J Integr. Sci. Technol, 2013, 1, 1, 48-53 Article

Journal of Integrated Science and Technology

High pressure properties of metals using various equation of state

R.S. Singh and Preeti Sen

[a] *Department of Physics, Jai Naraian Vyas University, Jodhpur (Rajasthan).*

Received: 23-03-2013 Accepted: 25-05-2013 Available Online: 31-05-13.

ABSTRACT

We have studied some high pressure properties of metals using various equation of state. The calculations have been performed using modified Rydberg EOS (equation of state), Hama Suito EOS, Stacey Reciprocal K-primed EOS, Kushwah logarithmic EOS and Kushwah Exponential EOS to find the pressure, bulk modulus and its pressure derivative for four metals at different values of compression V/V_0.The results for various parameters show systematic variations with the increase in pressure and compare well with the Stacey EOS.

Keywords: Equation of state, Metals, Pressure, Bulk modulus

Introduction

The equation of state (EOS) of a system describes the relationship among thermodynamic variables such as pressure, temperature and volume[1-3]. The study of equation of state for solid have been extremely useful in the field of Geophysics and condensed matter Physics[4-7]

The EOS`s have been derived by many authors based on different physical assumption. Among these EOS's its very difficult to choose appropriate EOS. Among These EOS's we have chosen the equation of state depend on free volume theory[8]. Equations involving K-prime are more advantageous for determining pressure derivative of bulk modulus than the pressure volume relationship[11-15]

In the present study we determine the pressure, bulk modulus and its pressure derivatives for four metals viz, Ag, Cu, Au and Al at different values of compression V/V_0 (from 0.8 to 1.0).

We have used five EOS`s (a) Modified Rydberg EOS, (b) Hama Suito EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS,(e) Kushwah Exponential EOS. The results for different metals obtained from these EOS's have been found to present good agreement with experimental data[6,9,10]

Equation of state:

The equation of state used in the present study are

(a) **Modified Rydberg EOS[2,17]**

$$P = 3K_0 x^{-K'_\infty}\left(1-x^{1/3}\right)\exp\left[t\left(1-x^{1/3}\right)\right]$$

$$K = 3K_0 x^{-K'_\infty}\exp\left\{t\left(1-x^{1/3}\right)\right\}\left\{K'_\infty\left(1-x^{1/3}\right)\right\} + \frac{t}{3}\left\{x^{1/3}\left(1-x^{1/3}\right)\right\} + \frac{x^{1/3}}{3}$$

$$K' = K'_\infty + t\frac{x^{1/3}}{3} + \frac{x^{1/3}}{3\left(1-x^{1/3}\right)} - \frac{P}{9K}tx^{1/3} + \frac{1}{1-x^{1/3}} + \frac{x^{1/3}}{\left(1-x^{1/3}\right)^2}$$

where

$$x = \frac{V}{V_0}$$

$$t = \frac{3}{2}K'_0 - 3K'_\infty + \frac{1}{2}$$

Address:
Dr. R.S. Singh
Jai Narain Vyas University, Jodhpur – 342 005 (Raj.) India
Tel: 0291-2724784
Email: rssinghkush@gmail.com

Cite as: singh et al *J Integr. Sci. Technol., 2013, 1(1), 48-53.*

Here K_0, K_0' and K_0'' are respectively zero pressure values of K , K' , K'' and K_∞' is the value of K' at P $\to \infty$.

(b) Hama Suito EOS [3,17]

$$P = 3K_0 x^{-K_\infty'}\left(1-x^{1/3}\right)$$

$$\exp\left[A\left(1-x^{1/3}\right)+B\left(1-x^{1/3}\right)^2\right]$$

$$K = \frac{P}{3}\left\{3K_\infty' + \frac{x^{1/3}}{1-x^{1/3}}\right\}$$

$$+x^{1/3}\left\{A+2B\left(1-x^{1/3}\right)\right\}$$

$$K' = \frac{K}{P}-\frac{1}{3}+\frac{P}{9K}$$

$$\left\{3K_\infty' + \left(x^{1/3}\right)^2\left(2B-\frac{1}{\left(1-x^{1/3}\right)^2}\right)\right\}$$

