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Research Article

COMPUTATION OF EFFECTIVE DEBYE TEMPERATURE (Θ_D) OF BINARY LIQUID MIXTURES

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ABSTRACT

On the basis of quasicrystalline model of liquid state effective Debye temperature (θ_D), of 32 binary liquid mixtures at 298.15 K has been computed using sound velocity and density data, mixtures under the present investigation contain benzene, toluene, p-xylene, 1-chloronaphthlene and 1-chlorobenzene with n- and br- alkanes. θ_D values of all the mixture were also calculated on the basis of Lorenz – Bertholet combination rule using heat capacity data. The results are found to be quite satisfactory which are discussed critically.

Keywords: Debye temperature, binary liquid mixtures, n- and br-alkanes, sound velocity.

INTRODUCTION

During the period 1974-1976, a number of workers[1-8] evaluated the effective Debye temperature of pure liquids as a fraction of temperature and pressure on the basis of quasicrystalline behavior and other experimental evidence. The approach utilized the experimental data of density, ultrasonic velocity and absorption of liquids. Subsequently the traditional method, having several approximations and limitations, was modified and extruded to binary[9] and multicomponent liquid mixture[10] for the computation of effective Debye temperature. Recently[11] an independent method for computing the specific heat ratio, Gruneisen parameter and Debye temperature of crude oil has been developed. Due to increasing importance of Debye temperature of liquids, we are reporting here the results of calculation of θ_D for several binary liquid mixtures.

For the present work we have taken 32 binary liquid mixtures of benzene, toluene, p-xylene, 1-chloronaphthlene and 1-chlorobenzene with n- and br- alkanes, all at 298.15 K. The experimental data of density, sound velocity, heat capacity, isothermal compressibility and thermal expansity were taken from the literature.[12-13]

FORMULA USED

The basic equation employed for the calculation of the effective Debye temperature are, θ_D, can be written as

$$\theta_D = \frac{h}{k}\left[\left(\frac{9N}{4\pi V} \right) \Big/ \left(\frac{1}{C_l^3} + \frac{2}{C_t^3} \right) \right] \qquad \text{……….. (1)}$$

Where all the symbols have their usual notations as given in earlier papers.[14] Without going into further details it can be shown that the resulting expression for computing θ_D

$$\theta_D = \left[\frac{9N/4\pi V}{(\rho\beta_a)^{3/2} \left\{ \left(\frac{1}{1+\gamma} \right)^{3/2} + 2\left(\frac{4}{3\gamma} \right)^{3/2} \right\}} \right]^{1/3} \qquad \text{…………………. (2)}$$

Where, $\gamma = \frac{C_P}{C_V} = \frac{\beta_T}{\beta_S}$

$$\beta_a = \left(\rho u^2\right)^{-1}$$

ρ and u being the density and isentropic compressibility of liquid mixture.
Now we are introducing two different methods for obtaining the value of Debye temperature of a liquid mixture.

1. Ideal mixture relation.

$$\theta_D = \sum X_i \,\theta_{Di} \qquad \text{……. (3)}$$

Where,
Xi is the mole fraction of i[th] component and θ_D the Debye temperature of i[th] component.

2. According to Lorenz – Bertholet combination rule,

$$m_1 s_1 (t_1 - t) = m_2 s_2 (t - t_2) \qquad \text{…….(4)}$$

Where m, s and t are the mass specific heat and temperature respectively. If we use the mole fraction, molar heat capacity and Debye temperature in place of mass, specific heat and temperature in equation (4), it becomes,

$$X_1 C_{P1} (\theta_{D1} - \theta_D) = X_2 C_{P2} (\theta_D - \theta_{D2})$$

$$X_1 C_{P1} \theta_{D1} - X_1 C_{P1} \theta_D = X_2 C_{P2} \theta_D - X_2 C_{P2} \theta_{D2}$$

$$\theta_D (X_1 C_{P1} - X_2 C_{P2}) = X_1 C_{P1} \theta_{D1} + X_2 C_{P2} \theta_{D2}$$

$$\theta_D = \frac{X_1 C_{P1} \theta_{D1} + X_2 C_{P2} \theta_{D2}}{X_1 C_{P1} + X_2 C_{P2}}$$

$$\theta_D = \frac{\sum X_i C_{Pi} \theta_{Di}}{\sum X_i C_{Pi}} \qquad \text{………………………….. (5)}$$

Where Cpi is the molar specific heat capacity at pressure of i[th] component. Using these methods we have calculated the Debye temperature of mixture and compared with the standered values obtained with the help of equation (2).

The Debye frequency v_m, was obtained from the equation

$$v_m = \frac{k}{h} \times \theta_D \qquad \text{………… (6)}$$

RESULT AND DISCUSSION

For the computation of effective Debye temperature θ_D and Debye frequency v_m of 32 equimolar binary mixtures of benzene, toluene, p-xylene, 1-chloronaphthlene and 1-chlorobenzene with normal and branched alkanes, at 298.15 K. The experimental data of density (ρ), sound velocity (u), adiabatic compressibility (βs) and thermal expansivety (α) were taken from literature.[12-13]

Equations (2-5,6) were used to obtain the values of θ_D and v_m for all the liquid mixtures. These values are reported in Tables -1,2,3,4 and 5 respectively for the mixtures benzene +n-C_6, +n-C_8, +n-C_{10}, +n-C_{12}, +n-C_{16}; toluene +n-C_6, +n-C_8, +n-C_{10}, +n-C_{12} and br-C_{12}; p-xylene +n-C_6, +n-C_{16}; 1-chloronaphthlene +n-C_6 to +n-C_{16}, +br-C_6 to br-C_{16}; and 1-chlorobenzene +n-C_6 to +n-C_{16}, +br-C_6 to br-C_{16}.

