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Excess molar volumes, viscosities, and refractive indices for binary and ternary mixtures of {cyclohexanone (1) + *N,N*-dimethylacetamide (2) + *N,N*-diethylethanolamine (3)} at (298.15, 308.15, and 318.15) K

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ABSTRACT

Densities ρ, viscosities η, and refractive indices n_D, of the binary and ternary mixtures formed by cyclohexanone + *N,N*-dimethylacetamide + *N,N*-diethylethanolamine were measured at (298.15, 308.15, and 318.15) K for the liquid region and at ambient pressure for the whole composition ranges. The excess molar volumes V_m^E, viscosity deviations $\Delta\eta$, and refractive index deviations Δn_D, were calculated from experimental densities and refractive indices. The excess molar volumes are positive over the mole fraction range for binary mixtures of cyclohexanone(1) + *N,N*-dimethylacetamide (2) and *N,N*-dimethylactamide (2) + *N,N*-diethylethanolamine (3) and increase with increasing temperatures from (298.15 to 318.15) K. The excess molar volumes of cyclohexanone (1) + *N,N*-diethylethanolamine (3) are S-shaped dependence on composition with negative values in the *N,N*-diethylethanolamine rich-region and positive values at the opposite extreme and increase with increasing temperatures from (298.15 to 318.15) K. The excess molar volumes are positive over the whole mole fraction ranges for the ternary mixtures at all temperatures. Viscosity deviations are negative over the mole fraction range for all binary and ternary mixtures and decrease with increasing temperatures from (298.15 to 318.15) K. Refractive index deviations are negative over the mole fraction range for all binary and ternary mixtures and increase with increasing temperatures from (298.15 to 318.15) K. The experimental data of constitute were correlated as a function of the mole fraction by using the Redlich–Kister equation for binary and , Cibulka, Jasinski and Malanowski , Singe et al., Pintos et al., Calvo et al., Kohler, and Jacob–Fitzner for ternary mixture, respectively. McAllister's three body, Hind, and Nissan–Grunberg models were used for correlating the kinematic and dynamic viscosity of binary mixtures. The experimental data of the constitute binaries are analyzed to discuss the nature and strength of intermolecular interactions in these mixtures.

1. Introduction

This paper is a continuation of our earlier work related to the study of thermodynamic properties of binary and ternary mixtures [1–6]. Multicomponent liquid mixtures have attracted the attention of researchers in the past decades. Physical properties are very important factors in chemical and engineering processes because of their influence upon the effectiveness of the operations. Mass and heat transfer processes and flow operations are evident examples of the importance of the knowledge for these properties [7,8]. It is well-known that the knowledge of the dependence of dynamic viscosity on both temperature and composition of the system is needed for many engineering processes and the study of fluid phenomena. There are several predictive equations [9] for estimating thermodynamic properties of multicomponent systems. Geometrical solution models are considered to predict excess molar volumes and deviations of the viscosity for the ternary mixture from binary contribution because of dependence of interactions in ternary systems on the interaction in binary systems [10–13]. Recently, new models have been developed for the prediction of viscosities of the mixtures. Some of them are based on the group contribution concept [14,15] and others are based on the molecular approach that requires binary interaction parameters for each binary system present in the multicomponent mixtures [16,17]. Such methods are rarely used for viscosity because some of them cannot be immediately extensible to multicomponent mixtures or they may require more parameters (such as three- and four-body interaction terms) for mixtures containing more than two components or require binary interaction parameters for each binary system present in the multicomponent mixtures.

Here, we have measured densities ρ, viscosities η, and refractive indices n_D, for the binary systems formed by cyclohexanone + *N,N*-dimethylacetamide, + *N,N*-diethylethanolamine, and *N,N*-dimethylacetamide + *N,N*-diethylethanolamine and ternary system

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Table 1
Purity grades, densities ρ, refractive indices n_D, and thermal expansion coefficients α, of the pure components at different temperatures and ambient pressure.

Component	Purity	T (K)	ρ (g cm^{-3})		n_D		$10^4\alpha$
	(Mass fraction)		Experimental	Literature	Experimental	Literature	
Cyclohexanone	0.995	298.15	0.94291	0.9418 [23]	1.4517[a]	1.4518 [32]	9.42
				0.9420 [26]		1.4503 [33]	
				0.9410 [25]		1.4507 [34]	
				0.9420 [24]			
		308.15	0.93467	0.9365 [25]	1.4440		9.52
				0.9334 [24]			
		318.15	0.92569	0.9242 [24]	1.4393		9.69
N,*N*-dimethylacetamide	0.99	298.15	0.93631	0.935287 [29]	1.4357	1.4357 [31]	9.93
				0.9366 [28]			
				0.93654 [27]			
		308.15	0.92708	0.926297 [29]	1.4313		10.81
		318.15	0.91782	0.917216 [29]	1.4267		11.72
N,*N*-diethylethanolamine	0.995	298.15	0.88234	0.883578 [30]	1.4276		9.60
		308.15	0.87378	0.875017 [30]	1.4233		9.88
		318.15	0.86508	0.866316 [30]	1.4187		10.11

[a] $T = 293.15$ K.

cyclohexanone + *N*,*N*-dimethylacetamide + *N*,*N*-diethylethanolamine at (298.15, 308.15, and 318.15) K for the liquid region and at ambient pressure for the whole composition ranges. The derived properties (excess molar volumes V_m^E, viscosity deviations $\Delta\eta$, and refractive index deviations Δn_D, in combination with other mixing properties, provide valuable information for qualitatively analyzing the molecular interactions between molecules.

