GIBBS FREE ENERGY, ABSORPTION COEFFICIENT, ACOUSTIC RELAXATION TIME, INTERNAL PRESSURE OF CHOLESTERYL OLEYL CARBONATE

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Abstract:

The ultrasonic velocity (U), density (ρ), viscosity (η) have been measured for Cholesteryl oleyl carbonate at different temperatures. From the experimental data, Adiabatic Compressibility (β), Free Length (LF), Free Volume (VF)), Internal Pressure (πi), Relaxation time (τ), Acoustic Impedance (Z), Gibbs Free Energy (ΔG), Absorption Coefficient (α) and Cohesive Energy (H) have been calculated. In addition to that the excess values of certain above parameters are also evaluated. The excess properties have been used to discuss the presence of significant interactions between the component molecules.

Keywords: cholesteryl oleyl carbonate, Ultrasonic Velocity, surface tension, acoustic impedance,
Gibbs Free Energy (ΔG), Absorption Coefficient

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INTRODUCTION

Cholesterol is a steroid alcohol that is essentially insoluble in aqueous solutions.

FORMULA	MOL WT.
$C_{46}H_{80}O_3$	681.14

Cholesterol can be esterified with a fatty acid to form cholesteryl esters. The latter form discrete lipid droplets in cells, especially in cells of steroidogenic tissues, and in the lipid core of low-density lipoproteins in the blood. Cholesterol is a fatty lipid sparingly insoluble in water but soluble in a number of organic solvents. Cholesteric materials are temperature sensitive and have color changing ability upon temperature.Not only emulsifying and humectant properties but also liquid crystal properties of cholesterol and its derivatives (salts and esters) make them useful in the commercial applications of cosmetics and pharmaceuticals. Measurement of Ultrasonic Velocity is generally made either by continuous wave method or by pulse methods. In the present study, the ultrasonic velocity was measured using a multi ultrasonic Interferometer (Mittal Enterprises Make) for the observation of ultrasonic velocity (C) and knowing the frequency we can find out various parameters such as adiabatic compressibility, acoustic impedance and temperature variation using temperature bath. The density at room temperature was measured using specific gravity bottle and single pan microbalance. Acoustical parameters were calculated using the measure values of velocity, density. The values of ultrasonic velocity,), Free Volume (VF)), Internal Pressure (πi), Relaxation time (τ), Acoustic Impedance (Z), Gibbs Free Energy (ΔG), Absorption Coefficient (α) of cholesteryl oleyl carbonate at different temperatures (303K, 308K, 313K, 318K and 323K) are given in Table 1. The study of intermolecular interaction plays an important role in the development of molecular sciences. A large number of studies have been made on the molecular interaction in liquid systems by various physical methods like Infrared [1,2], Raman effect [3,4], Nuclear Magnetic resonance, Dielectric constant[5], ultra violet[6] and ultrasonic method [7,8]

Some Formulae of the parameters to be calculated

Gibbs free energy is calculated from acoustic relaxation time (τ) following Eyring rate process theory [19]:

$$\Delta G = RT \ln(KT\tau /h)$$

Where K = 1.23×10^{-23} J/K, t is the temperature, τ is the relaxation time, h = 6.626×10^{-34} Js (Planck's Constant) Acoustic relaxation time (τ) is calculated using the following relation:

$\tau = [4\,\eta/3\rho\ C^2]$ Acoustical relaxation time indicates the presence of interactions.

The internal pressure is calculated from the free volume concept on the basis of statistical thermodynamics as,

$$\pi i = bRT\,[\,K\,\eta\,/\,C\,]^{1/2}\,[\,\rho^{2/3}\,/\,M^{7/6}\,]$$

Absorption coefficient (α) is calculated from the following equation $\alpha = \omega^2\,\tau/2\,C$ [19] where $\omega = 2\pi f$, C is the ultrasonic velocity, η is viscosity, ρ is the density and M is the molecular weight of the cholesteryl oleyl carbonate taken.

