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Densities and Viscosities of Binary Mixtures of Cyclohexanone and 2-Alkanols

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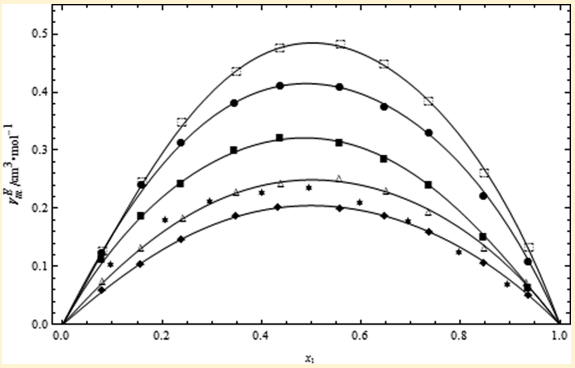
Supporting Information

ABSTRACT: Densities and viscosities of mixtures of cyclohexanone with 2-alkanols, namely, 2-propanol, 2-butanol, 2-pentanol, 2-hexanol, and 2-heptanol, have been measured as a function of composition range at T = (298.15, 303.15, 308.15, and 313.15) K and ambient pressure. Excess molar volumes V_m^E and viscosity deviations $\Delta\eta$ were calculated and correlated by the Redlich−Kister type function to derive the coefficients and estimate the standard error. For mixtures of cyclohexanone with used 2-alkanols, V_m^E is positive, and $\Delta\eta$ is negative over the entire range of mole fraction. The effect of temperature and chain length of the 2-alkanols on the excess molar volumes and viscosity deviations of its mixtures with cyclohexanone is discussed.



INTRODUCTION

Densities and viscosities of fluids and fluid mixtures are essential for many engineering and industrial applications. The mixture functions such as the excess molar volume, V_m^E, and the viscosity deviation, $\Delta\eta$, are often used to describe the intermolecular forces in mixtures to help us understand their real behavior and to develop models for their description as well as the simulation processes. Therefore, over the years, studies on multicomponent liquid systems have attracted the attention of many researchers.[1−4]

Thermodynamic properties of cyclohexanone with alkanols are important in the fundamental understanding of the mixing processes. Knowledge of the thermophysical properties of these liquids is of high interest on account of their wide usage in science and industrial processes. Those properties are crucial for the design of chemical processes as well as for progress in the thermodynamic theories of the liquid state. The densities and viscosities as functions of temperature and pressure, and their derivatives render some insight in the molecular structure of liquids and provide information on intermolecular interactions. This paper is a part of an ongoing research effort to measure and characterize the properties of mixtures containing alkanols.[5,6] It reports the densities, viscosities, excess molar volumes, and viscosity deviations of mixing for the binary mixtures of cyclohexanone + 2-alkanols at the temperatures of (298.15, 303.15, 308.15, and 313.15) K. The influences of temperature and chain length on the thermodynamic properties were investigated. No reported mixing properties of these studied systems at these temperatures were found.

EXPERIMENTAL SECTION

Cyclohexanone, 2-propanol, 2-butanol, 2-pentanol, and 2-heptanol were obtained from Merck with a mass purity of > 99 %, and 2-hexanol was supplied from Aldrich with a mass purity of > 99 %. All of the materials were used as purchased without further purification. The purity of reagents was checked by comparing the measured densities and viscosities at various temperatures with those reported in the literature;[7−10] the resultant values are in good agreement with values found in the literature and reported in Table 1.

The density of the pure compounds and mixtures was measured by means of an Anton Parr DMA 4500 oscillating U-tube densimeter, provided with automatic viscosity correction. The uncertainty of the density measurements was estimated to be ± $5{\cdot}10^{-5}$ g·cm^{-3}. The apparatus was calibrated once a day with dry air and bidistillated water. The temperature in the cell was regulated to ± 0.01 K with a solid state thermostat. Viscosities were measured with an Ubbleohde viscometer with an uncertainty of ± $1{\cdot}10^{-2}$ mPa·s. The temperature in the cell was regulated to ± 0.01 K. The mixtures were prepared by weighing known masses of pure liquids in airtight, narrow-mouth ground stoppered bottles taking due precautions to minimize evaporation losses. All of the mass measurements were performed on an electronic balance (Mettler AE 163, Switzerland) accurate to 0.01 mg. The uncertainty in the mole fraction was estimated to be ± $1{\cdot}10^{-4}$.