The excess and deviation quantities of binary mixtures have been fitted to the Redlich–Kister [18] and ternary mixture has been fitted to the Cibulka [19], Jasinski and Malanowski [19], Singe et al. [19], Pintos et al. [19], Calvo et al. [19], Kohler [19], and Jacob–Fitzner [19], equations to determine the coefficients. The viscosity data for the binary mixtures were correlated to the semi-empirical McAllister [20], Nissan and Grunberg [21], Hind et al. [22], models and their parameters have been calculated.

Table 2
Coefficients A_{pq} of Eq. (3) and standard deviations for the fitting of the binary excess molar volumes, V_m^E, viscosity deviations, $\Delta\eta$, and refractive index deviations, Δn_D, in the temperatures range at (298.15n to 318.15) K.

q	p					σ (V_m^E)
	0	1	2	3	4	
{cyclohexanone (1) + *N*,*N*-dimethylacetamide (2)}						
0	13.2215	−0.0865	0.0002	55.9296	−0.3452	0.003
1	0.0005	−36.9677	0.2465	−0.0004	−77.5186	
2	0.4937	−0.0008	25.7568	−0.1686	0.0003	
{cyclohexanone (1) + *N*,*N*-diethylethanolamine (2)}						
0	−40.6461	0.2405	−0.00034	49.5614	−0.3268	0.005
1	0.0005	130.612	−0.8521	0.0014	−153.857	
2	0.9821	−0.0016	−133.818	0.8712	−0.0014	
{*N*,*N*-dimethylacetamide (1) + *N*,*N*-diethylethanolamine (2)}						
0	−5.6679	0.0414	6.39×10^{-5}	6.1246	−0.0424	0.004
1	7.52×10^{-5}	3.1697	−0.0216	3.44×10^{-5}	−0.8318	
2	0.0032	-7.3×10^{-6}	−5.273	0.0328	5.53×10^{-5}	
						$\sigma(\Delta\eta)$
{cyclohexanone (1) + *N*,*N*-dimethylacetamide (2)}						
0	40.7541	−0.2563	0.0004	−47.238	0.3014	0.001
1	−0.0005	7686.15	−0.1089	0.0002	−24.318	
2	0.165	−0.0003	−105.421	0.06722	−0.0012	
{cyclohexanone (1) + *N*,*N*-diethylethanolamine (2)}						
0	42.9981	0.2756	0.0004	1.5006	0.0016	0.003
1	−0.00002	−274.957	1.7728	−0.0029	72.1874	
2	−0.4575	0.0007	186.887	−1.1939	0.0019	
{*N*,*N*-dimethylacetamide (1) + *N*,*N*-diethylethanolamine (2)}						
0	3.93843	−0.0176	6.6×10^{-7}	37.2531	−0.2520	0.003
1	0.00042	−84.1816	0.5627	−0.0009	−22.9196	
2	0.1480	−0.0002	98.1532	−0.6718	0.0011	
						$\sigma(\Delta n_D)$
{cyclohexanone (1) + *N*,*N*-dimethylacetamide (2)}						
0	−1.7519	0.0107	−0.00002	−3.8148	0.02447	4×10^{-5}
1	−0.00004	0.8504	−0.0053	8.48×10^{-6}	2.85791	
2	−0.0183	0.00003	−4.6045	0.0299	−0.00005	
{cyclohexanone (1) + *N*,*N*-diethylethanolamine (2)}						
0	−0.1312	0.0007	-9.5×10^{-7}	0.2262	−0.0015	2×10^{-5}
1	2.36×10^{-6}	−0.4993	0.0032	-4.9×10^{-6}	−0.0496	
2	0.0003	-5.2×10^{-6}	−1.7251	0.0113	-2×10^{-5}	
{*N*,*N*-dimethylacetamide (1) + *N*,*N*-diethylethanolamine (2)}						
0	0.0127	−0.0001	1.8×10^{-7}	−0.1915	0.0012	1.3×10^{-5}
1	-1.9×10^{-6}	−0.1562	0.0011	-1.8×10^{-6}	0.1901	
2	−0.0012	1.9×10^{-6}	0.2018	−0.0013	2.3×10^{-6}	