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An Approximation of Energy Difference, Bayer's Nonlinearity Parameter in Two Dissimilar Chain of Mesogens

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ABSTRACT

In the present work density measurements are carried out on P-Cyanobenzylidene P- Nonyloxyaniline , liquid crystalline compound. The density is observed to drop with grow of temperature in mesogic phases expect in the vicity of stage transition it shows steep grow before it attains equilibrium value of the next part. Using density facts the various thermodynamic parameters like Moelwin Hughes parameter, Isochoric hotness coordinated of internal pressure, Sharma parameter Huggin's parameter, Gruneisen parameter, etc. are assessed. The Bayer's nonlinearity parameter is also estimated. All variables exhibit discontinuity at phase transformation. The outcome is discussed with instance to the literature facts accessible on number of samples.

Keywords: Mesogens, density, phase transition, thermodynamic parameters, Bayer's nonlinearity parameter.

Preface

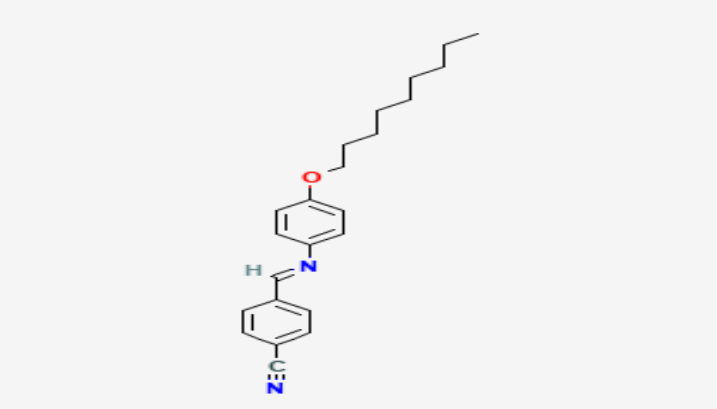
The Mesogenic materials shows a different mesophases with coin of hard core, side chain and terminal groups [1-4]. The lengthy terminal side chains quench the high temperature nematic phase thereby manifesting the smectic phases. The position of oxygen atom in the molecular moiety changes the transition temperatures. Further the dilatometric studies involving temperature variation across different phase transformation in liquid crystal materials provide information regarding the nature of phase transition and pre transitional effects [5-9]. The compound viz., P-Cyanobenzylidene P-Nonyloxyaniline differs from other compounds with electro negative oxygen atom on right side of the rigid core. The selected sample shows Nematic and Smectic phases.

In the present paper the density estimation as a function of temperature are carried out and the thermal expansion co-efficient at phase transition are noted. By using density and thermal expansion coefficient data the number of thermodynamic parameters is evaluated and outcomes are discussed.