RESULTS AND DISCUSSION

Densities and Excess Molar Volumes. The excess molar volumes of the solutions of molar composition, x, were calculated at the temperatures of (298.15, 303.15, 308.15, and 313.15) K from the densities of the pure liquids and their

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Table 1. Sources, Purity Grades, Densities, ρ, and Viscosities, η, of Pure Components at Various Temperatures

				ρ/(g·cm^{-3})		η/(mPa·s)	
chemical name	source	initial mass purity	T/K	exptl	lit.	exptl	lit.
cyclohexanone	Merck	0.995	298.15	0.94191	0.9418[a]	2.057	2.0205[a]
			303.15	0.93724	0.9374[b]	1.847	1.799[b]
			308.15	0.93267	0.9328[b]	1.694	1.635[b]
			313.15	0.92772		1.546	
2-propanol	Merck	0.995	298.15	0.78109	0.78098[c]	2.055	2.044[c]
			303.15	0.77657	0.77660[d]	1.788	1.763[d]
			308.15	0.77187	0.7725[a]	1.563	1.560[a]
			313.15	0.76736		1.387	
2-butanol	Merck	0.995	298.15	0.80301	0.80256[c]	3.104	3.132[c]
			303.15	0.79820	0.79851[d]	2.597	2.493[d]
			308.15	0.79357	0.7939[a]	2.152	2.125[a]
			313.15	0.78915		1.733	
2-pentanol	Merck	>0.99	298.15	0.80541	0.80524[c]	3.499	3.478[c]
			303.15	0.80121	0.80090[d]	2.801	2.774[d]
			308.15	0.79666	0.7966[a]	2.334	
			313.15	0.79251		1.993	
2-hexanol	Aldrich	>0.99	298.15	0.81014	0.81014[c]	4.101	4.100[c]
			303.15	0.80613	0.8064[a]	3.411	3.33[a]
			308.15	0.80206	0.80175[e]	2.819	2.920[e]
			313.15	0.79796	0.7984[a]	2.219	2.29[a]
2-heptanol	Merck	0.995	298.15	0.81318	0.81333[c]	5.023	5.088[e]
			303.15	0.80926		4.151	
			308.15	0.80501	0.80488[e]	3.748	3.683[e]
			313.15	0.80114		2.852	

[a]Reference 7. [b]Reference 8. [c]Reference 6. [d]Reference 9. [e]Reference 10.

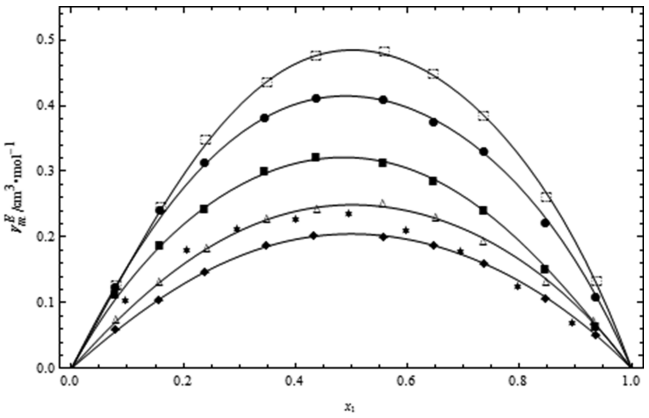

Figure 1. Excess molar volumes V_m^E vs mole fraction of cyclohexanone for binary mixtures of cyclohexanone with ◆, 2-propanol; △, 2-butanol; ★, ref 19 for 2-butanol; ■, 2-pentanol; ●, 2-hexanol; □, 2-heptanol; at 298.15 K. The solid curves were calculated from coefficients of eq 2 given in Table 3.

mixtures according to the following equation

$$V_E^m = \sum_{i=1}^{N} x_i M_i (\rho^{-1} - \rho_i^{-1}) \quad (1)$$

where ρ is the density of the mixture, ρ_i is the density of pure component i, x_i is the mole fraction, M_i is the molar mass of component i, and N stands for the number of components in the mixture.