where $x = \frac{V}{V_0}$

$$A = (3/2)\left(K_0' - 2K_\infty' + 1/3\right)$$

$$B = (3/8)\left(4K_0K_0'' + K_0'^2 + 2K_0' - 4K_\infty' + 5/9\right)$$

(c) Stacey Reciprocal k-primed EOS[4,17]

$$\ln\frac{V}{V_0} = \frac{K_0'}{K_\infty'^2}\ln\left(1-K_\infty'\frac{P}{K}\right)+\left(\frac{K_0'}{K_\infty'}-1\right)\frac{P}{K}$$

$$K = K_0\left(1-K_\infty'\frac{P}{K}\right)^{-\frac{K_0'}{K_\infty'}}$$

$$\frac{1}{K'} = \frac{1}{K_0'}+\left(1-\frac{K_\infty'}{K_0'}\right)\frac{P}{K}$$

(d) Kushwah Logarithmic EOS[5,17]

$$Px^{K_\infty'} = B_1\ln(2-x)$$

$$+B_2\left[\ln(2-x)\right]^2+B_3\left[\ln(2-x)\right]^3$$

$$K = K_\infty' P + \frac{x^{1-K_\infty'}}{2-x}$$

$$\left[B_1+2B_2\ln(2-x)+3B_3\left\{\ln(2-x)^2\right\}\right]$$

$$K' = 2K_\infty' - \frac{K_\infty'^2 P}{K}+\frac{2}{2-x}$$

$$\left[\frac{K_\infty' P}{K}+\frac{x^{2-K_\infty'}}{K(2-x)}\left\{B_2+3B_3\ln(2-x)\right\}-1\right]$$

Where

$$x = 1-\frac{V}{V_0}$$

$$B_1 = K_0$$

$$B_2 = \left(\frac{K_0}{2}\right)\left(K_0' - 2K_\infty' + 2\right)$$

$$B_3 = \left(\frac{K_0}{6}\right)\left(K_0K_0'' + K_0'^2 + 3K_\infty'^2\right.$$

$$\left.-3K_0'K_\infty' - 12K_\infty' + 6K_0' + 6\right)$$

(e) Kushwah Exponential EOS[6]

$$P\,(1-x)^{K_\infty'} = B_1\left(1-e^{-x}\right)$$

$$+B_2\left(1-e^{-x}\right)^2+B_3\left(1-e^{-x}\right)^3$$

$$K = K_\infty' P + \frac{e^{-x}}{(1-x)^{K_\infty'-1}}$$

$$\left[B_1+2B_2\left(1-e^{-x}\right)+3B_3\left\{\left(1-e^{-x}\right)^2\right\}\right]$$

$$K' = 2K_\infty' + x - 2 - K_\infty'\left(x+K_\infty'-2\right)\frac{P}{K}$$

$$+\frac{e^{-2x}}{K(1-x)^{K_\infty'-2}}\left[2B_2+6B_3\left(1-e^{-x}\right)\right]$$

Where

$$x = 1-\frac{V}{V_0}$$

$$B_1 = K_0$$

$$B_2 = \left(\frac{K_0}{2}\right)\left(K_0' - 2K_\infty' + 2\right) \text{ and}$$

$$B_3 = \left(\frac{K_0}{6}\right)\left(K_0 K_0'' + K_0'^2 + 3K_\infty'^2 - 3K_0' K_\infty' - 12K_\infty' + 6K_0' + 7\right)$$

We make use of these equations to calculate values of pressure.

Results and Discussion:

Values of input parameters used in the present calculations are given in table1. We determine pressure P, bulk modulus *K* and pressure derivative of bulk modulus K' for four metals.