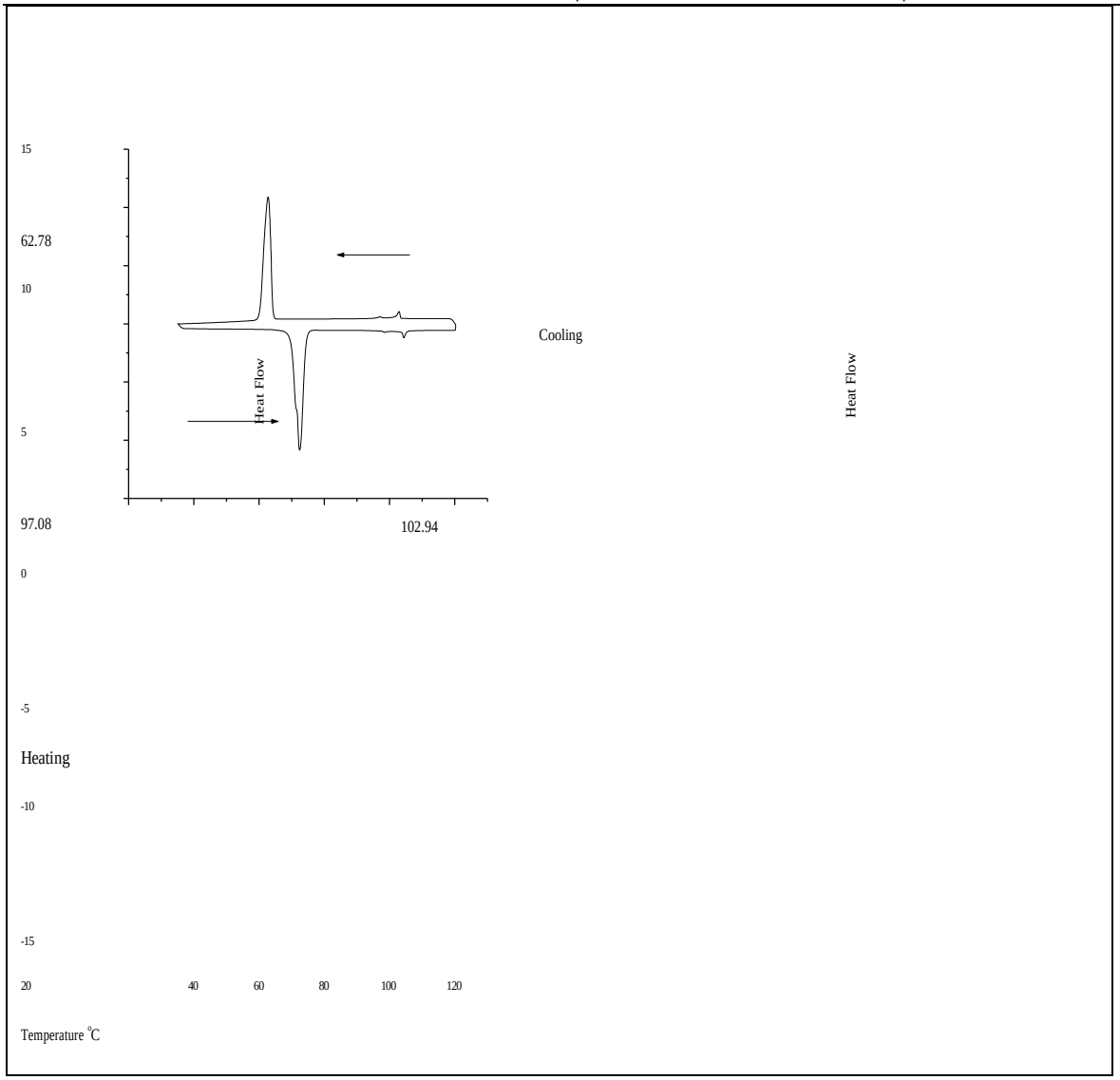
The molecular formula of the liquid crystals used is shown below.

C1: $NCC_6H_4CH = NC_6H_4O\,(CH_2)_8CH_3$ (P-Cyanobenzylidene P-Nonyloxyaniline)

The Structure of the sample as shown below:



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Thermograms and Transition temperature of compound P- Cyanobenzylidene P- Nonyloxyaniline shown in Fig.1, Table 1.

Table 1: Transition temperature in °C recorded by using Differential Scanning Calorimetry (DSC)

Compound	Transition temperature in °C		
	I-N	N-SmA	SmA-Cr
C1	102.94	97.08	62.78

Experimental

The density computation is done by using specially made pyknometer is used. The pyknometer made of capillaries with a radius of about 600μm and $5x10^{-2}$ to 8 $x10^{-2}$ meters of length is mounted on 'U' shaped designed glass tube. The pyknometer is adjusted by measuring the molar volume of water at various temperatures. The above liquid crystalline compound is loaded in pyknometer and its weight is noted using the highly accurate chemical balance.

The pyknometer is kept in heating block of dilatometer and the temperature of the heating block is raised 5°C above the clearing temperature. Then the sample is slowly cooled until the sample level reaches the marks in capillaries. The excess sample in the cups of the capillaries was removed by syringe. Conventional cathetometer was used to measure the liquid crystal level in the capillaries. The main scale and vernier scale is replaced with

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a digital scale. A CCD camera is attached to the telescope and the levels of the capillary were observed on a monitor with a high magnification. By this technique the temperature variation of density and hence thermal expansion coefficient was measured to estimate various thermo dynamical parameters.

