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Estimation of thermodynamic parameters in 3.Om and 3O.Om liquid crystalline compounds

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ABSTRACT

Thermodynamic parameters such as Moelwyn–Hughes parameter (C_1), reduced volume ($V^{\sim}$), reduced compressibility (β), isochoric temperature coefficient of internal pressure (X), Sharma parameter (S_0), Huggin's parameter (F), Grüneisen parameter (Γ_p), isothermal microscopic Grüneisen parameter (Γ), fraction free volume (f) and acoustical parameters like isothermal (K′), isobaric (K), isochoric (K″) acoustical parameters, isothermal Grüneisen parameter (Γ_{ith}), isobaric Grüneisen parameter (Γ_{iba}), isochoric Grüneisen parameter (Γ_{ich}), reduced Bulk modulus ($B^{\sim}$), isothermal Anderson–Grüneisen parameter (δ) and magnitude of repulsive exponent (n) are estimated from thermal expansion coefficient, α obtained from density variation with temperature, ρ in liquid crystalline N-(p-n-propyl/propyloxybenzylidene)-p-n-alkoxy anilines, 3.Om and 3O.Om with m = 6, 7 and 8. In addition to these, the parameters like molecular free length (L_f), molecular radius (m_r) and nonlinearity parameter, (B/A) are also evaluated. The variation of all these parameters are studied both with the temperature in an individual compound and with the chain length in a homologous series. Further, the results agree with the body of the data available.

1. Introduction

Liquid Crystal (LC) materials possessing anisotropic properties are gaining interest of several workers and have been recognized as new dynamic functional molecular materials with wide range of applications in electro-optic display devices. The nature of molecular interactions in LC compounds can be studied from different phase transformations and pretransitional effects [1]. Further, the study of thermo dynamical, anharmonic and acoustical parameters provide information regarding the physico-chemical behavior of the molecules. Moreover, the Bayer's nonlinearity parameter (B/A) provides [2] information regarding physical attributes of a material such as internal pressure, intermolecular spacing and acoustic scattering. Thus, the evaluation of these parameters in pure liquids and liquid mixtures has gained much interest from past decade [3–7]. In view of their importance, as a part of our systematic studies, in the present paper we made an attempt to extend the studies to the liquid crystalline compounds N-(*p*-*n*-propyl/propyloxybenzylidene)-*p*-*n*-alkoxy anilines, 3.Om and 3O.Om with m = 6, 7 and 8 which exhibit nematic phase with different nematic thermal ranges. The density and refractive index data required for the present compounds is taken from literature [8,9].

2. Theory and expressions

The procedure for the estimation of different thermodynamic parameters using the coefficient of thermal expansion (α) is taken from literature [10–13] and is given below.

The coefficient of volume expansion is given by $(\alpha) = 1/V_m\,(dV_m/dT)$, where $dT = T_2 - T_1$, $dV_m = V_{m2} - V_{m1}$.

The Moelwyns–Hughes parameter (C_1) and reduced molar volume ($V^{\sim}$) [3] are evaluated from the following expressions:

$$C_1 = \left(\frac{13}{3}\right) + \left(\frac{1}{\alpha T}\right) + \left(\frac{4\,\alpha T}{3}\right) \tag{1}$$

$$V^{\sim} = \left\{\frac{\left(\frac{\alpha T}{3}\right)}{(1+\alpha T)} + 1\right\}^3. \tag{2}$$

The isochoric temperature coefficient of internal pressure (X) is given by

$$X = -\frac{2(1+2\,\alpha T)}{V^{\sim C_1}} \tag{3}$$

where $V^{\sim C_1} = \beta$ is the reduced compressibility.