Table 1. Values of input data for different metals at room temperature and zero pressure[18,19,20]

Metals	Ag	Cu	Au	Al
K_0	99.65	133.4	166.7	72.67
K_0'	6.11	5.37	6.00	4.62
K_∞'	3.67	3.22	3.60	2.77
$K_0 K_0''$	-14.93	-11.53	-14.40	-8.54

Table 2. Values of pressure for the different metals calculated from (a) Modified Rydberg EOS, (b) Hama Suito EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS, (e) Kushwah Exponential EOS

Metals	V/V_0	P				
		(a)	(b)	(c)	(d)	(e)
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	2.14	2.14	2.14	2.14	2.14
	0.96	4.61	4.60	4.60	4.60	4.60
	0.94	7.45	7.42	7.43	7.42	7.42
	0.92	10.73	10.65	10.67	10.66	10.66
Ag	0.90	14.50	14.34	14.37	14.37	14.36
	0.88	18.85	18.55	18.62	18.61	18.61
	0.86	23.87	23.35	23.50	23.47	23.47
	0.84	29.67	28.81	29.07	29.04	29.03
	0.82	36.38	35.03	35.48	35.43	35.41
	0.80	44.15	42.11	42.82	42.76	42.74
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	2.82	2.84	2.85	2.85	2.84
	0.96	5.97	6.07	6.08	6.07	6.06
	0.94	9.48	9.72	9.73	9.72	9.72
Cu	0.92	13.42	13.85	13.86	13.85	13.85
	0.90	17.82	18.52	18.53	18.53	18.53
	0.88	22.75	23.78	23.82	23.83	23.82
	0.86	28.28	29.72	29.83	29.82	29.81
	0.84	34.50	36.42	36.62	36.61	36.59
	0.82	41.49	43.97	44.29	44.31	44.28
	0.80	49.37	52.48	53.04	53.05	53.00
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	3.58	3.58	3.57	3.58	3.57
	0.96	7.69	7.68	7.68	7.68	7.68
	0.94	12.42	12.38	12.38	12.38	12.38
	0.92	17.86	17.75	17.77	17.76	17.75
Au	0.90	24.11	23.87	23.91	23.91	23.90
	0.88	31.31	30.85	30.95	30.94	30.92
	0.86	39.60	38.79	38.99	38.97	38.95
	0.84	49.15	47.82	48.21	48.16	48.14
	0.82	60.18	58.09	58.73	58.68	58.65
	0.80	72.92	70.92	70.82	70.74	70.69
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	1.54	1.54	1.54	1.53	1.53
	0.96	3.26	3.26	3.26	3.25	3.25
	0.94	5.19	5.18	5.18	5.17	5.17
	0.92	7.35	7.32	7.32	7.32	7.32
Al	0.90	9.77	9.71	9.73	9.72	9.71
	0.88	12.49	12.37	12.40	12.40	12.39
	0.86	15.55	15.34	15.38	15.39	15.38
	0.84	18.98	18.66	18.74	18.74	18.73
	0.82	22.86	22.35	22.48	22.50	22.48
	0.80	27.22	26.48	26.70	26.71	26.68

Table 3. Values of bulk modulus and pressure derivative of bulk modulus for the different metals calculated from (a) Modified Rydberg EOS, (b) Hama Suito EOS, (c) Stacey reciprocal K- primed EOS, (d) Kushwah logarithmic EOS, (e) Kushwah Exponential EOS

Metals	V/V_0	K				
		(a)	(b)	(c)	(d)	(e)
	1.00	99.65	0.00	99.65	99.65	99.65
	0.98	112.55	112.41	12.39	112.42	112.42
	0.96	127.55	126.41	126.48	126.49	126.48
	0.94	143.28	141.79	142.08	142.03	142.01
	0.92	161.58	158.67	159.34	159.25	159.21
Ag	0.90	182.19	177.22	178.49	178.38	178.32