The corresponding V_m^E values of binary mixtures of [cyclohexanone (1) + 2-alkanols (2)] are calculated and plotted against the mole fraction of cyclohexanone at 298.15 K in Figure 1. The uncertainty for excess molar volume is $\pm 1 \cdot 10^{-3}$ cm^3·mol^{-1}. The values of density for binary mixtures are in Table 2. Each set of results was fitted using a Redlich–Kister polynomial,[11] which for binary mixtures is

$$Y^E = x_1(1 - x_1) \sum_{k=0}^{N} A_k (1 - 2x_1)^k \quad (2)$$

where $Y^E \equiv V_m^E$ or $\Delta\eta$ and x_1 is the mole fraction of cyclohexanone. A_k is an adjustable parameter obtained by the least-squares method, and k is the degree of the polynomials. In each case, the optimum number of coefficients was ascertained from an examination of the variation of standard deviation σ with

$$\sigma = [\sum (Y - Y_{cal})^2/(n - p)]^{1/2} \quad (3)$$

where Y and Y_{cal} are the experimental and calculated values of the property Y, respectively, and n and p are the number of experimental points and number of parameters retained in the respective equations. Table 3 presents the values of the parameters A_k together with the standard deviation σ.

Cyclohexanone is expected to exhibit dipole–dipole interactions in the pure state because of its fairly high dipole moment (μ = 3.01 D). However, the association between cyclohexanone molecules is weak (probably negligible) and does not compete with the high degree of association between alcohol molecules, which are strongly associated in the pure state through hydrogen bonding to form short-lived aggregates.[12,13] Alcohols represent an important class of hydrogen-bonded solvents, for which the degree of association is very sensitive to temperature and the presence of electrolytes.[14,15] Excess molar volumes of all binary mixtures are positive and increase slightly with increasing the temperature.

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Table 2. Densities, ρ, and Viscosities, η, for the Binary Mixtures as a Function of the Mole Fraction x_1 of Cyclohexanone[a]