Theory and expressions:

The theory for the estimation of different thermodynamic parameters using the coefficient of thermal expansion (α) is reported by several authors (Ranga Reddy et al., 1999[10]; Fakruddin et al., 2010[11]). The Moelwyn-Hughes parameter (Moelwyn-Hughes, 1951[12]), Beyer's nonlinearity parameter and the reduced molar volume ($\tilde{V}$) are evaluated from the following expression.

$$C = 13\,(\alpha T)^{-1} + 4^{4}\,(\alpha T) \qquad (1)$$

1 3 3

B

$$(_{A}) = C_1 = 1 \qquad (2)$$

$$V = [1 +$$

αT 3

$$3(1 + \alpha T)^{]} \qquad (3)$$

Using the coefficient of thermal expansion Haward and Parker(Haward and Parker, 1968[13]) obtained an expression for the isochoric temperature coefficient of internal pressure (X) as

$$X = \frac{-2(1 + 2T)}{V^{C_1}} \qquad (4)$$

The Sharma parameter (S_o) (Sharma, 1983[14]; Reddy et al., 2007[15]) is given by the expression

$$S_O = {}^{-X}(3 + 4\alpha T) \qquad (5)$$

The isothermal microscopic Gruneisen parameter (Γ) is a measure of volume dependence of the harmonicity of the normal mode frequency (ν) of a molecular vibrations of a polymer and is related to F and S_0 as

$$2\,\Gamma = (3\,2 + F + 4\alpha T)\,\alpha T + (\,2\alpha T) \qquad (6)$$

The fractional free volume (f) is a measure of disorder due to increasing mobility of molecules in a polymer and can be expressed in terms of the isothermal microscopic Gruneisen parameter (Γ) as

V α $_1 f = (\ ) = (\,)$ (7)

V r+1

Where V_a is the available volume of a liquid crystal.

Thermal parameter (A^*), is a dimensionless parameter which shows that at low temperatures, a liquid crystal tends to be ordered exhibiting a small thermal expansion and small fractional free volume, thereby making A^* equal to unity.

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A^{*1+f^2}

$= ( ) = 1 + (^{f})$ (8)

$1-f$ Γ

The Gruneisen parameter (Γ_P) for liquid crystals can be found from

$\Gamma_P = (21\ )\ \alpha T + ( ) + 2$ (9)

3 $2\alpha T$

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

$\Gamma_{ich} = \Gamma_{ith} + \Gamma_{iba}$ (10)

The isochoric Gruneisen parameter Γ_{ich} could be evaluated using the following equation

$E - F$

$\Gamma_{ich} = -$

Where (11)

$FE = -[2 + (\alpha T)^{-1}]\,[2\alpha(\tilde{V})^{C1^{-1}}]$ and F=-2α (12)

RESULTS AND DISCUSSIONS

The heat variation of (ρ) and thermal expansion coefficient (α) for the liquid crystalline compounds is measured and illustrated in Fig. 3 and Fig.4. The density is found to decrease with increase of temperature in LC phases but in the vicinity of phase transition there is a steep jump in density. The density data is used to estimate the number of thermodynamic parameter viz, Moelwyn - Hughes parameter(C1), reduced molar volume($\tilde{V}$), Isochoric Temperature Co-efficient of Internal Pressure(X), Sharma parameter(So), fractional free volume (f), Thermal parameter(A*), Gruneisen parameter(Γ_P), Huggin's parameter(F) isothermal microscopic Gruneisen parameter(Γ), isothermal Gruneisen parameter(Γ_{ith}), isochoric Gruneisen parameter(Γ_{ich}), isobaric Gruneisen parameter(Γ_{iba}) and Bayer's nonlinearity parameter(B/A) and shown in table 2 and table 3.

From our studies it is reported that the reduced molar volume and fractional free volume is found to increase with increase of temperature and there is a sudden increase in this values at phase transition. This is due to the fact that at phase transition the molecules in a compound align in a particular direction hence critical volume decreases, due to this reduced molar volume and fractional free volume increases. The percentage of increase in reduced molar volume in isotropic to nematic phase is 41% and Smectic to nematic phase is 24% in P-Cyanobenzylidene P-Nonyloxyaniline. temperature. Similar results are observed in fractional free volume also.

The Moelwyn - Hughes parameter (C1) and Bayer's nonlinearity parameter (B/A) falls with decreases of heat at phase transitions. There is a steep decrease in these values because these two parameters depend on compressibility. At phase transition the molecules in a compound are aligned in a particular direction and hence compressibility decreases therefore C1 and B/A values decreases. During isotropic- nematic transition the decreases in these values are very high when compared to smectic-nematic transitions. This is due to the fact that at higher temperatures compressibility is low; in liquid crystal research isotropic-nematic transition temperature is more than smectic - nematic transition temperature. Similarly, the values of the parameters viz, Isochoric Temperature Co-efficient of Internal Pressure(X), Sharma parameter(So), Thermal parameter(A*), Gruneisen parameter(Γ_P), Huggin's parameter(F) isothermal microscopic Gruneisen parameter(Γ), isothermal

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Gruneisen parameter(Γ_{ith}), isochoric Gruneisen parameter(Γ_{ich}), isobaric Gruneisen parameter(Γ_{iba}) decreases at phases transitions.

