{V_0}$ then

$$f = \left(1-y\right)^{-1}\exp\left(\alpha y\right)$$

$$f = (1+y+y^2+y^3+.....................)\exp(\alpha y)$$

The integration of f is so complicated then by the approximation f can be written as

$$f = (1+y+y^2+y^3)\exp(\alpha y) \tag{16}$$

At $V = V_0,\ f = f_0 = 1$ and $= 0$. Using equation (15) in the (14) then we get

$$P = B_0\left(\frac{V}{V_0}\right)^{-4/3}\int_0^y (1+y+y^2+y^3)e^{\alpha y}dy \tag{17}$$

Where B_0 bulk modulus at zero pressure.
Integrating equation (17), we get a new EOS as

$$P = B_0\left(\frac{V}{V_0}\right)^{-4/3}\left[\frac{\left(\alpha^3(1+y+y^2+y^3)+\alpha^2(-3y^2-2y-1)+\alpha(6y+2)-6\right)e^{\alpha y}-(\alpha^3-\alpha^2+2\alpha-6)}{\alpha^4}\right] \tag{18}$$

Using the boundary condition $B_T' = B_0'$ at $P = 0$ and $V = V_0$ in equations (11) and (15), then we obtain

$$\alpha = \frac{3B_0'-8}{3}$$

The Vinet EOS, Murnaghan EOS, Holzapfel EOS, Born-Mie EOS and Birch-Murnaghan third order EOS [25-34] are as follows

$$P = 3B_0x^{-2}\left(1-x\right)\exp\left\{\eta\left(1-x\right)\right\} \tag{19}$$

Where, $x = \left(V/V_0\right)^{\frac{1}{3}}$ and $\eta = \frac{3}{2}\left(B_0'-1\right)$

$$P = \frac{B_0}{B_0'}\left[\left(\frac{V}{V_0}\right)^{-B_0'}-1\right] \tag{20}$$

$$P = 3B_0x^{-5}\left(1-x\right)\exp\left[f\left(1-x\right)\right] \tag{21}$$

Where $x = \left(V/V_0\right)^{\frac{1}{3}}$ and $f = \frac{3}{2}\left(B_0'-3\right)$

$$P = \frac{3B_0}{3B_0'-8}\left[\left(\frac{V}{V_0}\right)^{\frac{4}{3}-B_0'}-\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}\right] \tag{22}$$

$$P = \frac{3B_0}{2}\left[\left(\frac{V}{V_0}\right)^{-7/3}-\left(\frac{V}{V_0}\right)^{-5/3}\right]\left[1+\frac{3}{4}\left(B_0'-4\right)\left\{\left(\frac{V}{V_0}\right)^{-2/3}-1\right\}\right] \tag{23}$$

The expression given above for P based on different EOS has been used in the present study to obtain the results discussed in the following section.

3. RESULT AND DISCUSSION

The present work has derived a new equation of state using the concept of third-order approximation of lattice potential energy, which is given in equation (18). We extended the calculations to the high compression value to validate our result.

Equations (19), (20), (21), (22), and (23) give the equations of state for Vinet, Murnaghan, Hozapfel, Born-Mie, and Birch-Murnaghan, respectively.

To estimate the compression behavior of Halides and test the validity of said EOS, we have taken NaF, NaCl, NaBr, and NaI samples whose experimental results are available. For computing the compression behavior of different halide samples, we need the input values of isothermal bulk modulus at zero pressure (B_0) and its pressure derivatives (B_0'), which are given in Table 1 [32, 33].

Table1. Values of input data B_0 (GPa), B_0' (GPa) all at P=0 [32,33].

Solids	B_0	B_0'
NaF	46.5	5.28
NaCl	24	5.39
NaBr	19.9	5.49
NaI	15.1	5.59

The computed results using different EOS for the selected samples of halides are tabulated in Table 2. For further clarity, we have also calculated the deviation of results obtained from different EOS with respect to the available experimental results [34, 35]. The variations of compression corresponding to different pressure P (GPa) for other samples, such as NaF, NaCl, NaBr, and NaI, are shown in Fig. 1, Fig. 2, Fig. 3, and Fig. 4, respectively.