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Sharma parameter [10–17] S_0 is given by the expression

$$S_0 = \left(-\frac{X}{2}\right)(3 + 4\ \alpha T). \tag{4}$$

The Huggins parameter [15] F of a liquid crystal is related to S_0 by the equation

$$F = 2\left[1 + \left(\frac{S_0}{(3 + 4\,\alpha T)}\right)\right] - \left(3 + \frac{4\alpha T}{3}\right). \tag{5}$$

Isothermal microscopic Grüneisen parameter (Γ) is a measure of volume dependence of the hormonicity of the normal mode frequency (ν) of molecular vibrations of a material is related to F and S_0 as

$$\Gamma = \left(\frac{2}{3}\right)\ \alpha T + \left(\frac{2 - F + 4\,\alpha T}{2\,\alpha T}\right). \tag{6}$$

The fraction free volume (f), is a measure of disorder due to increase of mobility of molecules in a liquid crystal and can be expressed in terms of isothermal Grüneisen parameter (Γ) as

$$f = \frac{1}{(\Gamma\ + 1)} = \frac{V_a}{V} \tag{7}$$

where V_a is the available volume. The estimation of V_a is described below.

Thermal parameter A* is a dimensionless parameter which shows that at low temperatures, a liquid crystal tends to be ordered, thereby makes A* equal to unity

$$A* \ = 1 + \left(\frac{f}{\Gamma}\right). \tag{8}$$

The Grüneisen parameter (Γ_p) for liquid crystals can be obtained from

$$\Gamma_p = \left(\frac{2}{3}\right)\alpha T + \left(\frac{1}{2\alpha T}\right) + 2. \tag{9}$$

The isochoric acoustical parameter, Δ is given as

$$\Delta = \left(\frac{-\alpha T}{2}\right). \tag{10}$$

The reduced Bulk modulus can be given as follows

$$B^{\sim} = \left[V^{\sim C_1}\right]^{-1} \tag{11}$$

where $B^{\sim} = B'/B_0$ is the reduced bulk modulus, and $V^{\sim} = V/V_0$ is the reduced volume. B′ and V is the bulk modulus and volume at temperature T, and B_0' and V_0 are the bulk modulus and volume at absolute zero.

The isothermal Anderson–Grüneisen parameter δ is known to be an important parameter in the theory of temperature dependence of bulk modulus in solids. It is defined as

$$\delta = 2\Gamma_{iba}. \tag{12}$$

The Anderson–Grüneisen parameter is distinguished from the Moelwyn–Hughes parameter by introducing a new parameter θ as

$$\theta = 2(\Gamma_{ith} - \Gamma_{iba}) + 1. \tag{13}$$

The isothermal, isobaric and isochoric Grüneisen parameters are identical to the corresponding acoustical parameters so one can write

$$\Gamma_{ith} = \Gamma_{iba} + \Gamma_{ich}. \tag{14}$$

The isothermal Grüneisen parameter is evaluated using the value of C_1 in Eq. (1). The isochoric Grüneisen parameter Γ_{ith} could be evaluated by using the following equation.

$$\Gamma_{ith} = (C_1 - 1)/2 \tag{15}$$

and

$$\Gamma_{ich} = -(E - F)/F \tag{16}$$

where $E = [2 + (\alpha T)^{-1}(-2\alpha)(V^{\sim C_1})]^{-1}$ and $F = -2\alpha T$.

Reddy et al. [18–20] demonstrated the following relationship between n, m and C_1 as

$$n = 3C_1 - 12 \tag{17}$$

and

$$m = 3C_1 - (n\ +\ 6) \tag{18}$$

where m and n are the exponents describing the magnitude of attractive and repulsive force, respectively.

Sharma [21] proposed a theoretical method to establish a relation between the molecular constant r and isochoric thermo acoustical parameter Δ as

$$r = (1 - \Delta)^{-1} = P_i/\varepsilon \tag{19}$$

where P_i and ε is internal pressure and cohesive energy density respectively.