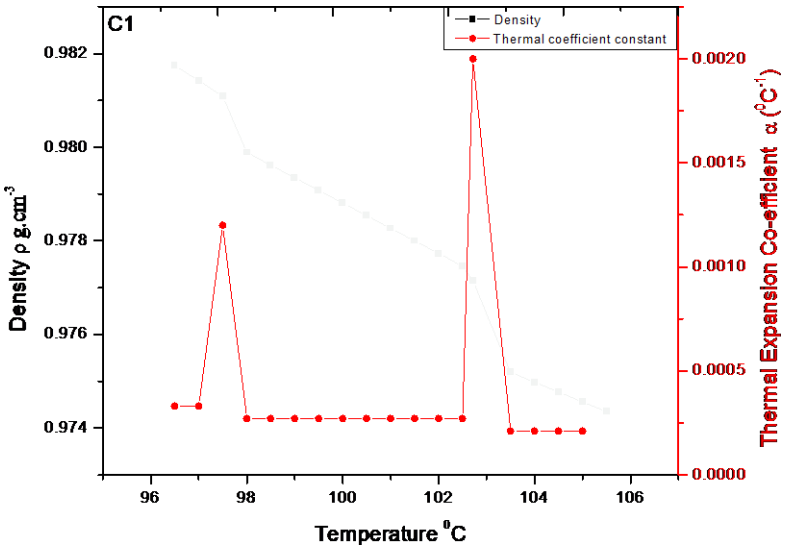


Fig. 3: Temperature versus density and thermal expansion coefficient graph of compound P-Cyanobenzylidene P-Nonyloxyaniline

Table 2: Thermodynamic parameters of liquid crystalline compound (C1) P-Cyanobenzylidene P-Nonyloxyaniline

T(K)	A	C1	$\tilde{V}$	X	So	f	A^*	Γp
369.5	0.00033	12.69326	1.112668	-0.64162	1.118897	0.074523	1.006001	6.181835
370	0.00033	12.6824	1.112808	-0.6415	1.118908	0.074593	1.006013	6.176404
370.5	0.0012	7.170531	1.34042	-0.4623	1.104525	0.146692	1.025218	3.421006
371	0.00027	14.44625	1.093841	-0.65704	1.117194	0.064816	1.004492	7.058294
371.5	0.00027	14.433	1.093959	-0.65694	1.117206	0.064879	1.004501	7.051666
372	0.00027	14.41978	1.094078	-0.65685	1.117218	0.064943	1.004511	7.045056
372.5	0.00027	14.40659	1.094196	-0.65675	1.117229	0.065007	1.00452	7.038464
373	0.00027	14.39344	1.094314	-0.65665	1.117241	0.065071	1.004529	7.03189
373.5	0.00027	14.38033	1.094433	-0.65655	1.117253	0.065134	1.004538	7.025334
374	0.00027	14.36725	1.094551	-0.65646	1.117265	0.065198	1.004547	7.018796
374.5	0.00027	14.35421	1.094669	-0.65636	1.117276	0.065261	1.004556	7.012275
375	0.00027	14.34121	1.094787	-0.65626	1.117288	0.065325	1.004566	7.005772
375.5	0.00031	13.07551	1.107934	-0.64548	1.118503	0.072162	1.005612	6.372951
376	0.00196	6.667083	1.487115	-0.35106	1.044021	0.167921	1.033888	3.16977

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376.5	0.00021	17.08298	1.075076	-0.67253	1.115146	0.054236	1.00311	8.376621
377	0.00021	17.06634	1.075171	-0.67245	1.115157	0.054291	1.003117	8.368304
377.5	0.00021	17.04975	1.075265	-0.67238	1.115169	0.054347	1.003123	8.360009
378	0.00021	17.03321	1.07536	-0.6723	1.11518	0.054403	1.00313	8.351736
378.5	0.00021	17.01671	1.075454	-0.67222	1.115191	0.054459	1.003137	8.343485

