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Elastic Properties of $MgSiO_3$ using Equation of State

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Abstract: Various equation of state (EOS) have been used to study pressure as a function of volume compression at a given temperature. The EOS,s for solids under low compression by evaluating the pressure-volume derivative properties viz., isothermal bulk modulus and its pressure derivatives calculated for $MgSiO_3$. The elastic moduli such as Bulk modulus, Shear modulus, Young's modulus and Poisson's ratio have been calculated as a function of pressure. The values of elastic moduli have been obtained using compressional wave velocity and shear wave velocity. It is found that all EOS's give satisfactory results which is in good agreement with Stacey EOS.

Keywords: Phase transition, Equation of state, Elastic properties.

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1. Introduction

The equation of state (EOS) of condensed matter is very important in many fields of basic and applied sciences including physics and geophysics.[1-3] An EOS provides useful information about the relationship among thermodynamic variables such as pressure (P), temperature (T) and volume (V) that helps us to understand the behaviour of materials under the effects of high pressure and high temperature.[4-5] The EOS is fundamentally important in studying the properties of materials at different pressure and at high temperature. The knowledge of the P-V-T EOS of relevant standard materials is one of the most basic information needed for pressure calibration. Various EOS are intended to account for the volumetric properties of solid whose structural configurations vary with pressure and temperature[1,6]. For performing calculations with the help of an EOS for a material at high pressures, we need the parameters K_0 , K'_0 , all at zero pressure. EOS can be made by studying the variation of $K' = dK/dP$ with pressure or compression (V/V_o). The P-V relationships reveal that the volume decreases continuously with the increase in pressure .The bulk modulus also increases with increase in pressure but its pressure derivatives K' decreases with the increase in pressure[7]. The purpose of the present study is to assess the validity of some important EOS's. A comparison of the result for P-V relationships, bulk modulus and its pressure derivative has been presented with various EOS's. In this paper, the EOS has been extended to calculate the theoretical values of both compressional and shear velocities of $MgSiO_3$ using isothermal EOS[8]. The other different elastic parameters viz., young's modulus, shear modulus, and poison's ratio are also determined by using pressure –density relationship for $MgSiO_3$.

2. Variation of pressure with compression at room temperature

The values of P, K and K' has been obtained as a function of compression V/V_0 from EOS's for $MgSiO_3$ with input parameters as (K_0 = 261 GPa and K'_0 = 4 GPa for $MgSiO_3$)[9]. We have used four EOS`s (a) Modified Rydberg EOS, (b) Birch Murnaghan EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS for calculating the pressure, bulk modulus and its pressure derivatives are as follows:

(a) Modified Rydberg EOS [4,10]

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

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

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

Where,

$$x = V/V_0$$
$$t = \frac{3}{2}K'_0 - 3K'_\infty + \frac{1}{2}$$
$$t = -3K_0K''_0 - \frac{3}{4}K'^2_0 + \frac{1}{12}$$

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) Birch Murnaghan EOS [8]

$$P = \frac{3}{4}K_0\left(x^{-7} - x^{-5}\right)\left[1 + \frac{3}{4}A_1\left(x^{-2} - 1\right)\right]$$
$$K = \frac{1}{2}K_0\left(7x^{-7} - 5x^{-5}\right) + \frac{3}{8}K_0A_1\left(9x^{-9} - 14x^{-7} - 5x^{-5}\right)$$
$$K' = \frac{K_0}{8K}\left[\left(K'_0 - 4\right)\left(81x^{-9} - 98x^{-7} - 25x^{-5}\right) + \frac{4}{3}\left(49x^{-7} - 25x^{-5}\right)\right]$$