2.1. Inter molecular free length (L_f)

The estimation of L_f is described below using the thermodynamic parameters. Using the equations (1 to 3), the isothermal (K′), isochoric (K″) and isobaric (K) acoustical parameters are obtained from the following expressions

$$K' = K + K'' = \frac{1}{2}\left[3 + \frac{(S*(1 + \alpha T) + X)}{\alpha T}\right] \tag{20}$$

$$K'' = 1 + \left(\frac{X}{2\alpha T}\right) \tag{21}$$

and

$$K = \frac{1}{2}\left[1 + \left(\frac{S*(1 + \alpha T)}{\alpha T}\right)\right] \tag{22}$$

where $S* = 1 + \left(\frac{4\,\alpha T}{3}\right)$. (23)

The isothermal acoustical parameter (K′) is related to the available volume (V_a) of the compound as

$$\frac{V_a}{V_m} = \frac{1}{(K' + 1)} = \frac{1}{(K'' + K + 1)} \tag{24}$$

where V_m is molar volume (molecular weight/density) and the available volume, (Va) can be deduced using the thermo acoustical parameter K′ as

$$V_a = \frac{V_m}{K' + 1}. \tag{25}$$

Then the intermolecular free-length [17] (L_f) is given by the relation

$$L_f = \frac{2V_a}{Y} \tag{26}$$

where V_a represents the available volume per mole and Y is surface area per mole given by

$$V_{01} = V - V_a \tag{27a}$$

where

$$Y = (36\pi N V_0^{\,2})^{1/3}. \tag{27b}$$

The molar volume at 0 K (V_0) can be also obtained by

$$V_{02} = \frac{V}{V^{\sim}}. \tag{28}$$

N is the Avogadro number and $V^{\sim}$ is taken from Eq. (2).

Further, V_0 can be obtained directly from molar volume data by extrapolating isotropic data to 0 K.

B^* is another dimensionless parameter and is related to isochoric and isothermal acoustical parameter is given by

$$B^* = [1 + (K - K'')(K' + 1)]^{-1}. \tag{28a}$$

2.2. Molecular radius (M_r)

M_r for the LC molecule can be obtained from density and refractive index results and the relevant expressions are given below [13]

(i) From density, ρ

$$M_r = \frac{1}{2} 3 \sqrt{\frac{M\sqrt{2}}{\rho N}} \tag{29}$$

where M is the molecular weight.

(ii) The refractive index data can be utilized in conjunction with molar volume to compute the molecular radius (M_r) using the following relation [13,14]

$$M_r = \left[\left(\frac{3}{4\pi N} \right) \frac{(n^2 - 1)}{(n^2 + 2)} V_m \right]^{1/3}. \tag{30}$$

2.3. Acoustic nonlinearity parameter, B/A

There are a number of reports in literature describing in detail the theoretical and empirical approach for the estimation of B/A from the thermal expansion coefficient, α and ultrasonic velocity, u respectively, the relevant expressions of the non-linearity parameter, B/A is given as [22]

$$B/A = 2u\rho[du/dp]_T. \tag{31}$$

General formalism for B/A in terms of the acoustical parameters for liquids and polymers has been made using Moelwyns–Hughes parameter (C_1), isobaric acoustic parameter (K) and the isothermal acoustic parameter (K″) (the detailed method of calculation of K and K″ from α is given elsewhere obtained from the thermal expansion coefficient, α, and from the ultrasonic velocity, u respectively). The expressions for B/A from density are given as