x_1	ρ / g·cm^{-3}	η / mPa·s
Cyclohexanone (1) + 2-Propanol (2), T/K = 298.15		
0.0000	0.7810	2.055
0.0812	0.7976	1.689
0.1576	0.8125	1.436
0.2398	0.8277	1.236
0.3495	0.8469	1.067
0.4363	0.8614	1.023
0.5601	0.8809	1.076
0.6502	0.8944	1.177
0.7403	0.9073	1.331
0.8481	0.9221	1.581
0.9384	0.934	1.845
1.0000	0.9419	2.057
T/K = 303.15		
0.0000	0.7765	1.788
0.0812	0.7929	1.489
0.1576	0.8076	1.268
0.2398	0.8228	1.081
0.3495	0.8419	0.934
0.4363	0.8562	0.899
0.5601	0.8757	0.951
0.6502	0.8892	1.056
0.7403	0.9021	1.202
0.8481	0.917	1.437
0.9384	0.929	1.675
1.0000	0.9372	1.847
T/K = 308.15		
0.0000	0.7718	1.563
0.0812	0.7881	1.301
0.1576	0.8027	1.098
0.2398	0.8176	0.934
0.3495	0.8365	0.809
0.4363	0.8510	0.779
0.5601	0.8705	0.845
0.6502	0.8840	0.949
0.7403	0.8972	1.087
0.8481	0.9122	1.301
0.9384	0.9244	1.537
1.0000	0.9326	1.694
T/K = 313.15		
0.0000	0.7673	1.378
0.0812	0.7832	1.142
0.1576	0.7977	0.961
0.2398	0.8127	0.817
0.3495	0.8317	0.715
0.4363	0.8462	0.689
0.5601	0.8653	0.751
0.6502	0.8789	0.854
0.7403	0.8921	0.995
0.8481	0.9070	1.211
0.9384	0.9193	1.412
1.0000	0.9277	1.546
Cyclohexanone (1) + 2-Butanol (2), T/K = 298.15		
0.0000	0.8030	3.104
0.0814	0.8149	2.511
0.1598	0.8263	2.067
0.2444	0.8385	1.737
0.3514	0.8537	1.472
0.4404	0.8661	1.361
0.5596	0.8826	1.332
0.6523	0.8953	1.400
0.738	0.9069	1.501
0.8494	0.9218	1.704
0.9361	0.9333	1.889
1.0000	0.9419	2.057
T/K = 303.15		
0.0000	0.7982	2.597
0.0814	0.8110	2.163
0.1598	0.8222	1.820
0.2444	0.8341	1.535
0.3514	0.8490	1.305
0.4404	0.8613	1.206
0.5596	0.8777	1.183
0.6523	0.8903	1.249
0.738	0.9019	1.354
0.8494	0.9169	1.558
0.9361	0.9285	1.716
1.0000	0.9372	1.847
T/K = 308.15		
0.0000	0.7935	2.152
0.0814	0.8051	1.828
0.1598	0.8163	1.561
0.2444	0.8281	1.330
0.3514	0.8431	1.128
0.4404	0.8556	1.039
0.5596	0.8721	1.036
0.6523	0.8849	1.108
0.738	0.8968	1.224
0.8494	0.9120	1.410
0.9361	0.9240	1.572
1.0000	0.9326	1.694
T/K = 313.15		
0.0000	0.7891	1.733
0.0814	0.8005	1.441
0.1598	0.8114	1.186
0.2444	0.8231	0.982
0.3514	0.8380	0.841
0.4404	0.8503	0.794
0.5596	0.8669	0.825
0.6523	0.8796	0.914
0.7380	0.8915	1.051
0.8494	0.9070	1.248
0.9361	0.9189	1.430
1.0000	0.9277	1.546
Cyclohexanone (1) + 2-Pentanol (2), T/K = 298.15		
0.0000	0.8054	3.499
0.0824	0.8153	2.631
0.1615	0.8251	2.178
0.2401	0.8350	1.822
0.3492	0.8491	1.465
0.4397	0.8611	1.277
0.5607	0.8777	1.191
0.6496	0.8901	1.230
0.7399	0.9030	1.354
0.8498	0.9192	1.597
0.9396	0.9327	1.855
1.0000	0.9419	2.057