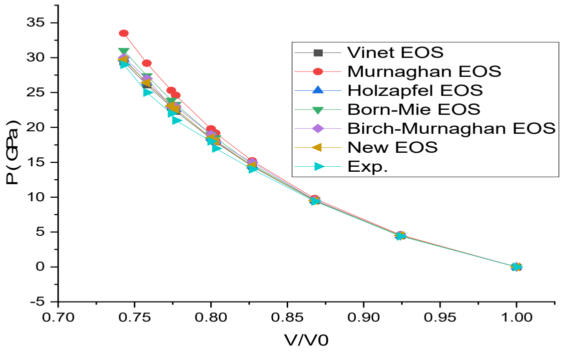

Figure 1. Compression behavior of NaF with pressure

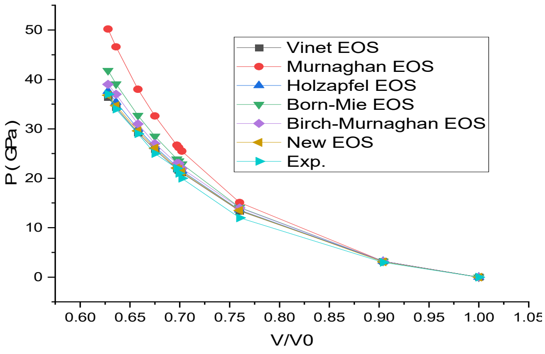

Figure 2. Compression behavior of NaCl with pressure

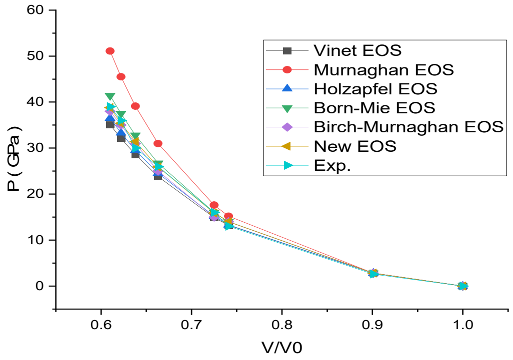

Figure 3. Compression behavior of NaBr with pressure

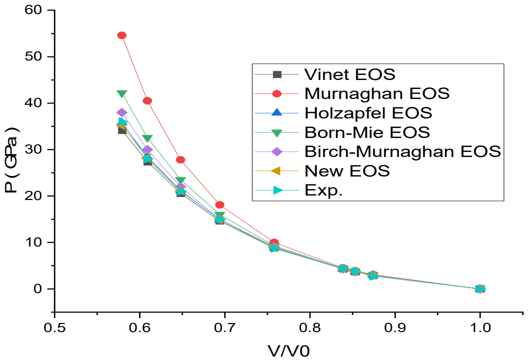

Figure 4. Compression behavior of NaI with pressure

It has also been compared with the experimental results in the respective figures. Deviation plots for different EOS for corresponding samples are shown in Fig. (5-8), respectively. Based on a comparative analysis of various equations of state (EOS), it has been observed that the Vinet EOS and New EOS produce pressure values that are closer to the experimental results than the Murnaghan EOS, Holzapfel EOS, Born-Mie EOS, and Birch-Murnaghan EOS. The analysis also revealed that the Vinet EOS is only suitable for some samples, while the new EOS consistently works for all the samples compared to other EOS. In conclusion, the new EOS is recommended for accurate pressure calculations.

From the close observation of results obtained from different equations of state for NaF, it is evident that all the results are almost the same as experimental values below 14 GPa. Still, above this pressure, the results obtained using all equations of state deviate from experimental values except Vinet EOS and NEOS. The same situation is observed for NaCl. However, when observed in the case of NaBr and NaI at higher pressure, the Vinet EOS also deviates from the experimental results. At the same time, the NEOS is still consistent and very close to the experimental results. The consistent validity of NEOS is based on the fundamental concept considered during its derivation. The NEOS has been derived by considering the third-order approximation of lattice potential energy, while in the other EOSs, only up to second-order approximation has been considered. The choice of third-order approximation not only includes the vibrational behavior of lattice parameters but also gives it the choice of odd and even numbers of higher degree approximations to include the change in the material's behavior at their atomic and molecular level at higher compression. Thus, the consistent NEOS can also be applied to predict the compression behavior of those halides for which the experimental results are still awaited.

Table 2. Values of P (GPa) calculated from Vinet EOS P(V), Murnaghan EOS P(M), Holzapfel EOS P(H), Born-Mie EOS (B) and new EOS P(N)