Table:1

Abs. Temp	C m/s	τ (relaxation time)	ΔG	πi	α	Vf
303	1748	1.11E-09	2.20E+04	6.11E+05	1.275022155	1.17E-06
304	1568	1.17E-09	2.22E+04	5.95E+05	1.498288025	1.27E-06
305	1492	1.20E-09	2.24E+04	5.87E+05	1.611565767	1.33E-06
306	1504	1.19E-09	2.24E+04	5.88E+05	1.585643054	1.33E-06
307	1420	1.23E-09	2.26E+04	5.80E+05	1.727882688	1.40E-06
308	1456	1.21E-09	2.27E+04	5.84E+05	1.663199766	1.38E-06
309	1616	1.15E-09	2.26E+04	5.99E+05	1.420397546	1.28E-06
310	1624	1.14E-09	2.27E+04	6.00E+05	1.407639041	1.28E-06
311	1644	1.13E-09	2.27E+04	6.01E+05	1.379806776	1.28E-06
312	1660	1.13E-09	2.28E+04	6.03E+05	1.357724825	1.28E-06
313	1764	1.09E-09	2.28E+04	6.12E+05	1.237459938	1.23E-06
314	1548	1.16E-	2.30E+	5.92E+05	1.5028994	1.36E-06

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		09	04		63	
315	1500	1.18E-09	2.32E+04	5.88E+05	1.573109748	1.40E-06
316	1524	1.17E-09	2.32E+04	5.90E+05	1.533663903	1.39E-06
317	1468	1.19E-09	2.33E+04	5.84E+05	1.619692135	1.44E-06
318	1444	1.20E-09	2.34E+04	5.82E+05	1.657627099	1.47E-06
319	1468	1.19E-09	2.35E+04	5.84E+05	1.614606747	1.46E-06
320	1416	1.20E-09	2.36E+04	5.79E+05	1.701693416	1.50E-06
321	1388	1.21E-09	2.37E+04	5.76E+05	1.750711048	1.53E-06
322	1368	1.22E-09	2.38E+04	5.74E+05	1.786463329	1.56E-06
323	1284	1.26E-09	2.40E+04	5.65E+05	1.961563587	1.65E-06

Table2:

Absolute Temp(T)	C(m/s)	Sigmax10^{-4}(σ)	Eta(η)	kg/m3
303	1748	4.53	2.510051	982.9000
304	1568	3.84	2.124227	980.7000
305	1492	3.55	1.964224	978.6000
306	1504	3.58	1.975388	976.5000
307	1420	3.28	1.807604	974.3000
308	1456	3.40	1.87161	972.2000
309	1616	3.97	2.180629	970.1000
310	1624	3.99	2.188548	968.0000
311	1644	4.06	2.220686	965.9000
312	1660	4.11	2.244912	963.9000
313	1764	4.49	2.449869	961.8000
314	1548	3.68	2.006363	959.7000
315	1500	3.51	1.906749	957.7000
316	1524	3.58	1.94553	955.7000

317	1468	3.38	1.832349	953.6000
318	1444	3.29	1.781042	951.6000
319	1468	3.36	1.818934	949.6000
320	1416	3.18	1.71683	947.6000
321	1388	3.08	1.660052	945.6000
322	1368	3.01	1.618347	943.6000
323	1284	2.73	1.466207	941.6000