	0.80	205.48	197.60	199.89	199.71	199.61
	0.86	231.03	220.01	223.90	223.54	223.40
	0.84	261.70	244.65	250.71	250.26	250.06
	0.82	295.65	271.78	280.89	280.28	280.01
	0.80	334.33	301.67	314.87	314.13	313.78
				K'		
	1.00	0.00	0.00	6.11	6.11	6.11
	0.98	5.94	5.82	5.83	5.83	5.83
	0.96	5.79	5.57	5.61	5.60	5.60
	0.94	5.65	5.34	5.41	5.40	5.40
	0.92	5.52	5.13	5.25	5.23	5.23
Ag	0.90	5.41	4.93	5.10	5.09	5.08
	0.80	5.30	4.76	4.97	4.96	4.95
	0.86	5.20	4.59	4.86	4.84	4.84
	0.84	5.11	4.44	4.76	4.74	4.74
	0.82	5.02	4.29	4.66	4.65	4.65
	0.80	4.94	4.16	4.58	4.57	4.57
				K		
	1.00	133.40	0.00	133.41	133.41	133.40
	0.98	145.90	148.38	148.39	148.37	148.35
	0.96	159.60	164.69	164.73	164.70	164.67
	0.94	174.66	182.45	182.62	182.53	182.53
	0.92	191.22	201.80	202.23	202.13	202.13
Cu	0.90	209.48	222.90	223.77	223.69	223.69
	0.88	229.64	245.92	247.59	247.48	247.48
	0.86	251.94	271.05	274.03	273.79	273.49
	0.84	276.66	298.51	303.29	302.98	302.98
	0.82	304.11	328.54	333.68	335.03	335.44
	0.80	334.67	361.40	371.94	372.44	371.64
				K'		
	1.00	0.00	0.00	5.37	5.37	5.37
	0.98	4.39	4.16	5.15	5.15	5.15
	0.96	4.32	4.96	4.97	4.97	4.97
	0.94	4.25	4.77	4.81	4.81	4.81
	0.92	4.18	4.60	4.68	4.68	4.67
Cu	0.90	4.12	4.45	4.55	4.56	4.55
	0.88	4.06	4.30	4.45	4.45	4.44
	0.86	4.00	4.17	4.35	4.36	4.34
	0.84	3.95	4.04	4.26	4.27	4.26
	0.82	3.90	3.92	4.18	4.20	4.18
	0.80	3.85	3.81	4.11	4.13	4.11
				K		
	1.00	166.70	0.00	166.7	166.7	166.7

	0.98	187.87	187.68	187.65	187.66	187.66
	0.96	211.57	210.68	210.74	210.72	210.71
	0.94	238.14	235.91	236.18	236.17	236.14
	0.92	268.00	263.59	264.49	264.32	264.27
Au	0.90	301.59	293.96	295.75	295.57	295.57
	0.88	339.45	327.31	330.65	330.35	330.17
	0.86	382.22	363.94	369.59	369.16	368.90
	0.84	430.63	404.19	413.25	412.60	412.22
	0.82	485.55	448.43	462.04	461.36	460.84
	0.80	548.00	497.19	517.15	516.24	515.56
				K'		
	1.00	0.00	0.00	6.00	6.00	6.00
	0.98	5.84	5.73	5.73	5.73	5.73
	0.96	5.69	5.49	5.51	5.51	5.51
	0.94	5.55	5.26	5.32	5.32	5.31
	0.92	5.43	5.06	5.15	5.16	5.15
Au	0.90	5.32	4.87	5.01	5.02	5.00
	0.88	5.21	4.70	4.88	4.89	4.88
	0.86	5.11	4.53	4.77	4.78	4.76
	0.84	5.02	4.38	4.68	4.68	4.67
	0.82	4.94	4.24	4.59	4.59	4.58
	0.80	4.86	4.11	4.51	4.51	4.50
				K		
	1.00	72.67	0.00	72.67	72.67	72.67
	0.98	79.70	79.63	79.65	79.64	79.64
	0.96	87.41	87.15	87.19	87.21	87.19
	0.94	95.87	95.26	95.38	95.37	95.36
	0.92	105.18	104.02	104.28	104.26	104.24
Al	0.90	115.43	113.50	113.98	113.96	113.91
	0.88	126.74	123.75	124.58	124.51	124.46
	0.86	139.24	134.85	136.19	136.03	136.01
	0.84	153.08	146.89	148.95	148.72	148.67
	0.82	168.44	159.94	162.99	162.61	162.59
	0.80	185.51	174.13	178.49	178.00	177.44
				K'		
	1.00	0.00	0.00	4.62	4.62	4.62
	0.98	4.52	4.45	4.46	4.46	4.46
	0.96	4.43	4.30	4.32	4.32	4.31
	0.94	4.35	4.16	4.20	4.19	4.19
	0.92	4.27	4.03	4.09	4.08	4.08
Al	0.90	4.19	3.91	4.00	3.99	3.98
	0.88	4.12	3.79	3.91	3.90	3.89
	0.86	4.06	3.68	3.83	3.82	3.82

