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Volumetric, acoustic and optical properties of binary mixtures of 2-propanol with *n*-alkanes (C_6-C_{10}) from 293.15 K to 303.15 K

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ABSTRACT

Densities, ultrasonic speeds and refractive indices of 2-propanol + *n*-alkanes (C_6-C_{10}) systems were experimentally determined at 293.15 K to 303.15 K. Calculated excess molar volume, deviation in ultrasonic speed, refractive index, excess isentropic compressibility and excess intermolecular free length were correlated with Redlich-Kister equation. The excess volume was also interpreted by Flory-Treszczanowicz-Benson (FTB) model and Prigogine-Flory-Patterson (PFP) theory. While the excess molar volume were predicted well with FTB model, PFP theory able to describe sign and magnitude of excess molar volume values in propanol rich region but failed to describe in propanol lean region. For the theoretical estimation of ultrasonic speed and refractive index values, various correlation and mixing rules were also applied.

1. Introduction

To reduce pollution and toxic emissions of carbon monoxide, it is essential to add oxygen rich chemical species to the gasoline to ensure the complete combustion [1, 2]. Oxygenates with good anti-knocking properties such as ethers, alcohols etc. have become gasoline additive in place of tetraethyl–lead [3]. The thermophysical properties of liquid mixtures of associating and non-associating liquids play vital role in designing and formulating gasoline and diesel motor [4, 5]. These thermophysical properties help us to predict their molecular structure and intermolecular arrangements of different possible combinations formed by mixing of two components. Alcohols are mainly self-associated hydrogen bonded polar organic compound, whereas alkanes are homologous acyclic and nonpolar compounds [6, 7]. The mixture of alcohol and alkane is widely used in petrochemical and rectification processes for azeotropic mixtures [8, 9].

In continuation to earlier work [10–25] in this paper, densities (ρ), ultrasonic speeds (u) and refractive indices (n_D) of 2-propanol with *n*-alkanes (C_6-C_{10}) mixtures were measured at 293.15 K to 303.15 K. The excess isentropic compressibility (k_S^E) and intermolecular free length (L_f^E) were calculated from experimental u data. These results were discussed in terms of packing effect, disorder in the orientation order and cohesion forces. The u data were predicted with various empirical relations [26–30]. The acoustic data were further analyzed in terms of Jacobson's free length theory (FLT) and Schaaff's collision factor theory (CFT). The ${V_m}^E$ values were also predicted with Prigogine-Flory-Patterson (PFP) theory and Flory-Treszczanowicz-Benson model (FTB).

2. Experimental section

2-propanol and *n*-alkane were simply distilled and specifications are given in Table 1. The purities of the compounds were checked by measuring their ρ, u and n_D as given in Table 2 while for mixtures these are reported in Table 3. For the measurement of u and ρ Anton Paar DSA-5000 M was used with uncertainty of ± 0.1 m $s^{-1}$and $\pm 10^{-6}$ g cm^{-3}, respectively.

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Table 1
Chemicals specifications.

S. No.	Sample	CAS No.	Make	Mass fraction purity	Purification method
1.	2-propanol	67-63-0	Sigma-Aldrich	≥0.995	Distillation
2.	*n*-hexane	110-54-3	Merck	≥0.985	Distillation
3.	*n*-heptane	142-82-5	Merck	≥0.990	Distillation
4.	*n*-octane	111-65-9	Merck	≥0.990	Distillation
5.	*n*-nonane	111-84-2	Sigma-Aldrich	≥0.990	Distillation
6.	*n*-decane	124-18-5	Sigma-Aldrich	≥0.990	Distillation

Refractive indices were measured with refractometer Abbemat-200 with temperature controlled within ±0.01 K having accuracy up to $\pm 1 \times 10^{-4}$. The binary mixtures were weighed using balance of ±0.1 mg precision (OHAUS, AR224CN). The accuracy of measured data was checked by comparing ${V_m}^E$ values of the benzene + cyclohexane mixtures at 298.15 K mixture at 298.15 K which agreed with their corresponding literature values [45].

3. Results

3.1. Excess molar volume

The V_m^E recorded in Table 3 were calculated using following relation:

$$V_m^E = \frac{(x_1M_1 + x_2M_2)}{\rho_m} - \frac{x_1M_1}{\rho_1} - \frac{x_2M_2}{\rho_2} \tag{1}$$

and compared well with literature [16, 46] at $x_1 = 0.5$ in Table 4 and also shown in Fig. 1 (a) except for 2-propanol + *n*-hexane [8] system. We have also compared our data for this system with the literature reported by various workers in Fig. 1(b) [8, 47–49].