Fig 1:
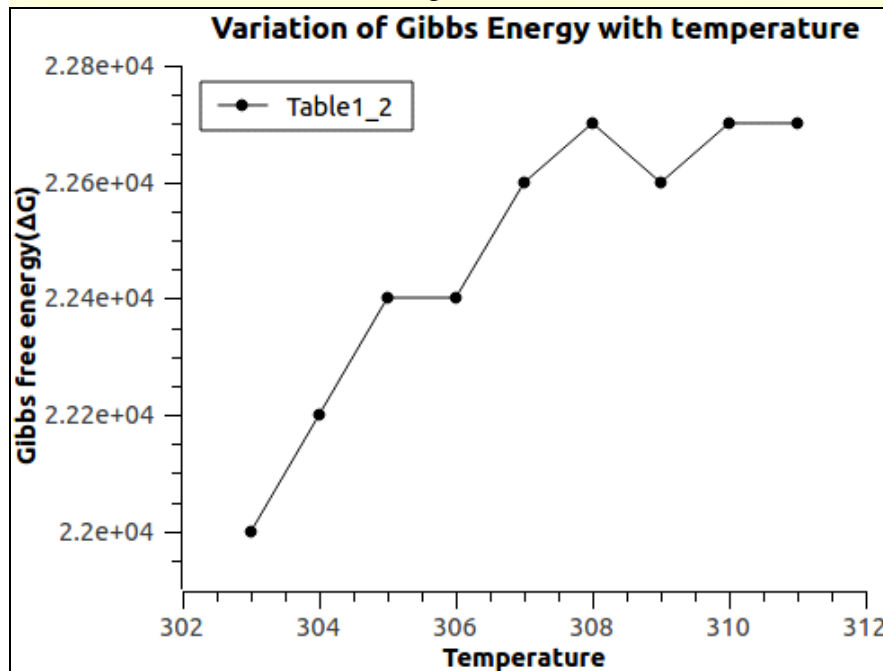
The Gibbs free energy (ΔG) increases with the increase in frequency. An increasing value of ΔG suggests that the closer approach of unlike molecules is due to hydrogen bonding. The increase in ΔG suggests shorter time for the