Table 2(continued)

T(K)	F	Γ	Γith	Γich	Γiba	B/A
369.5	1.479037	12.41861	5.846632	3.072015	2.774617	11.69326
370	1.478702	12.40612	5.841201	3.069195	2.772005	11.6824
370.5	0.869499	5.816981	3.085265	1.574987	1.510278	6.170531
371	1.523481	14.42836	6.723127	3.520581	3.202546	13.44625
371.5	1.523204	14.41319	6.716499	3.517164	3.199335	13.433
372	1.522927	14.39807	6.709889	3.513757	3.196132	13.41978
372.5	1.522649	14.38299	6.703297	3.510358	3.192938	13.40659
373	1.522372	14.36794	6.696722	3.506969	3.189753	13.39344
373.5	1.522095	14.35294	6.690166	3.503589	3.186577	13.38033
374	1.521818	14.33798	6.683627	3.500218	3.183409	13.36725
374.5	1.52154	14.32306	6.677106	3.496856	3.18025	13.35421
375	1.521263	14.30818	6.670603	3.493504	3.177099	13.34121
375.5	1.490278	12.85773	6.037757	3.169746	2.868012	12.07551
376	0.368445	4.955182	2.833541	1.352442	1.481099	5.667083
376.5	1.567112	17.43807	8.041489	4.191147	3.850342	16.08298
377	1.566894	17.41912	8.033172	4.186884	3.846287	16.06634
377.5	1.566676	17.40021	8.024877	4.182633	3.842243	16.04975
378	1.566457	17.38136	8.016604	4.178393	3.83821	16.03321
378.5	1.566239	17.36255	8.008353	4.174165	3.834188	16.01671

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Fig. 4: The variation of Beyer's parameter of nonlinearity (B/A) Isochoric Temperature Co-efficient of Internal Pressure (X) with temperature in P-Cyanobenzylidene P-Nonyloxyaniline compound

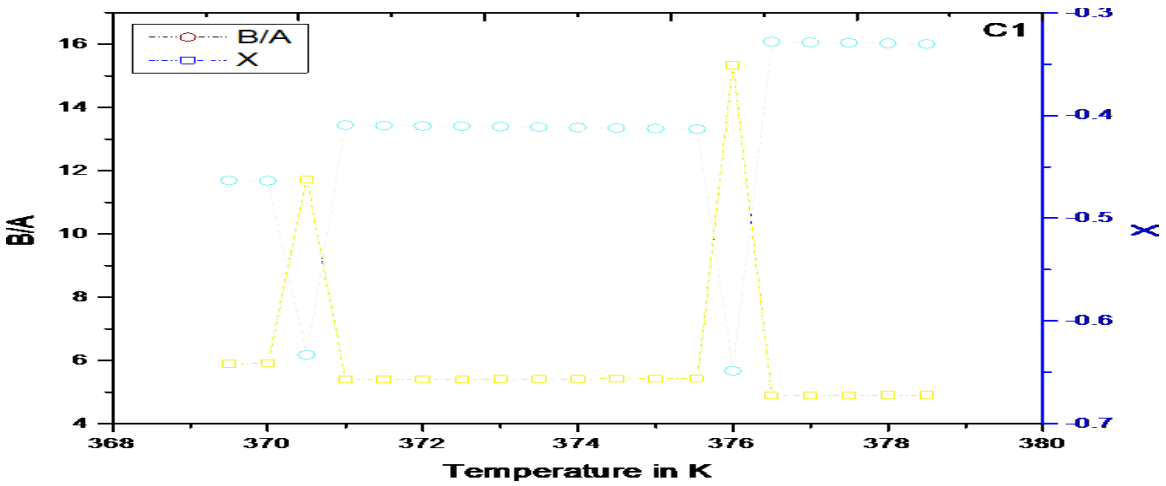


Fig. 5: The variation of reduced volume ($\tilde{V}$), Fractional free volume (f) with temperature in P-Cyanobenzylidene P-Nonyloxyaniline compound