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Table 2. continued

x_1	ρ / g·cm^{-3}	η / mPa·s
	T/K = 303.15	
0.0000	0.8012	2.801
0.0824	0.8109	2.307
0.1615	0.8206	1.893
0.2401	0.8305	1.580
0.3492	0.8446	1.241
0.4397	0.8565	1.081
0.5607	0.8729	1.016
0.6496	0.8854	1.072
0.7399	0.8982	1.205
0.8498	0.9144	1.417
0.9396	0.9281	1.685
1.0000	0.9372	1.847
	T/K = 308.15	
0.0000	0.7966	2.334
0.0824	0.8063	1.891
0.1615	0.8159	1.541
0.2401	0.8256	1.265
0.3492	0.8395	1.007
0.4397	0.8514	0.881
0.5607	0.8677	0.865
0.6496	0.8801	0.935
0.7399	0.8931	1.062
0.8498	0.9094	1.294
0.9396	0.9233	1.523
1.0000	0.9326	1.694
	T/K = 313.15	
0.0000	0.7925	1.993
0.0824	0.8019	1.596
0.1615	0.8115	1.285
0.2401	0.8210	1.056
0.3492	0.8347	0.838
0.4397	0.8464	0.750
0.5607	0.8626	0.771
0.6496	0.8750	0.848
0.7399	0.8880	0.982
0.8498	0.9043	1.194
0.9396	0.9179	1.388
1.0000	0.9277	1.546
Cyclohexanone (1) + 2-Hexanol (2), T/K = 298.15		
0.0000	0.8101	4.101
0.0821	0.8184	3.432
0.1612	0.8266	2.879
0.2409	0.8352	2.406
0.3496	0.8478	1.896
0.4391	0.8589	1.591
0.5600	0.8746	1.359
0.6490	0.8868	1.325
0.7391	0.8998	1.388
0.8492	0.9167	1.576
0.9395	0.9314	1.842
1.0000	0.9419	2.057
	T/K = 303.15	
0.0000	0.8061	3.411
0.0821	0.8141	2.834
0.1612	0.8222	2.346
0.2409	0.8308	1.932
0.3496	0.8433	1.477
0.4391	0.8543	1.230
0.5600	0.8699	1.080
0.6490	0.8820	1.082
0.7391	0.8951	1.173
0.8492	0.9120	1.400
0.9395	0.9266	1.662
1.0000	0.9372	1.847
	T/K = 308.15	
0.0000	0.8020	2.819
0.0821	0.8098	2.278
0.1612	0.8180	1.823
0.2409	0.8264	1.453
0.3496	0.8388	1.122
0.4391	0.8497	0.949
0.5600	0.8652	0.873
0.6490	0.8773	0.907
0.7391	0.8904	1.026
0.8492	0.9071	1.249
0.9395	0.9219	1.505
1.0000	0.9326	1.694
	T/K = 313.15	
0.0000	0.7979	2.219
0.0821	0.8059	1.686
0.1612	0.8140	1.307
0.2409	0.8224	1.024
0.3496	0.8347	0.781
0.4391	0.8454	0.679
0.5600	0.8608	0.655
0.6490	0.8729	0.727
0.7391	0.8859	0.850
0.8492	0.9027	1.068
0.9395	0.9172	1.326
1.0000	0.9277	1.546
Cyclohexanone (1) + 2-Heptanol (2), T/K = 298.15		
0.0000	0.8131	5.023
0.0826	0.8203	4.282
0.1625	0.8276	3.640
0.2415	0.8352	3.081
0.3506	0.8466	2.401
0.4400	0.8568	1.954
0.5603	0.8717	1.513
0.6494	0.8837	1.308
0.7394	0.8969	1.243
0.8500	0.9146	1.391
0.9392	0.9302	1.727
1.0000	0.9419	2.057
	T/K = 303.15	
0.0000	0.8092	4.151
0.0826	0.8162	3.546
0.1625	0.8233	2.986
0.2415	0.8309	2.473
0.3506	0.8421	1.874
0.4400	0.8522	1.468
0.5603	0.8669	1.107
0.6494	0.8789	0.971
0.7394	0.8921	0.976
0.8500	0.9099	1.193
0.9392	0.9255	1.535
1.0000	0.9372	1.847

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Table 2. continued

x_1	ρ / g·cm^{-3}	η / mPa·s	x_1	ρ / g·cm^{-3}	η / mPa·s
	T/K = 308.15			T/K = 313.15	
0.0000	0.8050	3.478	0.0000	0.8011	2.852
0.0826	0.8116	2.940	0.0826	0.8076	2.412
0.1625	0.8188	2.449	0.1625	0.8145	1.989
0.2415	0.8262	1.999	0.2415	0.8218	1.604
0.3506	0.8374	1.482	0.3506	0.8329	1.151
0.4400	0.8474	1.141	0.4400	0.8427	0.862
0.5603	0.8621	0.849	0.5603	0.8573	0.627
0.6494	0.8741	0.773	0.6494	0.8692	0.576
0.7394	0.8872	0.816	0.7394	0.8823	0.647
0.8500	0.9050	1.054	0.8500	0.9000	0.910
0.9392	0.9207	1.411	0.9392	0.9158	1.256
1.0000	0.9326	1.694	1.0000	0.9277	1.546

[a]Standard uncertainties u are $u(T) = 0.01$ K, $u(x) = 0.0001$; the combined expanded uncertainty U_c is $U_c(\rho) = 2{\cdot}10^{-2}$ kg·m^{-3} and for viscosity U_c is $U_c(\eta)$ is $2{\cdot}10^{-3}$ mPa·s (0.95 level of confidence).