$$B/A = C_1 - 1 \tag{32a}$$

$$B/A = 2K + 2\gamma K''. \tag{32b}$$

3. Results and discussion

The thermodynamic parameters such as reduced volume ($V^{\sim}$), reduced compressibility (β), isochoric temperature coefficient of internal pressure (X), Sharma parameter (S_0), Huggin's parameter (F), Grüneisen parameter (Γ_p), isothermal microscopic Grüneisen parameter (Γ), fraction free volume (f) parameters are evaluated from the coefficient of thermal expansion obtained from density data. The parameter such as Moelwyn–Hughes parameter (C_1), is an important parameter to obtain acoustical parameters like isothermal (K'), isobaric (K), isochoric (K'') acoustical parameters, isothermal Grüneisen parameter, (Γ_{ith}), isobaric Grüneisen parameter, (Γ_{iba}), isochoric Grüneisen parameter, (Γ_{ich}), reduced Bulk modulus, ($B^{\sim}$), isothermal Anderson–Grüneisen parameter, (δ) and magnitude of repulsive exponent, (n). It is already known that C_1 offers the simplest scale for the determination of molecular ordering, structure, interactions and anharmonicity in some materials [12]. In addition to these, the parameters like molecular free length (L_f), molecular radius (M_r) and nonlinearity parameter, (B/A) are also evaluated. The results are compared with those obtained for similar nature of compounds viz., nO.Om compounds. Recently, extensive studies are reported regarding the estimation of the thermodynamic parameters for a number of nO.m liquid crystalline compounds utilizing the available dilatometric, ultrasonic velocity and birefringence data [13]. The data pertinent to the above parameters for all the compounds are presented in Tables 1 to 5 and their variation with temperature and chain length is given in Figs. 1 to 6.

The salient features observed from the study are

1. All the parameters exhibit a constant value in a particular phase except in the vicinity of phase transition where they exhibit singularity, (Figs. 1 to 4).

Table 1
Variation of anharmonic parameters such as Moelwyn–Hughes parameter (C_1), reduced volume ($V^{\sim}$), reduced compressibility (β), isochoric temperature coefficient of internal pressure (X), Sharma parameter (S_0), Huggin's parameter (F), fraction free volume (f) in isotropic and nematic LC of all the compounds.

Comp.	Temp.	Phase	$V^{\sim}$	C_1	$\beta = V^{\sim C_1}$	X_1	X	S_0	F	Γ	f	A*
3.O6	83.9	Iso	1.12	11.93	4.02	−1.27	−0.63	1.12	1.45	4.12	0.20	1.05
	68.0	N	1.24	8.17	5.87	−1.58	−0.54	1.12	1.15	3.66	0.21	1.06
3.O7	81.0	Iso	1.13	11.63	4.08	−1.28	−0.63	1.12	1.44	4.08	0.20	1.05
	68.0	N	1.25	8.09	5.97	−1.59	−0.53	1.12	1.14	3.65	0.22	1.06
3.O8	83.1	Iso	1.14	11.22	4.17	−1.30	−0.62	1.12	1.42	4.03	0.20	1.05
	70.0	N	1.25	7.99	6.12	−1.62	−0.53	1.12	1.12	3.64	0.22	1.06
3O.O6	114	Iso	1.24	8.13	5.92	−1.59	−0.54	1.12	1.14	3.65	0.21	1.06
	98.5	N	1.28	7.68	6.66	−1.69	−0.51	1.11	1.05	3.61	0.22	1.06
3O.O7	111	Iso	1.26	7.89	6.28	−1.64	−0.52	1.12	1.10	3.63	0.22	1.06
	97.0	N	1.30	7.51	7.06	−1.75	−0.49	1.11	1.00	3.59	0.22	1.06
3O.O8	109	Iso	1.26	7.90	6.25	−1.64	−0.52	1.12	1.10	3.63	0.22	1.06
	96.5	N	1.30	7.50	7.08	−1.75	−0.49	1.11	1.00	3.59	0.22	1.06

Table 2
Variation of parameters such as isothermal (K′), isochoric (K″) and isobaric (K) acoustical parameters, available volume (V_a) and molecular free length (L_f) in isotropic and nematic LC phases of all the compounds.

