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Study of molecular interactions of binary mixtures DEC with alkoxyalkanols at various temperatures

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ABSTRACT

Density (ρ), speed of sound (u), and refractive index (n_D), values have been measured for the binary mixture of diethyl carbonate (1) and 2-alkoxyethanols (2) over the entire range of mole fraction at intervals of 5 °C temperatures from T = (298.15 to 323.15) K under atmospheric pressure (0.1 MPa). Using the basic experimental values, excess molar volume (V_m^E), excess isentropic compressibility (κ_s^E), excess molar isentropic compressibility ($K_{s,m}^E$), excess speed of sound (u^E), deviation in refractive index ($\Delta_\phi n_D$) and deviation in molar refraction (ΔR_M) of liquid mixtures have been calculated. The excess values have fitted to the Redlich–Kister smoothing polynomial equation to estimate the binary coefficients and standard deviation between the experimental and calculated values. The excess partial molar volume, $\overline{V}_{m,1}^E$, $\overline{V}_{m,2}^E$ over the whole composition range; and partial molar volume, $\overline{V}_{m,1}$, $\overline{V}_{m,2}$ excess partial molar volume at infinite dilution, $\overline{V}m,1^{E,\infty}$, $\overline{V}_{m,2}^{E,\infty}$ have also been calculated. The variations of these parameters with composition and temperature have discussed in terms of intermolecular interactions prevailing in these mixtures.

1. Introduction

The study of excess thermodynamic, structural and dynamics properties of mixed solvents is a classical area of chemistry of liquids. The long-standing interest in mixed solvents is largely due to their importance as tuneable reaction media. Accurate knowledge of various thermophysical properties such as excess molar volume, density, speed of sound and refractive index of mixtures of organic liquids is essential for the right design of several types of relevant industrial equipment [1–3]. From molecular perspective, binary liquid mixtures are also interesting because they often exhibit complex structural and dynamical features, especially when the components are capable of specific interactions with one another, which may result in strong interspecies molecular associations [4].

The 2-alkoxyethanols belonging to the group of cellosolves, and amphiphilic compounds has both alcoholic –OH and partially etheric –O– in its structure, and is noted for its donating and accepting ability, which makes it possible to form inter- and intra-molecular hydrogen bond [5,6]. The physical and chemical properties shown by 2-alkoxyalkanols resulting from its self-associated structure like alcohols allow one to place it between protic and aprotic solvents. The 2-alkoxyethanols in pure form and with aqueous solutions used as a solvent of electrolytes up to some extent as an aprotic solvent [7,8]. For that reason it is often defined as a "quasi-aprotic" solvent. The physicochemical behaviour of ethylene glycol derivatives (or) amphiphilic compounds with various molecular compounds has been systematically studied over the past few years [9–22]. Knowing the detailed knowledge of the behaviour of mixtures (DEC + 2-alkoxyethanols) is important for both industry and fundamental research and it turns out that very interesting features emerge from a purely thermodynamic point of view. Furthermore, accurate thermophysical (volumetric properties, volume expansivity and isothermal compressibility) are required for the optimization of the design of any industrial process [23]. These properties provide helpful thermodynamic information of solution non-ideality and component similarity. Furthermore, their variation as a function of the composition of the mixture permits a link between the molecular phenomena and the observed excess-property behaviour. The present study was therefore undertaken to evaluate the influence of particular specific interactions on the excess properties with the increase of temperature, and the alkyl group size of 2-alkoxyethanols.

Volumetric data of DEC with 2-ME/2-EE were reported by Francesconi et al. [59] at 298.15 K and 313.15 K and Pal et al. [60] for 2-ME at 298.15 K. On the basis of our preliminary experiments, diethylcarbonate (DEC) has been found to be totally miscible with 2-alkoxyethanols at all proportions. Hence, in the present study, it

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is proposed to measure the physical properties (density, ρ, speed of sound, u, refractive index, n_D) of the binary mixtures of DEC with 2-alkoxyethanols within the temperature range from (298.15–323.15) K and over the whole composition range and to estimate their excess/deviation properties for their potential applications. On the basis of the measured values; thermodynamic, acoustical and optical parameters such as excess molar volume (V_m^E), excess isentropic compressibility (κ_s^E), excess partial molar compressibility ($K_{s,m}^E$), excess speed of sound (u^E), deviation in refractive index ($\Delta_\phi n_D$), deviation in molar refraction (ΔR_M), excess partial molar volume, $\overline{V}_{m,1}^E$, $\overline{V}_{m,2}^E$ over the whole composition range; and partial molar volume, $\overline{V}_{m,1}$, $\overline{V}_{m,2}$ and excess partial molar volume at infinite dilution,$\overline{V}_{m,1}^{E,\infty}$, $\overline{V}_{m,2}^{E,\infty}$ have been determined for the binary

Table 1
Details of chemical source, purification method, purity and analysis method.