Table 3. Parameters A_k and Standard Deviations, σ, for Cyclohexanone + 2-Alkanols at Different Temperatures

		T/K	A_0	A_1	A_2	σ
cyclohexanone + 2-propanol	V_m^E (cm^3·mol^{-1})	298.15	0.820	0.027	0.080	0.002
		303.15	1.068	0.096	0.016	0.007
		308.15	1.328	0.051	0.045	0.008
		313.15	1.496	0.069	0.161	0.005
	$\Delta\eta$ (mPa·s)	298.15	4.080	0.737	0.224	0.005
		303.15	3.629	0.683	0.151	0.004
		308.15	3.314	0.635	0. 134	0.007
		313.15	3.014	0.671	0.299	0.002
cyclohexanone + 2-butanol	V_m^E (cm^3·mol^{-1})	298.15	0.996	0.036	0.043	0.004
		303.15	1.302	0.071	0.027	0.003
		308.15	1.524	0.053	0.132	0.005
		313.15	1.845	0.139	0.141	0.004
	$\Delta\eta$ (mPa·s)	298.15	4.991	1.745	0.541	0.005
		303.15	4.178	1.216	0.264	0.005
		308.15	3.591	0.802	0.595	0.003
		313.15	3.385	0.957	0.438	0.008
cyclohexanone + 2-pentanol	V_m^E (cm^3·mol^{-1})	298.15	1.283	0.128	0.019	0.005
		303.15	1.432	0.140	0.006	0.009
		308.15	1.740	0.014	0.013	0.008
		313.15	1.988	0.050	0.048	0.009
	$\Delta\eta$ (mPa·s)	298.15	5.654	0.861	0.180	0.003
		303.15	5.175	0.828	0.474	0.009
		308.15	4.628	0.887	0.300	0.004
		313.15	4.087	1.022	0.188	0.007
cyclohexanone + 2-hexanol	V_m^E (cm^3·mol^{-1})	298.15	1.656	0.005	0.176	0.006
		303.15	1.859	0.014	0.348	0.005
		308.15	2.033	0.042	0.476	0.008
		313.15	2.404	0.034	0.424	0.008
	$\Delta\eta$ (mPa·s)	298.15	6.494	0.333	0.285	0.005
		303.15	5.994	0.494	0.715	0.005
		308.15	5.475	0.921	0.153	0.009
		313.15	4.899	1.055	0.683	0.005
cyclohexanone + 2-heptanol	V_m^E (cm^3·mol^{-1})	298.15	1.939	0.150	0.022	0.008
		303.15	2.212	0.114	0.039	0.004
		308.15	2.470	0.099	0.279	0.007
		313.15	2.739	0.042	0.383	0.005
	$\Delta\eta$ (mPa·s)	298.15	7.334	1.516	0.628	0.006
		303.15	6.957	1.503	0.316	0.005
		308.15	6.463	1.224	0.480	0.008
		313.15	5.918	1.312	0.61	0.005

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Table 4. Partial Molar Volumes at Infinite Dilution, $\bar{V}^0_{m,i}$ for Cyclohexanone + 2-Alkanols at Different Temperatures

system	T/K = 298.15	T/K = 303.15	T/K = 308.15	T/K = 313.15
		Cyclohexanone + 2-Propanol		
$\bar{V}^0_{m,1}$ ($cm^3 \cdot mol^{-1}$)	105.00	105.68	106.55	107.28
$\bar{V}^0_{m,2}$ ($cm^3 \cdot mol^{-1}$)	77.77	78.53	79.20	79.93
		Cyclohexanone + 2-Butanol		
$\bar{V}^0_{m,1}$ ($cm^3 \cdot mol^{-1}$)	105.18	105.98	106.76	107.70
$\bar{V}^0_{m,2}$ ($cm^3 \cdot mol^{-1}$)	93.34	94.21	94.83	95.60
		Cyclohexanone + 2-Pentanol		
$\bar{V}^0_{m,1}$ ($cm^3 \cdot mol^{-1}$)	105.55	106.19	106.92	107.72
$\bar{V}^0_{m,2}$ ($cm^3 \cdot mol^{-1}$)	110.64	111.34	112.39	113.28
		Cyclohexanone + 2-Hexanol		
$\bar{V}^0_{m,1}$ ($cm^3 \cdot mol^{-1}$)	105.91	106.66	107.36	108.30
$\bar{V}^0_{m,2}$ ($cm^3 \cdot mol^{-1}$)	127.84	128.72	129.63	130.64
		Cyclohexanone + 2-Heptanol		
$\bar{V}^0_{m,1}$ ($cm^3 \cdot mol^{-1}$)	106.07	106.86	107.69	108.57
$\bar{V}^0_{m,2}$ ($cm^3 \cdot mol^{-1}$)	144.93	145.90	147.01	147.96