Comp	Temp °C	Phase	k″	k	k′	V_a	V_{01}	V_{02}	L_{f1}	L_{f2}
3.O6	83.9	Iso	−1.357	8.670	7.314	40.624	297.114	300.579	0.447	0.434
	68.0	N	0.053	4.808	4.861	56.771	275.986	267.907	0.656	0.669
3.O7	81.0	Iso	−1.246	8.367	7.121	43.531	309.990	313.265	0.466	0.462
	68.0	N	0.082	4.728	4.810	59.978	288.515	279.431	0.673	0.687
3.O8	83.1	Iso	−1.095	7.955	6.860	47.045	322.717	325.557	0.49	0.487
	70.0	N	0.124	4.615	4.739	63.634	301.545	291.049	0.693	0.71
3O.O6	113.5	Iso	0.067	4.771	4.838	60.402	292.197	283.345	0.672	0.686
	98.5	N	0.245	4.285	4.530	62.724	284.147	271.014	0.711	0.734
3O.O7	111	Iso	0.159	4.518	4.677	65.322	305.525	293.950	0.705	0.724
	97.0	N	0.316	4.094	4.409	67.560	297.879	281.696	0.742	0.77
3O.O8	109	Iso	0.156	4.527	4.683	67.669	316.876	304.962	0.713	0.732
	96.5	N	0.318	4.086	4.405	70.052	308.554	291.692	0.751	0.78

Table 3
Variation of parameters such as Grüneisen parameter (Γ_p), isothermal microscopic Gruneisen parameter (Γ),isothermal Anderson–Grüneisen parameter (δ), Anderson–Grüneisen parameter (θ), exponents describing the magnitude of attractive and repulsive force m and n in isotropic and nematic LC phase of all the compounds.

Comp.	Temp.	Phase	Γ	Γ_P	Δ	B^-	E	F	Γ_{ith}	Γ_{ich}	Γ_{iba}	δ	θ	θ*	r	m
3.O6	83.9	Iso	4.12	5.80	112.85	0.25	0.51	−0.27	5.46	2.87	2.59	5.17	6.75	5.17	2.72	6.00
	68	N	3.66	3.92	91.71	0.17	0.51	−0.58	3.58	1.88	1.71	3.41	4.75	3.41	2.17	6.00
3.O7	81	Iso	4.08	5.65	111.23	0.25	0.51	−0.28	5.31	2.80	2.51	5.03	6.59	5.03	2.69	6.00
	68	N	3.65	3.88	91.03	0.17	0.51	−0.59	3.54	1.86	1.69	3.38	4.71	3.38	2.15	6.00
3.O8	83.1	Iso	4.03	5.44	110.84	0.24	0.51	−0.30	5.11	2.69	2.42	4.83	6.38	4.83	2.65	6.00
	70	N	3.64	3.83	90.55	0.16	0.51	−0.62	3.49	1.83	1.67	3.33	4.65	3.33	2.12	6.00
3O.O6	113.5	Iso	3.65	3.90	103.59	0.17	0.51	−0.59	3.56	1.87	1.70	3.40	4.73	3.40	2.16	6.00
	98.5	N	3.61	3.68	94.44	0.15	0.51	−0.69	3.34	1.74	1.60	3.21	4.47	3.21	2.04	6.00
3O.O7	111	Iso	3.63	3.78	100.34	0.16	0.51	−0.64	3.45	1.80	1.65	3.30	4.60	3.30	2.10	6.00
	97	N	3.59	3.59	91.55	0.14	0.51	−0.75	3.25	1.68	1.57	3.14	4.36	3.14	1.98	6.00
3O.O8	109	Iso	3.63	3.79	99.91	0.16	0.51	−0.64	3.45	1.80	1.65	3.30	4.60	4.60	2.10	6.00
	96.5	N	3.59	3.58	91.33	0.14	0.51	−0.75	3.25	1.68	1.57	3.14	4.36	4.36	1.98	6.00