0.84	4.00	3.58	3.77	3.74	3.74
0.82	3.94	3.49	3.70	3.67	3.68
0.80	3.88	3.40	3.65	3.61	3.62

The above calculations for pressure, bulk modulus and pressure derivative of bulk modulus for metals Ag (Fig.1-3), Cu (Fig.4-6), Au (Fig.7-9) and Al (Fig.10-12) have been shown by the various graphs as follows:

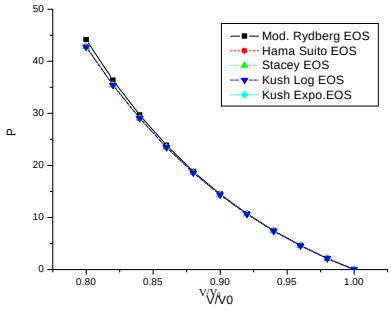

Figure1:Pressure P (GPa) versus relative volume (V/V_0) for Ag.

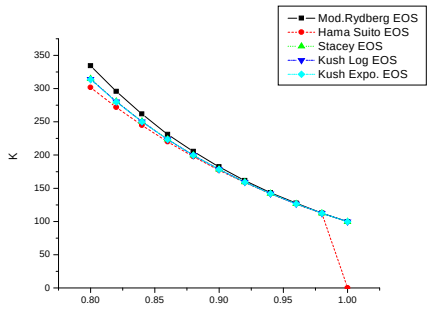

Figure 2. Bulk modulus K versus relative volume (V/V_o) for Ag.

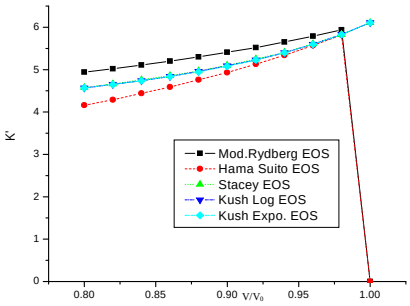

Figure 3. Pressure Derivative of Bulk modulus K' versus relative volume (V/V_o) for Ag.

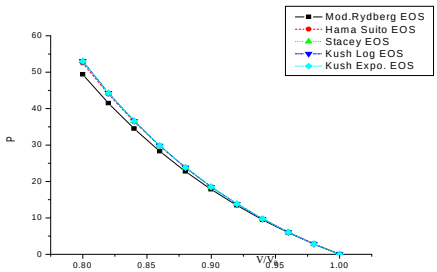

Figure 4.Pressure P(GPa) versus relative volume (V/V_o) for Cu.

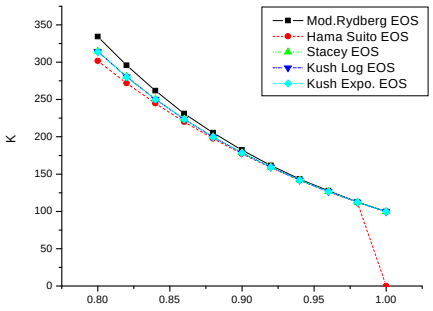

Figure 5. Bulk modulus K versus relative volume (V/V_o) for Cu.