Where

$$x = \left(V/V_0\right)^{1/3} \text{ and}$$
$$A_1 = \left(K'_0 - 4\right)$$

(c) Stacey Reciprocal k-primed EOS[10,11]

$$\ln\frac{V}{V_0} = \frac{K'_0}{K'^2_\infty}\ln\left(1 - K'_\infty\frac{P}{K}\right) + \left(\frac{K'_0}{K'_\infty} - 1\right)\frac{P}{K}$$
$$K = K_0\left(1 - K'_\infty\frac{P}{K}\right)^{-\frac{K'_0}{K'_\infty}}$$
$$\frac{1}{K'} = \frac{1}{K'_0} + \left(1 - \frac{K'_\infty}{K'_0}\right)\frac{P}{K}$$

(d) Kushwah Logarithmic EOS [2,10]

$$Px^{K'_\infty} = B_1\ln\left(2 - x\right)$$
$$B_2\left[\ln\left(2 - x\right)\right]^2 + B_3\left[\ln\left(2 - x\right)\right]^3$$
$$K = K'_\infty P + \frac{x^{1-K'_\infty}}{2 - x}$$
$$\left[B_1 + 2B_2\ln\left(2 - x\right) + 3B_3\left\{\ln\left(2 - x\right)^2\right\}\right]$$
$$K' = 2K'_\infty - \frac{K'^2_\infty P}{K} + \frac{2}{2 - x}$$
$$\left[\frac{K'_\infty P}{K} + \frac{x^{2-K'_\infty}}{K\left(2 - x\right)}\left\{B_2 + 3B_3\ln\left(2 - x\right)\right\} - 1\right]$$

Where,

$$x = V/V_0$$

$$B_1 = K_0$$

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

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

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

The results for P, K and K' as function of V/Vo down to 0.915 are given in table1-3. The results obtained from various EOS are found to present in general fair agreement with each other.

3. Elastic Moduli of $MgSiO_3$

There are mainly two types of sound velocities V_P and V_S i.e. for compressional or longitudinal and shear or transverse waves, respectively. These are related to bulk modulus (K), shear modulus (G) and density (ρ) as :

$$V_P = \left(\frac{K + \frac{4}{3}G}{\rho}\right)^{1/2}$$

$$V_S = \left(\frac{G}{\rho}\right)^{1/2}$$

The Shear modulus (G), Young's modulus (Y) and Poisson's ratio are as follows:

$$G = \frac{3}{5}\left(K - 2P\right)$$

$$Y = \left(\frac{9KG}{3K - G}\right)$$

$$\sigma = \left(\frac{3K + 4P}{12K - 4P}\right)$$

We make use of these equations for calculating shear modulus, Young's modulus and Poisson's ratio with help of K and P as a function of density .The results for these elastic moduli and sound velocities from various EOS's at different compression for $MgSiO_3$ at different compression are presented in table 4-7 respectively. [($\rho_O =$ 4.108 Kg/m^3) for $MgSiO_3$][1]

4. Result and Conclusion

For determining the values of pressure, isothermal bulk modulus and its derivatives, equations of state have been used exclusively. We have theoretically determined the variation of different elastic parameters viz., young's modulus, shear modulus, and poison's ratio of $MgSiO_3$ with compression. In this study, we have employed the equations to calculate the young's modulus, shear modulus, poison's ratio and have been reported in table 4 . It has been observed that the pressure increases with decrease in compression of the material as depicted in Fig. 1.The pressures calculated are found to be in good agreement with Stacey EOS. Bulk modulus also increases with decrease in compression as depicted in Fig. 2, but pressure derivative of bulk modulus decreases with decrease in compression as depicted in Fig. 3. It is also observed that the elastic moduli increase with increase in pressure and density . Moreover the density determined from the above calculations increases linearly with the calculated pressures. The nature of young's modulus, shear modulus, poisson's ratio with compression have been predicted and tabulated. The dependence of sound velocities has been determined using the pressure-density relationship . Furthermore we have predicted the variation of shear and compression wave velocity with different pressures as depicted in Fig-4.