2. From the data, it is observed that if coefficient of volume expansion is low its C_1 value is high. From Table 1 it is known that C_1 is low in nematic phase and high in isotropic phase. The parameters reduced volume, V^-, reduced compressibility, $V^{\sim C_1}$, and the isochoric temperature coefficient of internal pressure, (X) and their variation with temperature is similar to that of thermal expansion coefficient α, as excepted and in all compounds as these parameters are proportional to α. The variation of reduced volume V^- and C_1 with the temperature in 3O.O6 is shown in Fig. 1.
3. From Table 1 it is observed that the parameters C_1, X′, F, Γ, Δ, Γ_p are exhibiting low values in liquid crystalline phases compared to the isotropic phase which shows the molecular ordering increases as the temperature decreases in liquid crystal phases.
4. From Fig. 2 it is known that the Sharma parameter, S_0 is constant around 1.13 ± 0.05 irrespective of the nature and state of the compound including the liquid crystals. S_0 tends to be independent of the value of α for any material. However, at and in the immediate vicinity of the liquid crystalline phase transformations the value of S_0 abruptly falls to a minimum as the parameter S_0 [20] is indirectly proportional to α.
5. The fractional free volume (f) which determines the disorder due to the mobility of molecules in the compound. Hence, the relations viz., $S_0 = 5.5 * f$ and $A^* = 5.25 * f$ hold good in these compounds also as in the case of other nO.m compounds [14].
6. It is observed that the available volume, V_a is more in liquid crystalline phase than in isotropic phase and its variation with temperature for the case of all the compounds is given in Table 2 and Fig. 5. From the Figure it is known that V_a is more in 3O.Om compounds than in 3.Om compounds.
7. The isothermal Anderson–Grüneisen parameter δ is known to be an important parameter in the theory of temperature dependence of bulk modulus in solids [23]. Fig. 3 depicts its variation with temperature in 3.O6 compound. From Table 3 the magnitude of m is recognized as 6 in the case of liquid crystalline compounds which is in agreement with the literature [23].

Table 4
Variation of non linearity parameter, B/A in isotropic and nematic LC phase of all the compounds.

Comp.	Temp.	Phase	B/A (K)	B/A (C_1)
3.O6	83.9	Iso	8.238	10.924
	68	N	7.313	7.167
3.O7	81	Iso	8.161	10.624
	68	N	7.297	7.092
3.O8	83.1	Iso	8.057	10.219
	70	N	7.275	6.986
3O.O6	113.5	Iso	7.306	7.132
	98.5	N	7.215	6.683
3O.O7	111	Iso	7.256	6.896
	97	N	7.184	6.508
3O.O8	109	Iso	7.258	6.904
	96.5	N	7.183	6.502

Table 5
Variation of molecular radius, M_r obtained from Eqs. (29) and (30) in isotropic and nematic LC phase of all the compounds.

Comp.	Temp.	Phase	$M_{r(density)}$	M_r optics
3.O6	83.9	Iso	4.638	3.476
	68	N	4.605	3.557
3.O7	81	Iso	4.699	3.540
	68	N	4.676	3.600
3.O8	83.1	Iso	4.770	3.581
	70	N	4.750	3.681
3O.O6	113.5	Iso	4.700	3.570
	98.5	N	4.720	3.651
3O.O7	111	Iso	4.773	3.600
	97	N	4.751	3.691
3O.O8	109	Iso	4.832	3.599
	96.5	N	4.807	3.699

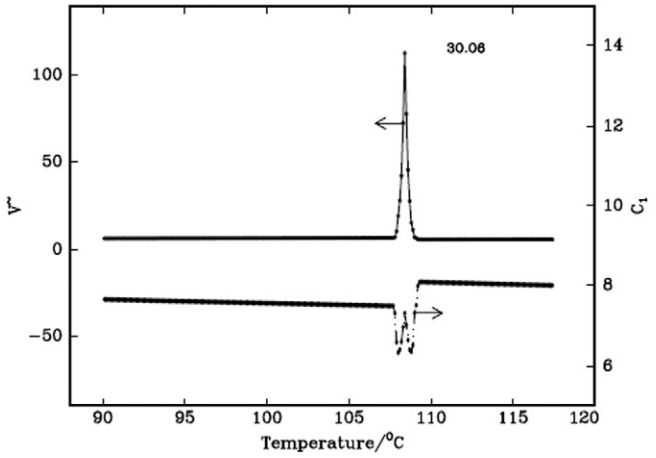

Fig. 1. Variation of reduced volume (V^*) and Moelwyn–Hughes parameter (C_1) with temperature in 3O.O6 compound.