It has been pointed out that excess molar volumes are the consequence and the sum of some different contributions deriving from a structural modification (stabilization of particular rotamers and conformers) of the mixed species, changes in the free volumes, and interstitial accommodation of unlike molecules. Furthermore, the specific intermolecular interactions that take place during the mixing process can be classified as follows: (i) favorable interactions (attractive and charge transfer) between polar groups (−C═O and −OH), responsible for a negative contribution to V^E_m, (ii) unfavorable interactions involving polar substituents and apolar groups (−CH_2− and alkyl chains). In this light, we can assert that the positive deviations of V^E_m for the cyclohexanone and 2-alkanols system should be dominated by steric hindrances of molecule components which overcome each effect due to specific interactions between different species.

Figure 1 shows that V^E_m, at equimolar concentrations of cyclohexanone, increases with the increase in carbon number of 2-alkanols. This fact can be described by considering the steric-hindrance effects of the heterocyclic ring of the cyclohexanone and of the alkyl chain of the 2-alkanols, because the hydrophobic character of the 2-alkanol is amplified by an increase in chain length and, consequently, the molecular interactions between 2-alkanol and cyclohexanone molecules weaken.

The partial molar volumes $\bar{V}_{m,i}$ in these mixtures were calculated over the whole composition range using eqs 4 and 5.[16,17]

$$\bar{V}_{m,1} = V^E_m + V^*_{m,1} + (1 - x_1)(\partial V^E_m/\partial x_1)_{T,P} \quad (4)$$

$$\bar{V}_{m,2} = V^E_m + V^*_{m,2} - x_1(\partial V^E_m/\partial x_1)_{T,P} \quad (5)$$

where $V^*_{m,1}$ and $V^*_{m,2}$ are pure molar volumes of components 1 and 2, respectively. The partial properties at infinite dilution are of interest since at the limit of infinite dilution the solute−solute interactions disappear and only interactions present are solute−solvent interactions. Values of partial molar volumes at infinite dilution $\bar{V}^0_{m,i}$ are in Table 4.

Partial molar volumes at infinite dilution of each component are not very different from the corresponding molar volumes $V^*_{m,1}$. Partial molar volumes close to pure component molar volumes indicate ideal behavior. As a matter of fact, in ideal solutions, partial molar volumes are equal to the pure component molar volume over the whole composition range. $\bar{V}^0_{m,i}$ increase slightly with increasing temperature.

Dynamic Viscosities. The viscosity deviation can be calculated as

$$\Delta\eta = \eta - x_1\eta_1 - x_2\eta_2 \quad (6)$$

where η is the viscosity of the mixture and η_1 and η_2 are pure component viscosities. The values of η for binary systems are listed in Table 2. The uncertainty for viscosity deviation is ± $4 \cdot 10^{-3}$ mPa·s. The $\Delta\eta$ values were fitted to Redlich−Kister eq 2, and the adjustable parameters and standard deviations are given in Table 3.

The viscosity deviations for the mixtures of cyclohexanone with the 2-alkanols at 298.15 K are presented graphically in Figure 2. It is observed that the $\Delta\eta$ values are negative for all of the investigated systems and tend systematically to larger negative values with an increase in size of the 2-alkanol; the negative values of $\Delta\eta$ for all of the binary systems fall in the order: 2-heptanol > 2-hexanol > 2-pentanol > 2-butanol > 2-propanol. Our results are in agreement with Vogel and Weiss[18] who have shown that mixtures with a positive deviation of Raoult's law and without strong specific interactions present the negative viscosity deviation.