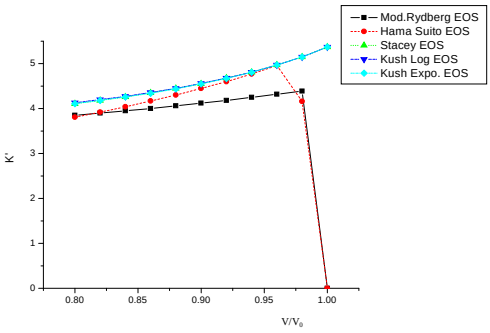

Figure 6. Pressure Derivative of Bulk modulus K' versus relative volume (V/Vo) for Cu.

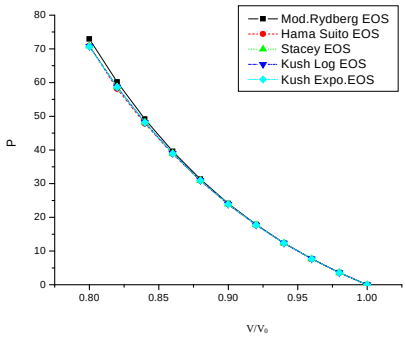

Figure 7.Pressure P(GPa) versus relative volume (V/V_o) for Au.

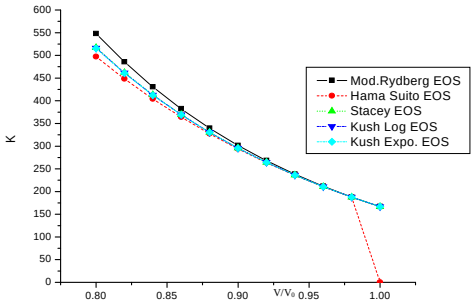

Figure 8. Bulk modulus K versus relative volume (V/V_o) for Au.

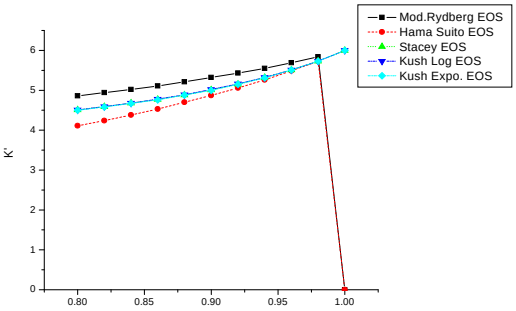

Figure 9. Pressure Derivative of Bulk modulus K' versus relative volume (V/V_o) for Au.

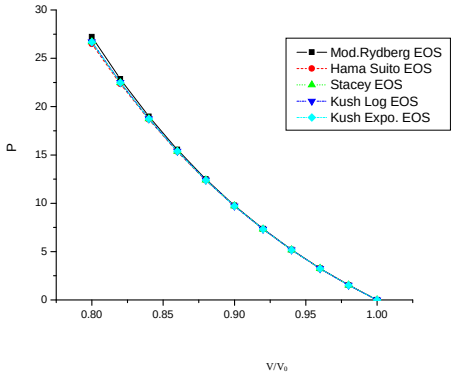

Figure10.Pressure P(GPa) versus relative volume (V/V_o) for Al.

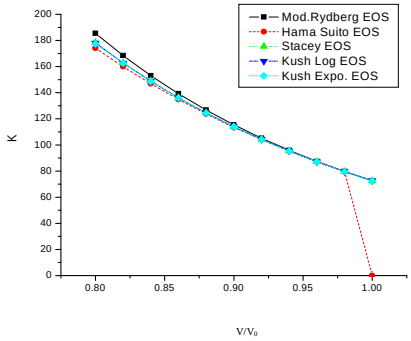

Figure 11. Bulk modulus K versus relative volume (V/V_o) for Al.

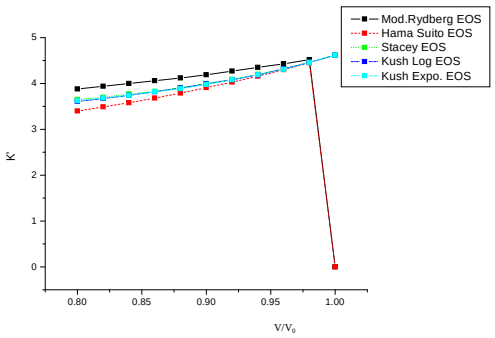

Figure 12. Pressure Derivative of Bulk modulus K' versus relative volume (V/V_o) for Al.