8. The isothermal Grüneisen parameter Γ_{ith} is a measure of anharmonicity of molecular vibration, the isothermal, isochoric, isobaric Grüneisen parameters also show the consistent values in any particular phase but decreases slightly in LC phases from isotropic phase. The values of Γ_{ith}, Γ_{iba}, Γ_{ich} are given in Table 3 for the all the present studied compounds. The variation of Γ_{ith}, Γ_{iba}, Γ_{ich} with temperature is shown for the compound 3.O8 in Fig. 4. The parameter Γ_{iba} exhibits almost a similar trend as Γ_{ith} and Γ_{iba} is less than Γ_{ith},
9. The molecular free length (L_f) are calculated from available volume V_a and molar volume (V_o). However, V_o can be evaluated using different expressions. The V_o is estimated in two ways and the values at different temperatures in LC phases given in Table 2 reveal that V_o values show agreement with one another. It has been reported earlier, from the systematic studies on the benzoic acids as well as in a number of nO.m compounds [13] found that the slope value should be around 8×10^{-4} to obtain reasonable agreement. The molecular free length values in all the compounds in both the series are of comparable magnitude and the isotropic values are slightly lower compared to LC phases. The variation of L_f with temperature is depicted in Fig. 6 for the case of all compounds.
10. The data from Table 4 reveals that the B/A value almost remains constant in a particular phase except in the vicinity of the phase transition where it shows a peak and the peak magnitude depends on α, and further, the magnitude of B/A is slightly smaller in LC phases compared to that in isotropic phase.

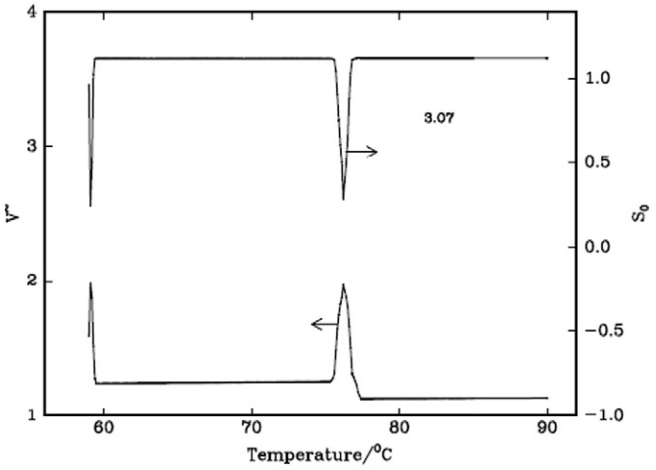

Fig. 2. Variation of reduced volume (V^*) and Sharma parameter (S_0) with temperature in 3.O7 compound.

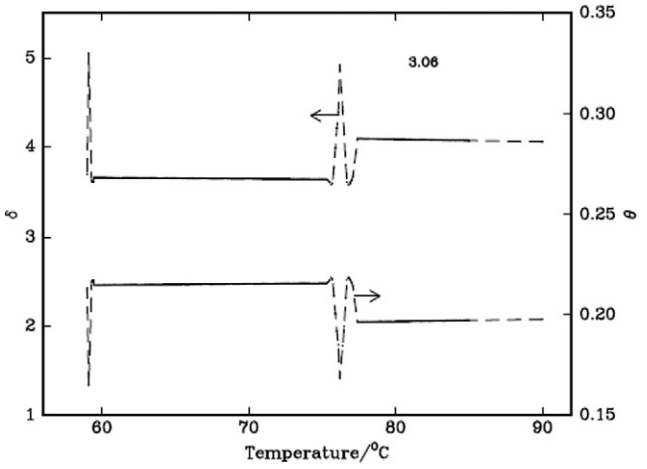

Fig. 3. Variation of isothermal Anderson–Gruneisan parameter (δ) and Anderson Gruneisan parameter (θ) with temperature in 3.O6 compound.