Our theoretical investigations are in accordance with existing literature and few evidences. The calculated Poisson's ratio is in agreement with current studies[12]. Most practical materials typically have poisson's ratio □ values between 0 and 0.5[13]. Metal oxides usually have □ values around 0.25[14]. The shear sound velocity has agreed with previous literature[15]. The rate of increase of compression velocity with pressure is faster than shear velocity. The present work has predicted various parameters for low pressures. The EOS's employed in our study are found to be in accordance with each other over the whole analysis including all elastic parameters.

TABLE 1: Values of pressure for $MgSiO_3$ calculated from (a) Modified Rydberg EOS, (b) Birch Murnaghan EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS.

	P			
V/V_0	(a)	(b)	(c)	(d)
1.000	0.000	0.000	0.000	0.000
0.999	0.262	0.262	0.249	0.262
0.994	1.590	1.590	1.585	1.590
0.989	2.952	2.951	2.962	2.951
0.984	4.348	4.348	4.337	4.347
0.979	5.780	5.780	5.792	5.779
0.974	7.248	7.248	7.232	7.246
0.969	8.754	8.754	8.745	8.750
0.964	10.298	10.298	10.289	10.292
0.958	12.203	12.203	12.178	12.194
0.953	13.836	13.835	13.824	13.823
0.947	15.851	15.849	15.817	15.832
0.942	17.577	17.575	17.537	17.552
0.936	19.708	19.705	19.656	19.674
0.930	21.905	21.902	21.877	21.860
0.924	24.170	24.166	24.118	24.113
0.918	26.506	26.502	26.417	26.434
0.915	27.702	27.697	27.607	27.621

Table 2: Values of bulk modulus K for $MgSiO_3$ calculated from (a) Modified Rydberg EOS, (b) Birch Murnaghan EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS.

	K			
V/V_0	(a)	(b)	(c)	(d)
1.000	261.000	261.000	261.000	261.000
0.999	262.046	262.046	261.995	262.046
0.994	267.341	267.340	267.310	267.329
0.989	272.745	272.743	272.745	272.703
0.984	278.262	278.256	278.133	273.166
0.979	283.893	283.883	283.788	283.736
0.974	289.641	289.627	289.346	289.401
0.969	295.510	295.489	295.145	295.166
0.964	301.503	301.474	301.019	301.037
0.958	308.861	308.821	308.156	308.223
0.953	315.137	315.086	314.327	314.333
0.947	322.845	322.779	321.746	321.816
0.942	329.420	329.339	328.104	328.18
0.936	337.496	337.396	335.882	335.977
0.930	345.784	345.661	343.975	343.953
0.924	354.288	354.14	352.081	352.113
0.918	363.016	362.839	360.34	360.465
0.915	367.466	367.274	364.595	364.714

Table 3: Values of pressure derivative of bulk modulus K' for $MgSiO_3$ calculated from (a) Modified Rydberg EOS, (b) Birch Murnaghan EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS.

	K’			
V/V_0	(a)	(b)	(c)	(d)
1.000	4.000	4.000	4.000	4.000
0.999	3.996	3.996	3.994	3.994
0.994	3.978	3.977	3.962	3.962
0.989	3.960	3.958	3.932	3.932
0.984	3.942	3.939	3.903	2.826
0.979	3.924	3.921	3.874	3.874
0.974	3.906	3.903	3.846	3.847
0.969	3.889	3.885	3.819	3.820
0.964	3.872	3.867	3.793	3.794
0.958	3.852	3.846	3.762	3.764
0.953	3.836	3.829	3.737	3.740
0.947	3.816	3.809	3.708	3.711
0.942	3.800	3.792	3.685	3.688
0.936	3.781	3.773	3.658	3.661
0.930	3.763	3.754	3.631	3.635
0.924	3.745	3.735	3.605	3.610
0.918	3.727	3.716	3.580	3.586
0.915	3.718	3.707	3.568	3.574

Table 4: Values of elastic moduli calculated from Modified Rydberg EOS with different compression for $MgSiO_3$.