Element	V/V0	P(V)	P(M)	P(H)	P(B)	P(BM)	P(N)	P(Exp.)	% Dev. (V)	% Dev. (M)	% Dev. (H)	% Dev. (B)	% Dev. (BM)	% Dev. (N)
NaF	1	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.924	4.5	4.6	4.5	4.5	4.5	4.5	4.4	2.7	4	2.7	2.3	2.3	2.3
	0.868	9.5	9.8	9.5	9.6	9.6	9.5	9.4	1.1	4	1.4	2.1	2.1	1.1
	0.827	14.4	15.2	14.5	14.7	15	14.5	14	2.9	9	3.6	5	7.1	3.6
	0.803	17.9	19.2	18	18.5	18	18	17	5.3	13	5.9	8.8	5.9	5.9
	0.8	18.4	19.8	18.5	19	19	18.5	18	2.2	10	2.8	5.6	5.6	2.8
	0.777	22.3	24.6	22.6	23.3	23	22.6	21	6.2	17	7.6	11	9.5	7.6
	0.774	22.9	25.3	23.2	23.9	23	23.1	22	4.1	15	5.5	8.6	4.5	5
	0.758	26.1	29.2	26.4	27.4	27	26.4	25	4.4	17	5.6	9.6	8	5.6
	0.743	29.4	33.5	29.8	31	30	29.7	29	1.4	16	2.8	6.9	3.4	2.4
NaCl	1	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.904	3.2	3.2	3.2	3.2	3.2	3.1	3	6.7	7	6.7	6.7	6.7	3.3
	0.76	13.4	15.1	13.6	14.1	14	13.5	12	12	26	13	18	17	13
	0.702	21.1	25.5	21.5	22.9	22	21.3	20	5.5	28	7.5	15	10	6.5
	0.699	21.6	26.2	22	23.5	23	21.8	21	2.9	25	4.8	12	9.5	3.8
	0.697	21.9	26.7	22.4	23.9	23	22.1	22	0	21	1.8	8.6	4.5	0.5
	0.675	25.8	32.6	26.4	28.5	27	26.1	25	3.2	30	5.6	14	8	4.4
	0.658	29.2	38	30	32.7	31	29.6	29	0.7	31	3.4	13	6.9	2.1
	0.636	34.3	46.6	35.4	39.1	37	34.7	34	0.9	37	4.1	15	8.8	2.1
	0.628	36.3	50.2	37.6	41.8	39	36.8	37	2	36	1.6	13	5.4	1
NaBr	1	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.901	2.8	2.8	2.8	2.8	2.8	2.8	2.6	7.7	7.7	7.7	7.7	7.7	7.7
	0.741	13.2	15.2	13.3	14	14	14	13	1.5	17	2.3	7.7	7.7	7.7
	0.725	14.9	17.6	15.2	16	15	15.9	16	7	10	5	0	6.3	1
	0.663	23.8	31	24.5	26.7	25	25.9	26	8	19	5.8	2.7	3.8	0
	0.638	28.6	39.1	29.5	32.8	31	31.4	30	5	30	1.7	9.3	3.3	4.7
	0.622	32.1	45.5	33.3	37.5	35	35.4	36	11	26	7.5	4.2	2.8	2
	0.61	35.1	51.1	36.5	41.4	38	38.8	39	10	31	6.4	6.2	2.6	1
NaI	1	0	0	0	0	0	0	0	0	0	0	0	0	0
	0.874	2.9	3.1	3	3	3	2.9	2.7	7.4	15	11	11	11	7.4
	0.853	3.7	3.9	3.7	3.8	3.7	3.8	3.8	3	3	2.6	0	2.6	0
	0.839	4.3	4.5	4.3	4.4	4.3	4.3	4.4	2	2	2.3	0	2.3	2
	0.758	8.8	10	8.9	9.3	9.1	8.9	8.7	1.1	15	2.3	6.9	4.6	2.3
	0.694	14.6	18.1	14.9	16	15	14.9	15	3	21	0.7	6.7	0	1
	0.648	20.6	27.8	21.2	23.5	22	21.1	21	2	32	1	12	4.8	0.5
	0.609	27.4	40.5	28.5	32.6	30	28.2	28	2	45	1.8	16	7.1	0.7
	0.579	34.2	54.6	35.8	42.2	38	35.2	36	5	52	0.6	17	5.6	2

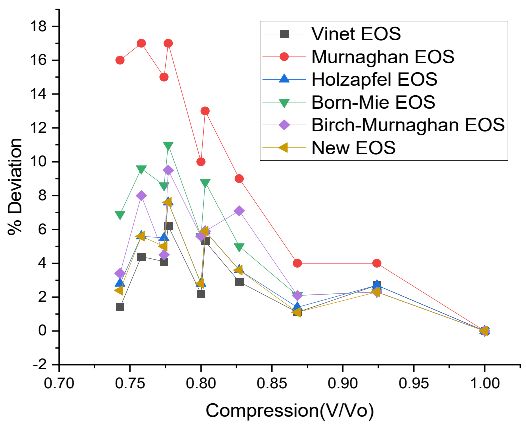

Figure 5. Percentage deviation of calculated value using different EOS with experimental value NaF