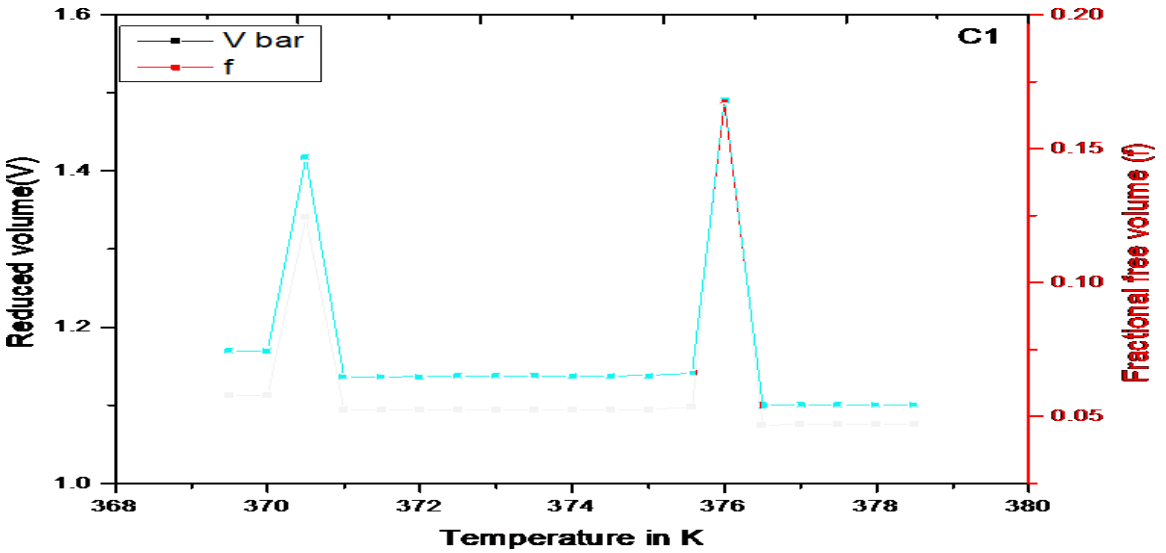
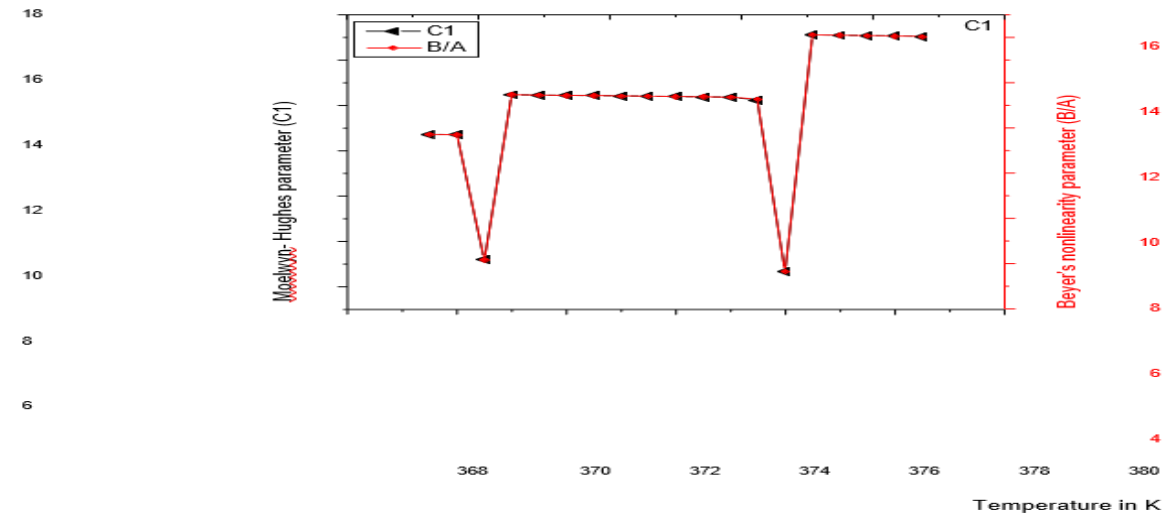


Fig. 6: The variation of Moelwyn- Hughes parameter (C1), Beyer's nonlinearity parameter (B/A) with temperature in P-Cyanobenzylidene P-Nonyloxyaniline compound



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CONCLUSION

From these studies it is noted that the sudden change in density and discontinuity in thermal expansion co-efficient attributes to the sudden change from ordered liquid crystal phases disordered isotropic phase. These phases differs mainly in the degree molecular orientation due to this the thermodynamic parameters also changes at phase transitions.

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