Chemical name (CAS number)	Source	Initial mole fraction purity	Purification method	Final mole fraction purity	Analysis method
Diethyl Carbonate (CAS 105-58-8)	Sigma-aldrich	>0.99	Fractional distillation	>0.993	GC
2-Methoxyethanol (109-86-4)	Sigma-aldrich	>0.99	Fractional distillation	>0.998	GC
2-Ethoxyethanol (110-80-5)	Sigma-aldrich	>0.99	Fractional distillation	>0.996	GC
2-Propoxyethanol (2807-30-9)	Sigma-aldrich	>0.99	Fractional distillation	>0.996	GC

GC-Gas Chromatography.

Table 2
Experimental values of density (ρ), speed of sound (u), refractive index(n) and heat capacity, C_p of pure liquids along with corresponding values available in the literature at T = (298.15–323.15) K, at P = 0.1 MPa.

T/K	Density/kg·m^{-3}		Speed of sound/m·s^{-1}		Refractive index n_D		Cp/
	Expt	Lit	Exp	Lit	Expt	Lit	(J·K^{-1}·mol^{-1})
2-Methoxyethanol							
298.15	960.32	960.05 [10] 960.29 [11] 960.28 [12] 960.45 [13]	1342.09	1341.58 [14]	1.4001	1.4004 [10] 1.4001 [15] 1.4002 [16]	176.40 [13]
303.15	955.71	955.75 [11] 955.68 [12] 955.83 [13]	1324.72	1324.29 [14]	1.3980	1.3981 [15] 1.3983 [16]	177.76 [13]
308.15	951.08	950.81 [10] 951.09 [11] 951.02 [12] 951.21 [13]	1307.38		1.3961	1.3961 [15] 1.3964 [16]	179.12 [13]
313.15	946.42	946.29 [11] 946.30 [12] 946.56 [13]	1290.05		1.3943	1.3942 [15] 1.3950 [16]	180.48 [13]
318.15	941.72	941.45 [10] 941.62 [11] 941.62 [12] 941.86 [13]	1272.73		1.3923	1.3922 [15]	181.84 [13]
323.15	936.89	936.89 [11] 936.87 [12]	1255.43		1.3902	1.3902 [15]	183.03 [35]
2-Ethoxyethanol							
298.15	925.54	925.99 [9] 925.60 [18]	1302.81	1303.06 [9] 1303.96 [18]	1.4055	1.4058 [18] 1.4054 [20]	211.1 [33]
303.15	920.99	921.45 [9] 921.19 [17] 920.70 [19]	1285.05	1285.42 [9]	1.4042	1.4042 [20] 1.4038 [6]	212.8 [33]
308.15	916.41	916.86 [9] 916.43 [17] 916.52 [18]	1267.32	1267.68 [9] 1269.53 [18]	1.4028	1.4017 [18] 1.4025 [20]	214.6 [33]
313.15	911.8	912.24 [9] 911.58 [17] 911.30 [19]	1249.63	1250.01 [9]	1.4016	1.4018 [20] 1.3995 [6]	216.5 [33]
318.15	907.15	907.58 [9] 907.76 [17] 907.31 [18]	1231.53	1232.39 [9] 1234.11 [18]	1.4001	1.3975 [18]	218.3 [33]
323.15	902.46	903.45 [17] 901.80 [19]	1214.29		1.3988	1.3954 [6]	220.2 [33]
2-Propoxyethanol[29]							
298.15	907.16	907.15 [21] 908.00[22]	1300.92	1298.58 [21]	1.4103	–	241.78[34]
303.15	902.74	902.74[21]	1283.65	1281.14[21]	1.4081	–	243.85 [34]
308.15	898.32	899.20 [22]	1266.41	–	1.4058	–	245.91 [34]
313.15	893.89	–	1249.17	–	1.4034	–	247.98 [34]
318.15	889.45	889.00 [22]	1231.93	–	1.4011	–	250.05 [34]
323.15	885.00	–	1214.95	–	1.3988	–	252.11 [34]

Standard uncertainties u are as follows: u(ρ) = ±0.5 kg·m^{-3}, u(u) = ± 0.6 m·s^{-1}, u(n_D) = ± 0.0008 and u(T) = ± 0.05 K, u(T) for n_D = ±0.02 K, u (p) = ±0.002 MPa.

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