It is clear from the Fig. 1(b) that reported data are not consistent. Since our data compared well with reported literature for other systems like 2-propanol (1) +*n*-octane or *n*-decane (2) and also for the known system (benzene + cyclohexane), this authenticates the accuracy of our data.

Other excess properties in Table 3 were calculated from experimental values of u and n_D using following equation

$$X_m^E = X_m - x_1X_1^o - x_2X_2^o \tag{2}$$

where X_m^E, X_m and ${X_i}^o$ represent excess property, mixture property and pure component property, respectively. The ${X_m}^E$ was correlated with Redlich-Kister (RK) equation [52] and shown in Figs. 1–3. The parameters of RK equation and standard deviations $\sigma(X_m^E)$ are reported in Table 5.

The V_m^E data was further analyzed in term of PFP theory and FTB model discussed in detail in earlier paper [53].

3.2. Prigogine-Flory-Patterson (PFP) theory

According to this theory [54]

$$V^E = V_{inter}^E + V_{freevol}^E + V_{P^*}^E \tag{3}$$

$$\frac{V^E}{x_1V_1^* + x_2V_2^*} = \frac{\left(\tilde{V}^{1/3} - 1\right)\tilde{V}^{2/3}\psi_1\theta_2\left(\chi_{12}^*/P_1^*\right)}{\left((4/3)\tilde{V}^{-1/3} - 1\right)} - \frac{\left(\tilde{V}_1 - \tilde{V}_2\right)^2\left((14/9)\tilde{V}^{-1/3} - 1\right)\psi_1\psi_2}{\left((4/3)\tilde{V}^{-1/3} - 1\right)\tilde{V}} + \frac{\left(\tilde{V}_1 - \tilde{V}_2\right)\left(P_1^* - P_2^*\right)\psi_1\psi_2}{P_2^*\psi_1 + P_1^*\psi_2} \tag{4}$$

where all the terms have their usual meaning [55, 56] The various parameters of pure compounds used in these calculations were tabulated in Table 6 [38, 42, 57–59]. The contribution of three terms to V_m^E at equimolar composition and interactional parameter χ_{12}^* are given in Table 7. PFP model able to describe only sign and magnitude of V_m^E values in propanol rich region but failed to describe in propanol lean region as shown in Fig. 4 and Table 8.

3.3. Flory-Treszczanowicz- Benson (FTB) model

According to this model ${V_m}^E$ is made of two factors: a chemical contribution (V_{MK}^E) due to Mecke-Kempter association and a physical contribution [55, 56].

$${V_m}^E = V_{MK}^E + V_{Phys}^E \tag{5}$$

Table 2
Purities, measured densities (ρ), refractive indices (n_D) and ultrasonic speeds (u) of the pure components.

Compound	T/K	$\rho/10^3 \times$ g cm^{-3}		n_D		u/ms^{-1}	
		This work	Literature	This work	Literature	This work	Literature
2- propanol	293.15	785.07	785.28 [31]	1.3773	–	1156.18	1156.00 [32]
	298.15	780.74	780.56 [33]	1.3752	1.3753 [34]	1138.58	1139.00 [32]
	303.15	776.61	776.76 [35]	1.3730	–	1121.00	1121.00 [32]
n-hexane	293.15	659.91	659.57 [36]	1.3761	1.3756 [37]	1099.65	1099.30 [38]
	298.15	655.38	655.10 [39]	1.3734	1.37234 [39]	1076.97	1076.50 [38]
							1077.00 [40]
	303.15	650.82	650.37 [41]	1.3708	–	1054.40	1054.20 [41]
							1054.10 [38]
n-heptane	293.15	683.85	683.92 [36]	1.3878	1.3878 [37]	1150.47	1152.00 [40]
	298.15	679.60	679.40 [39]	1.3852	1.38512 [39]	1128.92	1130.00 [39]
	303.15	675.33	675.47 [36]	1.3826	–	1107.50	–
n-octane	293.15	702.76	702.62 [36]	1.3928	–	1192.68	–
	298.15	698.71	698.60 [8]	1.3951	1.39519 [42]	1171.49	1172.70 [41]
	303.15	694.66	694.50 [41]	1.3925	–	1150.85	1152.10 [41]
n-nonane	293.15	717.87	717.85 [36]	1.4056	1.4058 [37]	1226.59	1227.30 [43]
	298.15	713.97	714.01 [36]	1.4032	1.40326 [42]	1205.98	1207.20 [43]
	303.15	710.07	710.11 [36]	1.4009	–	1185.80	1187.20 [43]
n-decane	293.15	730.07	730.05 [36]	1.4119	1.4120 [37]	1253.79	–
	298.15	726.29	726.90 [8]	1.4097	1.4099 [44]	1233.84	1234.80 [41]
	303.15	722.50	722.51 [36]	1.4074	–	1214.07	1215.20 [41]