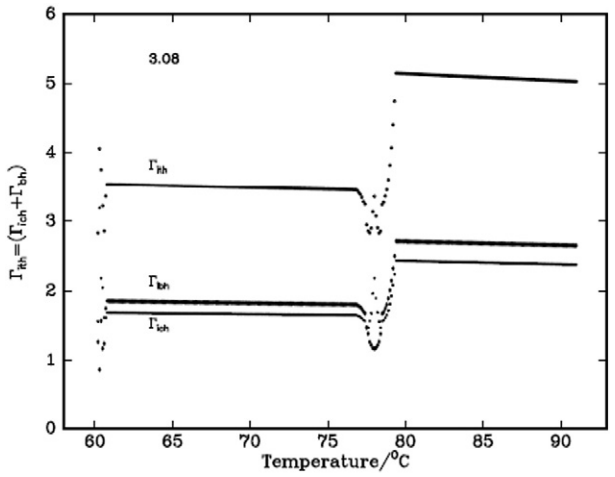

Fig. 4. Variation of isothermal Gruneisan parameter $\Gamma_{ith} = \Gamma_{iba} + \Gamma_{ich}$ with temperature in 3.O8 compound.

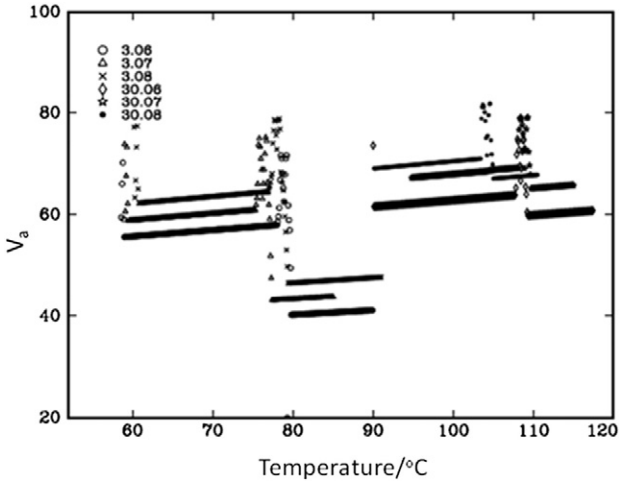

Fig. 5. Variation of available volume (V_a) with temperature in 3.Om and 3O.Om compounds.

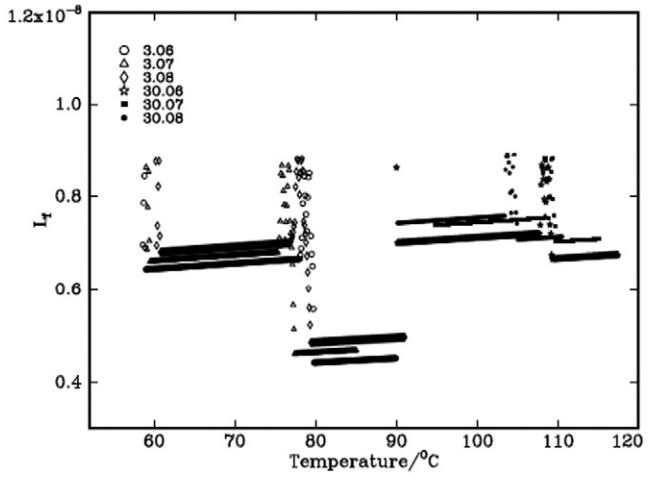

Fig. 6. Variation of Molecular free length (L_f) with temperature in 3.Om and 3O.Om compounds.

11. Generally this parameter, B/A lies in the range 5.5 to 9.5, with extreme variations of 2 and 13. These extreme values are reported in some cases [24] and
12. The molecular radius, M_r, estimated from birefringence is low compared to that obtained from α. Further, it is found from the Table 5 the increment of molecular radius for methylene unit is found to be 0.066 Å from density and 0.053 Å from birefringence and 0.066 Å from density and 0.057 Å from birefringence in 3.Om and 3O.Om materials respectively.

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