rearrangement of molecules in the liquid. When frequency increases, the energy imparted to the molecules obviously expedites the rearrangement procedure.
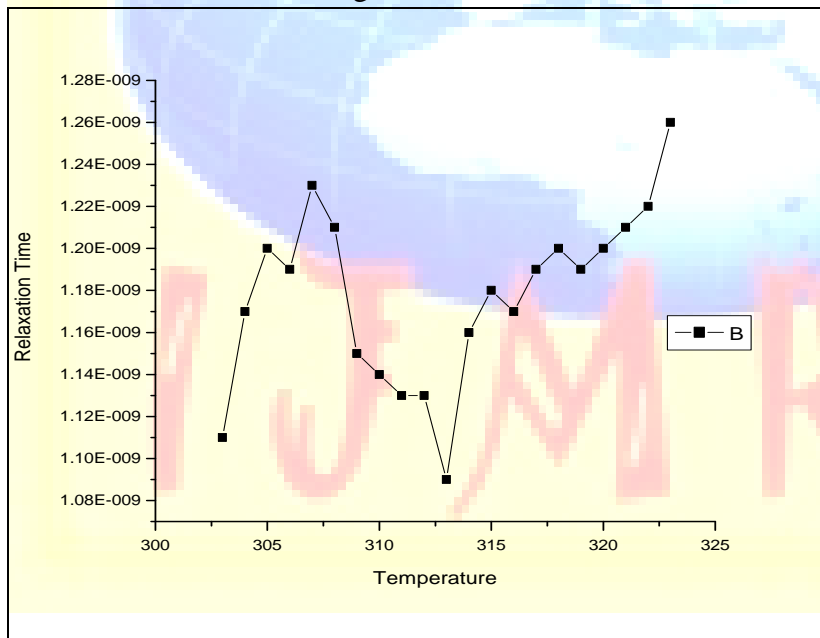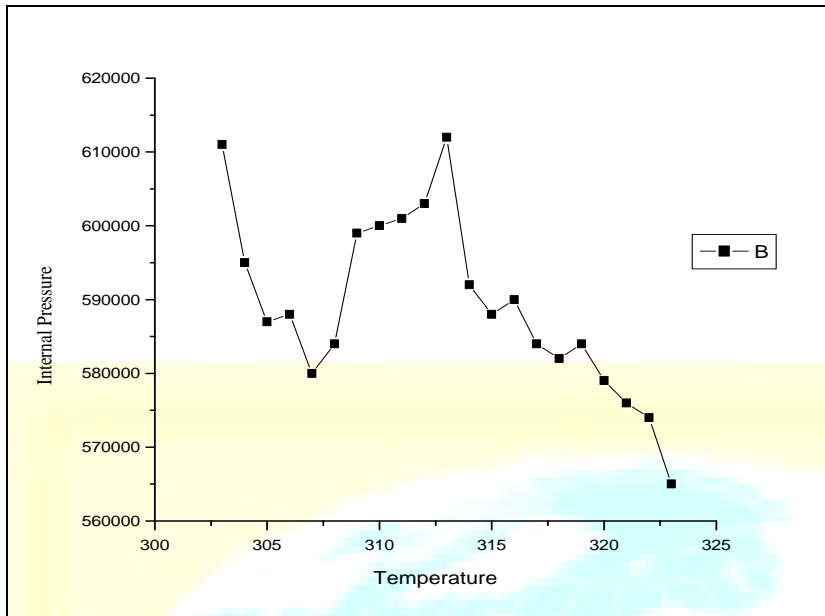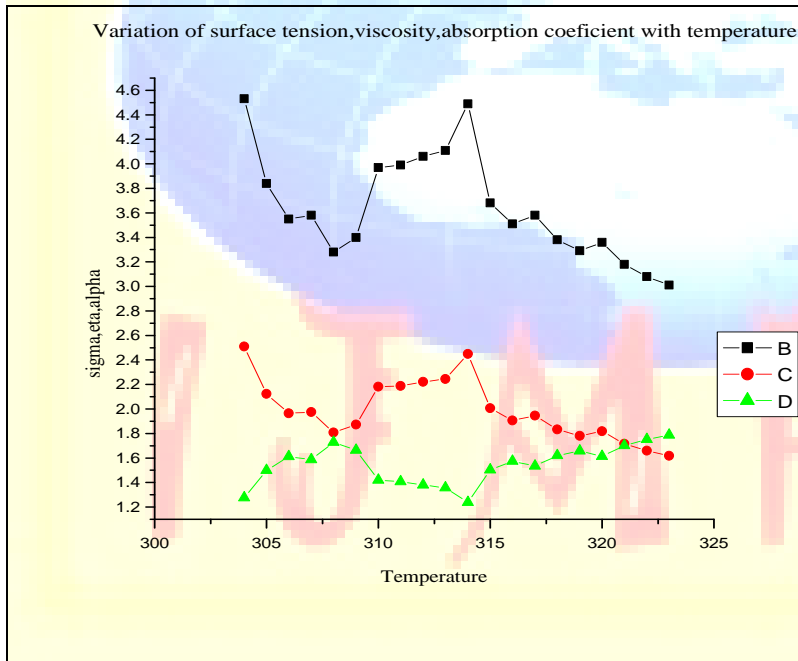
Fig 2:

Fig 3:

Fig 4:

Fig 5:

Variation of surface tension,viscosity,absorption coeficient with temperature
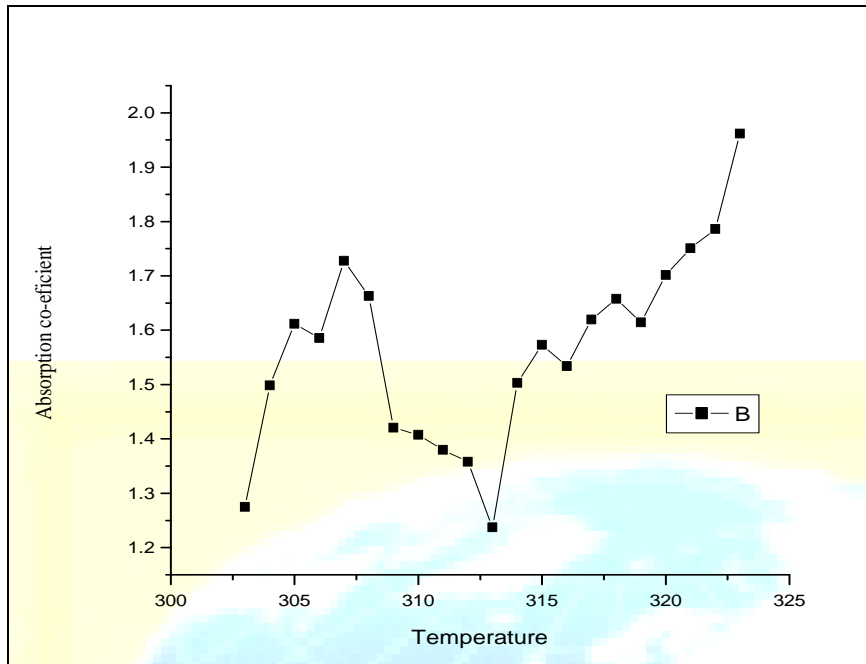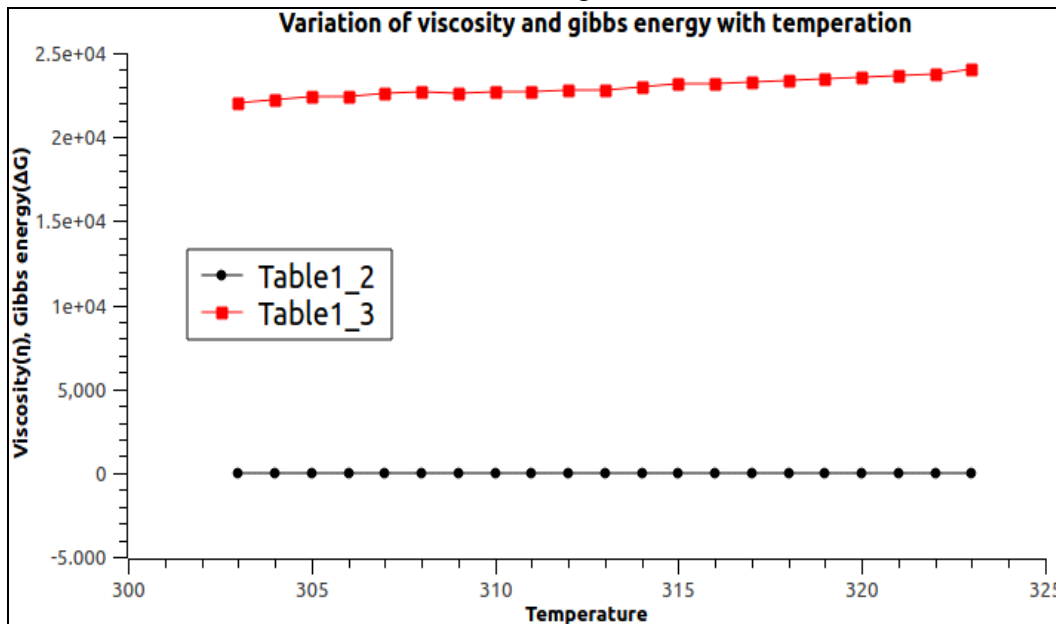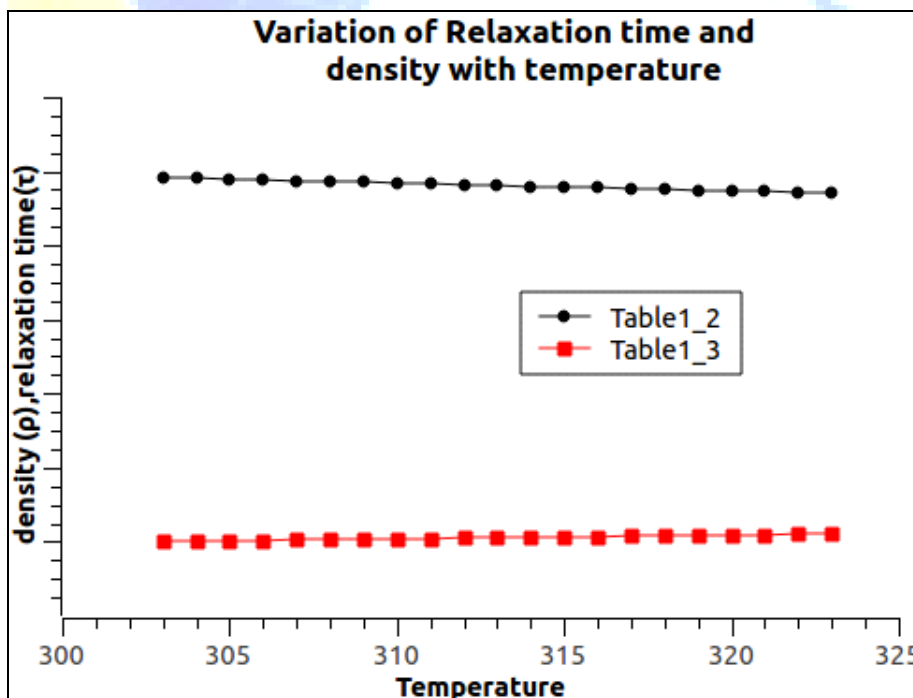
Fig 6:

Fig 7:

RESULTS AND DISCUSSION:

Table 1 represents the experimentally measured values of ultrasonic velocity(U) , Gibbs free energy(ΔG), Classical Absorption Coefficient, Free Volume (VF) ,), Internal Pressure(πi), Relaxation time(τ),   at different temperatures. Table 2 represents the variation of density (ρ), viscosity(η),surface tension, density(ρ) .The excess values of relaxation time, internal pressure, acoustic impedance, and Gibbs free energy indicate that the interaction between the molecules does not seem to vary very much in strength with changing frequency. Hence, intermolecular interaction in the case of cholesteryl oleyl carbonate is large. However, with rise in temperature increase in free volume and decrease in internal pressure are noticed.From the table (1) Gibbs Free Energy, Classical Absorption Coefficient increases with the increase in temperature.Increase in Gibbs' free energy suggests shorter time for rearrangement of molecules. Relaxation time is the time taken for the excitation energy to appear as translational energy. The above fact confirms the minimum interaction between the molecules in cholesteryl oleyl carbonate . Viscous relaxation time and the Gibbs' free energy both decreases as temperature increases. As temperature increases, excitation energy increases and hence relaxation time decreases. Further, since the kinetic energy of the molecule increases, longer time is taken for rearrangement of molecules and this suggest a decrease in Gibbs' free energy. Free volume is the average volume in which the centre of a molecule can move due to the repulsion of the surrounding molecules. . This suggests that there is a closed packing of molecules inside the shield. Such an increase in internal pressure generally indicates association through hydrogen bonding and hence supports the present investigation. Figure 5 shows variation of surface tension with

temperature. From the graph it is observed that the surface tension decreases with the increasing value of temperature, but a clearly visible change of the temperature evolution occurs at 307 and 313 , which may point to BP II and BP I [3] phase transitions. Recently the stabilization of blue phases over a temperature range of more than 60 K including room temperature (260–326 K) has been demonstrated [17,18] . Highly chiral liquid crystals, on the other hand, may exhibit one or more blue phases (BP) as they are heated from the helical phase to the isotropic phase. In addition, the blue phases possess a much higher viscosity than either the helical or isotropic phase. Their viscosity has been found to be on the order of 106 times larger than the viscosity of their corresponding helical phases (Wright [3]). In both cases, it is likely that the crystalline ordering of the blue phases is responsible for giving these liquids properties which one usually associates with solids. The phase of a thermotropic liquid crystal is temperature dependent. As temperature is varied, the conditions on the translational and orientational order of the constituent molecules which produce the most energetically favorable system may also change.

Conclusion

The results obtained for the present study indicate that the thermodynamic parameters are sensitive to the molecular interactive present in cholesteryl oleyl carbonate . From Ultrasonic velocity and related acoustical parameters for cholesteryl oleyl carbonate at varying temperature, it is concluded that there exists a strong molecular interaction due to hydrogen bonding.

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