V/V0	ρ/ρ0	ρ	G	Y	σ	Vp	Vs
1.000	1.000	4.108	156.600	391.500	0.25	10.694	6.174
0.999	1.001	4.112	156.914	392.415	0.25	10.705	6.177
0.994	1.006	4.133	158.497	397.029	0.25	10.762	6.193
0.989	1.011	4.153	160.105	401.713	0.26	10.820	6.209
0.984	1.016	4.174	161.740	406.466	0.26	10.878	6.225
0.979	1.021	4.194	163.400	411.291	0.26	10.938	6.242
0.974	1.026	4.215	165.087	416.189	0.26	10.997	6.258
0.969	1.032	4.239	166.802	421.163	0.26	11.053	6.273
0.964	1.038	4.264	168.544	426.213	0.26	11.109	6.287
0.958	1.044	4.289	170.673	432.377	0.27	11.184	6.308
0.953	1.050	4.313	172.479	437.602	0.27	11.242	6.324
0.947	1.056	4.338	174.686	443.982	0.27	11.319	6.346
0.942	1.062	4.363	176.559	449.391	0.27	11.378	6.362
0.936	1.069	4.391	178.849	455.998	0.28	11.452	6.382
0.930	1.075	4.416	181.185	462.733	0.28	11.533	6.405
0.924	1.082	4.445	183.569	469.600	0.28	11.609	6.426
0.918	1.090	4.478	186.002	476.604	0.28	11.681	6.445
0.915	1.093	4.490	187.237	480.158	0.28	11.724	6.458

Table 5: Values of elastic moduli calculated from Birch Murnaghan EOS with different compression for $MgSiO_3$.

V/V0	ρ/ρ0	ρ	G	Y	σ	Vp	Vs
1.000	1.000	4.108	156.600	391.500	0.25	10.694	6.174
0.999	1.001	4.112	156.914	392.415	0.25	10.705	6.177
0.994	1.006	4.133	158.497	397.028	0.25	10.762	6.193
0.989	1.011	4.153	160.104	401.709	0.26	10.820	6.209
0.984	1.016	4.174	161.736	406.458	0.26	10.878	6.225
0.979	1.021	4.194	163.394	411.277	0.26	10.937	6.242
0.974	1.026	4.215	165.079	416.168	0.26	10.997	6.258
0.969	1.032	4.239	166.789	421.132	0.26	11.052	6.272
0.964	1.038	4.264	168.527	426.170	0.26	11.108	6.287
0.958	1.044	4.289	170.650	432.318	0.27	11.183	6.308
0.953	1.050	4.313	172.449	437.527	0.27	11.241	6.323
0.947	1.056	4.338	174.648	443.885	0.27	11.318	6.345
0.942	1.062	4.363	176.513	449.274	0.27	11.377	6.361
0.936	1.069	4.391	178.791	455.852	0.28	11.451	6.381
0.930	1.075	4.416	181.114	462.555	0.28	11.531	6.404
0.924	1.082	4.445	183.484	469.387	0.28	11.607	6.425
0.918	1.090	4.478	185.902	476.351	0.28	11.679	6.443
0.915	1.093	4.490	187.128	479.884	0.28	11.720	6.456

Table 6: Values of elastic moduli calculated from Stacey reciprocal K-primed EOS with different compression for $MgSiO_3$.