Conclusion:

To conclude, the results obtained for four metals(Ag, Cu, Au and Al) using the input data (table1)are reported in tables(2&3)for pressure, bulk modulus and its pressure derivative at different values of V/V_0 (from 0.8-1.0) and graphs are shown from figure (1-12).

It is found that these equations for pressure, bulk modulus and is pressure derivative yield results which are most identical with the corresponding values obtained from the Stacey reciprocal K-primed EOS for all metals.

Acknowledgments

We are extremely grateful to UGC, New Delhi for the financial assistance.

References and notes

1. Anderson, O. L.; Equation of state of solids for Geophysics and ceramic science; New York, Oxford University Press: **1995**.
2. Stacey, F.D.; High pressure equation of state and planetary Interiors. Rep. Prog. Physics **2005**, 68, 341.
3. Hama ,J.; and Suito, K.; J. Phys. Chem. Solids **2004**,65, 1581 .
4. Stacey, F.D.; The K-primed approach to high pressure equation of state. Geophys. J. Int. **2000** ,143, 621.
5. Singh, B.P.; Gajendra, S.; Analysis of compatibility of the generalized Rydberg equation. Int. J. of Pure & Appl. Phys.**2011,**49,467.
6. Shrivastava, H.C.; Generalized pressure volume equations mimicking the Stacey reciprocal K-primed equation of state. Physica B, **2009**,404, 251-254.
7. Singh, P.K.; Pressure dependence of bulk modulus for solids based on the first principles results. J. Indian of Pure & App. phy. **2011**,49 829.
8. Vashchenko, V. Ya; Zubarev ,V. N. ; Sov. Phy.Solid State **1963**,5,653.
9. Kushwah, S. S.; Srivastava, H. C.; Singh, K. S.; Study of pressure – volume relationships and higher derivatives of bulk modulus based on generalized equation of state. Physica B **2007,**20,388.
10. Kushwah, S. S.; Tomar, Y. S.; Sharma, M. P.; A new Method for thermal pressure using equation of state For MgO. Solid state Sciences **2011,**13,1162.
11. Shanker, J.; Singh, B. P.; & Shrivastva, S. K.;Volume temperature relationship for iron at 330 GPa and the Earth's core density deficit. Phys. Earth Planet Inter **2004,**147,333.
12. Shanker, J.; Singh, B. P.; & Baghel, H. K.; Physica B, **2007,**387,409.
13. Shanker, J.; Singh, B. P. ;& Jitendra, K.; Analysis of thermal expansivity of solids at extreme compression. Condensed Matter Phys. **2008,**11,681.
14. Shanker, J.; Singh, B. P.; & Jitender, K.; Extreme compression behaviour of higher derivative properties of solids based on the generalized Rydberg equation of state. Condensed Matter Phys. **2009,**12, 205.
15. Shanker, J.; Dulari, P.; & Singh, P.K.; Extreme compression behaviour of equation of state. Physica B, **2009,**40,4083.
16. Hama, J.; & Suito, K.; J. Phys. Condensed Matter, **1996,**7, 8.
17. Kushwah, S.S.; Bhardwaj, N.K.; Higher order thermoelastic properties of the earth lower mantle and core. Int. J.of Modern Physics B, **2010,**24, 1187-1200.
18. Holzaphel, W. B., Hartwig, M., Sievers, W.; Equation of state for Ag, Cu and Au for wide ranges in temperature and pressure up to 500 GPa and above. J.Phys. Chem. Ref. Data **2001,**30,515.
19. Dorogokupets, P.I.; Oganov, A. R.; Equation of state of Al, Au, Cu, Pt, Ta and W and revised ruby pressure scale. Doklady earth Sciences **2006,**410,1091.
20. Holzaphel, W. B.; Progress in the realization of a practical pressure scale for the range 1-300 GPa High Press Res.**2005,**25,87