A perusal of results reported in Tables 1-5 show that the calculated values of θ_D and v_m in all system decrease with the number of carbon atom from C_6 to C_{16}. Similar treand is also observed in case of vm. The role of common liquids benzene, toluene, p-xylene, 1-chloronaphthlene and 1-chlorobenzene in all the mixture is not significant towards the change in the value of θ_D and v_m. Increase in C- atoms of alkanes results in the attaining the more crystalline character of liquids that reduce the θ_D values.

Table 1: Calculated values of the effective Debye temperature (θ_D) and Debye frequency of benzene with n-alkane at 298.15 K

Liquids	X_1	T(^{0}K)	ρ (kgm^{-3})	u (ms^{-1})	θ_D (^{0}K)	v_m (10^9)
Benzene with						
n-C_6	0.50	298.15	687.15	1155.56	116.76	5.61
n-C_8	0.50	298.15	687.15	1201.71	115.99	5.57
n-C_{10}	0.50	298.15	687.15	1236.20	114.61	5.50
n-C_{12}	0.50	298.15	687.15	1263.15	110.53	5.42
n-C_{16}	0.50	298.15	687.15	1305.30	109.67	5.26

Table 2: Calculated values of the effective Debye temperature (θ_D) and Debye frequency of toluene with n-alkane at 298.15 K

Liquids	X_1	T(^{0}K)	ρ (kgm^{-3})	u (ms^{-1})	θ_D (^{0}K)	v_m (10^9)
Toluene with						
n-C_6	0.50	298.15	687.9	1177.67	116.16	5.58
n-C_8	0.50	298.15	687.9	1214.59	114.80	5.51
n-C_{10}	0.50	298.15	687.9	1250.97	113.84	5.47
n-C_{12}	0.50	298.15	687.9	1273.83	112.02	5.38
n-C_{16}	0.50	298.15	687.9	1316.79	109.12	5.24

Table 3: Calculated values of the effective Debye temperature (θ_D) and Debye frequency of p-xylene with n-alkane at 298.15 K

Liquids	X1	T(^{0}K)	ρ (kgm^{-3})	u (ms^{-1})	θ_D (^{0}K)	v_m (10^9)
p-xylene with						
n-C_6	0.50	298.15	687.9	1186.51	114.43	5.49
n-C_{16}	0.50	298.15	687.9	1321.08	108.02	5.19

Table 4: Calculated values of the effective Debye temperature (θ_D) and Debye frequency of 1-chloronaphthalene with n-alkane at 298.15 K

Liquids	X_1	$T(^0K)$	ρ (kgm^{-3})	u (ms^{-1})	θ_D (^0K)	v_m (10^9)
1-chloronaphthalene with						
n-C_6	0.50	298.15	687.9	1266.97	120.60	5.79
n-C_8	0.50	298.15	687.9	1298.18	118.84	5.71
n-C_{10}	0.50	298.15	687.9	1320.93	116.72	5.62
n-C_{12}	0.50	298.15	687.9	1338.68	114.65	5.50
n-C_{14}	0.50	298.15	687.9	1357.10	112.92	5.42
n-C_{16}	0.50	298.15	687.9	1373.59	111.30	5.34
br-C_6	0.50	298.15	687.9	1224.32	116.28	5.58
br-C_8	0.50	298.15	687.9	1252.78	114.43	5.49
br-C_{12}	0.50	298.15	687.9	1287.98	110.22	5.29
br-C_{16}	0.50	298.15	687.9	1324.46	107.65	5.17

Table 5: Calculated values of the effective Debye temperature (θ_D) and Debye frequency of 1-chlorobenzene with n-alkane at 298.15 K

Liquids	X_1	$T(^0K)$	ρ (kgm^{-3})	u (ms^{-1})	θ_D (^0K)	v_m (10^9)
1-chlorbenzene with						
n-C_6	0.50	298.15	850	1158.43	93.2	4.47
n-C_8	0.50	298.15	850	1200.37	92.43	4.44
n-C_{10}	0.50	298.15	850	1232.41	91.27	4.38
n-C_{12}	0.50	298.15	850	1260.28	90.15	4.33
n-C_{14}	0.50	298.15	850	1200.89	83.23	4.00
n-C_{16}	0.50	298.15	850	1303.70	87.7	4.22
br-C_6	0.50	298.15	850	1118.72	89.78	4.31
br-C_8	0.50	298.15	850	1151.69	88.46	4.25
br-C_{12}	0.50	298.15	850	1206.74	86.26	4.14
br-C_{16}	0.50	298.15	850	1259.15	84.13	4.04

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