V/V0	ρ/ρ0	ρ	G	Y	σ	Vp	Vs
1.000	1.000	4.108	156.600	391.501	0.25	10.694	6.174
0.999	1.001	4.112	156.898	392.370	0.25	10.705	6.177
0.994	1.006	4.133	158.484	396.995	0.25	10.762	6.193
0.989	1.011	4.153	160.092	401.685	0.26	10.820	6.209
0.984	1.016	4.174	161.675	406.298	0.26	10.876	6.224
0.979	1.021	4.194	163.322	411.103	0.26	10.935	6.240
0.974	1.026	4.215	164.929	415.787	0.26	10.992	6.258
0.969	1.032	4.239	166.593	420.636	0.26	11.046	6.269
0.964	1.038	4.264	168.265	425.511	0.26	11.100	6.282
0.958	1.044	4.289	170.280	431.382	0.27	11.171	6.301
0.953	1.050	4.313	172.007	436.416	0.27	11.227	6.315
0.947	1.056	4.338	174.067	442.418	0.27	11.299	6.335
0.942	1.062	4.363	175.818	447.518	0.27	11.355	6.348
0.936	1.069	4.391	177.942	453.706	0.28	11.424	6.365
0.930	1.075	4.416	180.133	460.086	0.28	11.501	6.387
0.924	1.082	4.445	182.308	466.419	0.28	11.571	6.404
0.918	1.090	4.478	184.504	472.815	0.28	11.637	6.419
0.915	1.093	4.490	185.629	476.088	0.28	11.676	6.430

Table 7: Values of elastic moduli calculated from Kushwah logarithmic EOS with different compression for $MgSiO_3$.

V/V0	ρ/ρ0	ρ	G	Y	σ	Vp	Vs
1.000	1.000	4.108	156.600	391.500	0.25	10.694	6.174
0.999	1.001	4.112	156.913	392.414	0.25	10.705	6.177
0.994	1.006	4.133	158.489	397.011	0.25	10.762	6.193
0.989	1.011	4.153	160.080	401.649	0.25	10.819	6.208
0.984	1.016	4.174	158.731	398.924	0.26	10.778	6.167
0.979	1.021	4.194	163.308	411.059	0.26	10.934	6.240
0.974	1.026	4.215	164.945	415.834	0.26	10.993	6.256
0.969	1.032	4.239	166.600	420.656	0.26	11.046	6.269
0.964	1.038	4.264	168.271	425.528	0.26	11.100	6.282
0.958	1.044	4.289	170.301	431.442	0.27	11.172	6.301
0.953	1.050	4.313	172.012	436.429	0.27	11.227	6.315
0.947	1.056	4.338	174.091	442.485	0.27	11.300	6.335
0.942	1.062	4.363	175.845	447.593	0.27	11.356	6.349
0.936	1.069	4.391	177.977	453.801	0.28	11.426	6.366
0.930	1.075	4.416	180.139	460.095	0.28	11.501	6.387
0.924	1.082	4.445	182.332	466.479	0.28	11.572	6.405
0.918	1.090	4.478	184.558	472.956	0.28	11.639	6.420
0.915	1.093	4.490	185.683	476.230	0.28	11.678	6.431

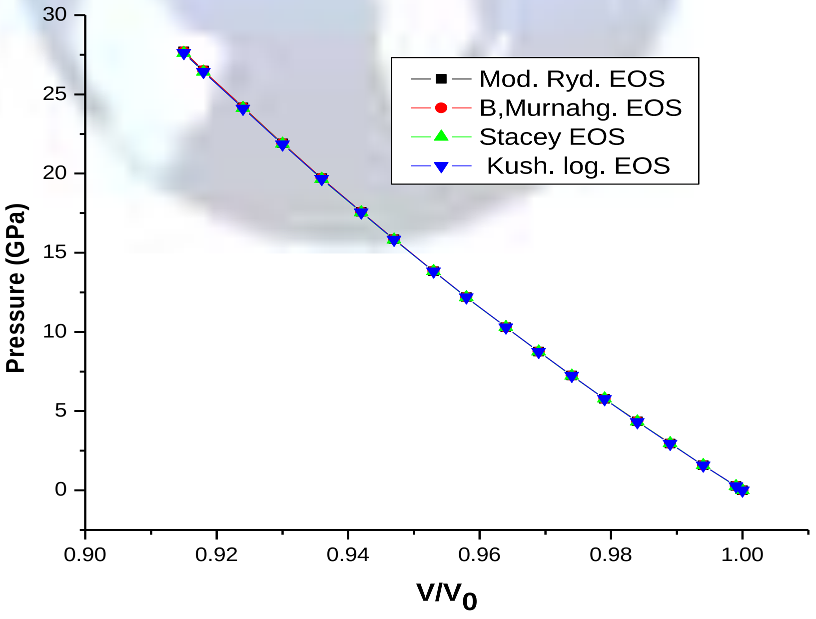

Fig.1: Pressure P(GPa) versus Compression(V/V_0) for $MgSiO_3$.