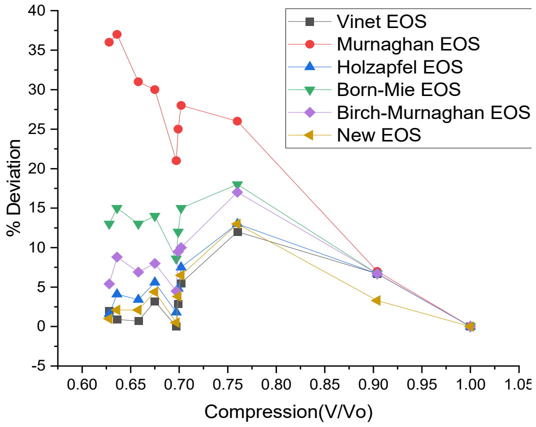

Figure 6. Percentage deviation of calculated value using different EOS with experimental value NaCl

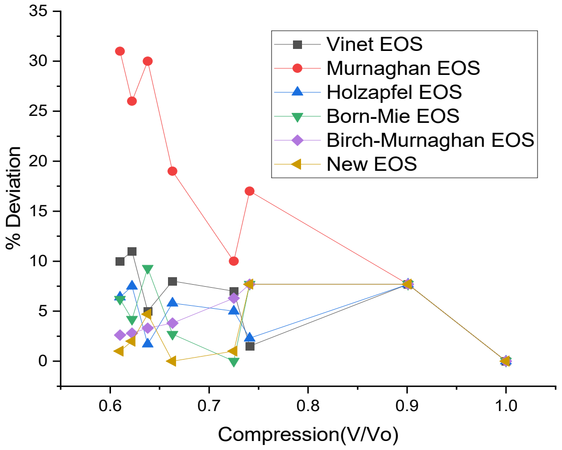

Figure 7. Percentage deviation of calculated value using different EOS with experimental value NaBr

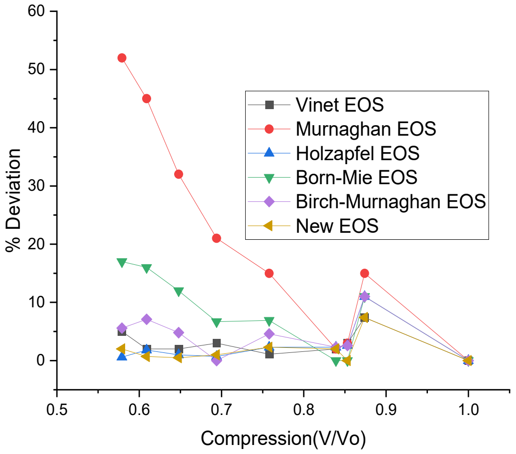

Figure 8. Percentage deviation of calculated value using different EOS with experimental value NaI

4. CONCLUSIONS

The Present study concludes that Vinet EOS and NEOS help calculate the pressure at different compressions. They agree with experimental results at the low-pressure range (≤ 14GPa) at the higher compression, the Vinet EOS deviates from experimental results. Still, the pressure calculated by NEOS is very close to the experimental values at high compressions. Thus, NEOS is the best EOS for the theoretical prediction of pressure at high compression for Halides.

Ethical Approval. The authors confirm that the manuscript is original and unpublished.
Competing interests. The authors of this paper declare no known financial interests or personal relationships that could have affected the presented work.
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ПРОГНОЗУВАННЯ ЗМІНИ ТИСКУ В ГАЛОІДАХ ПІД СТИСНЕННЯМ

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Нове рівняння стану (NEOS) для галогенідів було розроблено з використанням теорії потенціалу гратки та концепції об’ємної залежності короткодіючої силової постійної. Виведення цього рівняння стану передбачало використання третього порядку наближення потенціалу гратки. Було проведено порівняльний аналіз між ізотермічними рівняннями стану, включаючи EOS Віне, EOS Мурнагана, EOS Хольцапфеля, EOS Борна-Мі, EOS Берча-Мурнагана та нещодавно отриману NEOS. NEOS використовувався для аналізу поведінки стиснення галогенідів, і було виявлено, що Vinet EOS і NEOS узгоджуються з експериментальними даними для галогенідів до високого стиснення. Однак EOS Мурнагана, EOS Борна-Мі, EOS Хольцапфеля та EOS Берча-Мурнагана зазвичай менш чутливі до обчислення тиску при високому стисненні. Було також помічено, що для деяких галогенідів, таких як NaBr і NaI, Vinet EOS не може дати результати, які відповідають експериментальним висновкам. Навпаки, NEOS послідовно давав результати, які збігалися з експериментальними результатами для всіх зразків галоїдів, недвозначно демонструючи свою надійність і точність.

Ключові слова: *рівняння стану (EOS); Vinet EOS; Murnaghan EOS; Holzapfel EOS; Born-Mie EOS; Бірч-Мурнаган EOS; новий EOS (NEOS); галоїди*