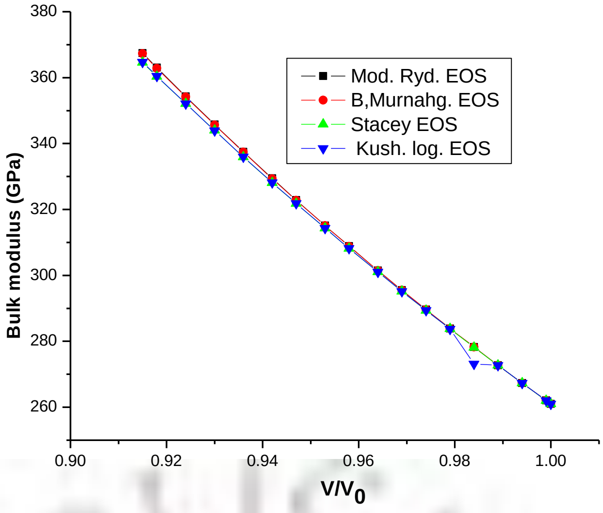

Fig.2: Bulk modulus K (GPa) versus Compression(V/V_0) for $MgSiO_3$.

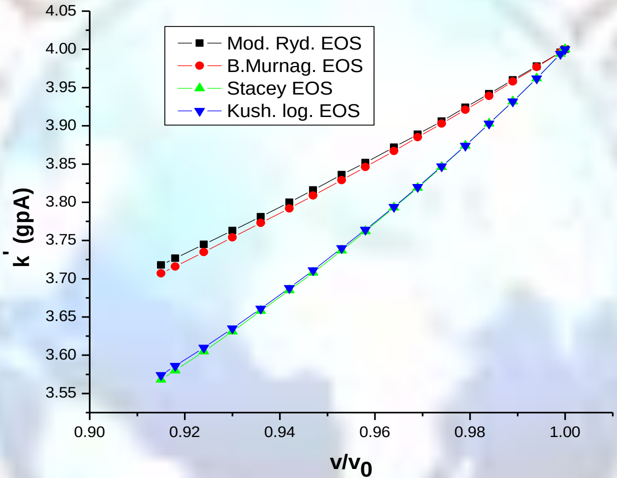

Fig.3: Pressure derivative of bulk modulus K′ P(GPa) versus Compression(V/V_0) for $MgSiO_3$.

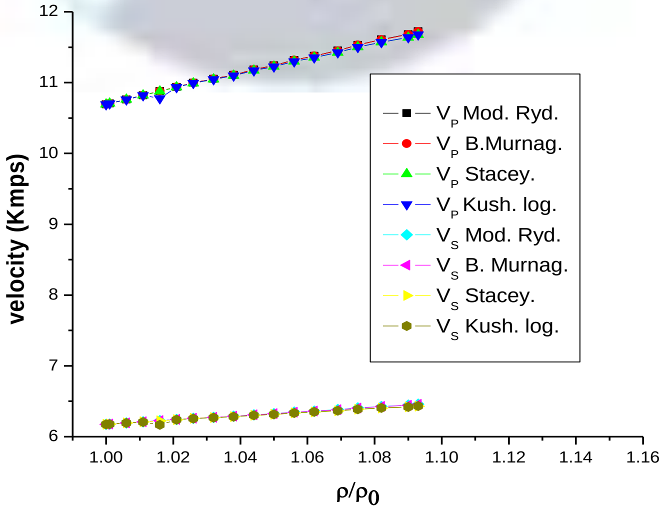

Fig.4: Reduced velocities versus normalized density for $MgSiO_3$.

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