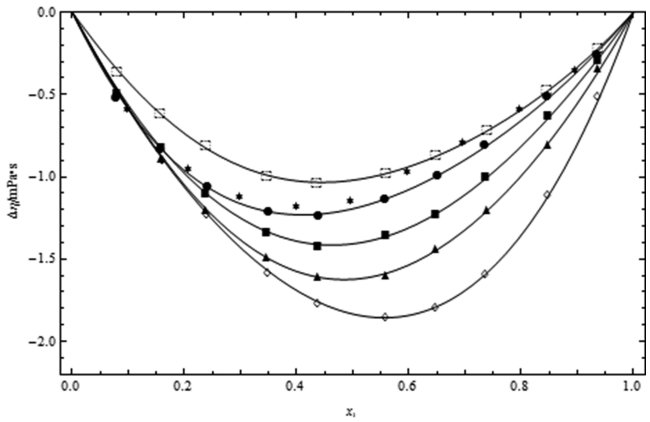

Figure 2. Viscosity deviations $\Delta\eta$ vs mole fraction of cyclohexanone, for binary mixtures of cyclohexanone with □, 2-propanol; ●, 2-butanol; ★, ref 19 for 2-butanol; ■, 2-pentanol; ▲, 2-hexanol; ◊, 2-heptanol; at 298.15 K. The solid curves were calculated from coefficients of eq 2 given in Table 3.

Also in Figures 1 and 2, we compare our data of excess molar volumes and viscosity deviations for binary mixtures of

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cyclohexanone and 2-butanol at 298.15 K with data of ref 19. The discrepancy between experimental data and the literature value may be due to the difference between the applied apparatus. In Figures 3 and 4 the differences between experimental and literature data and the fitted equation are graphically represented.

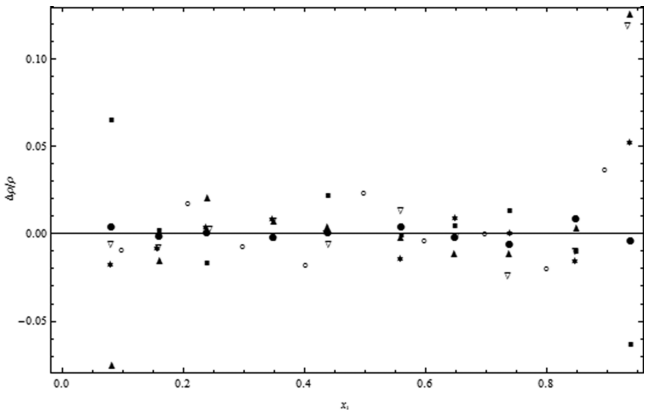

Figure 3. Differences $\Delta\rho = \rho(\text{experimental}) - \rho(\text{calculated})$ between experimental and literature data and the fitted equation for the cyclohexanone and ★, 2-propanol; ▽, 2-butanol; ○, ref 19 for 2-butanol; ■, 2-pentanol; ●, 2-hexanol; ▲, 2-heptanol; at 298.15 K.

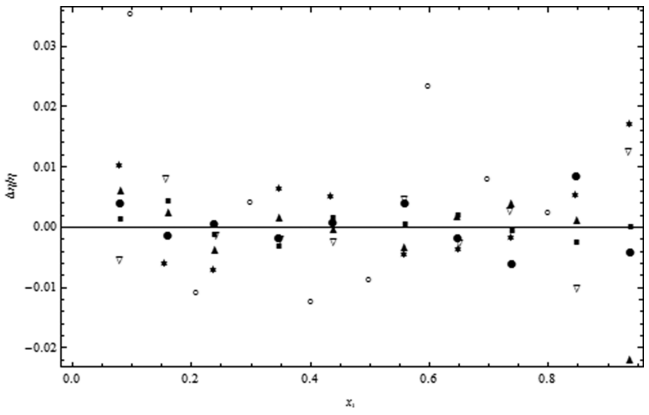

Figure 4. Differences $\Delta\eta = \eta(\text{experimental}) - \eta(\text{calculated})$ between experimental and literature data and the fitted equation for the cyclohexanone and ★, 2-propanol; ▽, 2-butanol; ○, ref 19 for 2-butanol; ■, 2-pentanol; ●, 2-hexanol; ▲, 2-heptanol; at 298.15 K.

CONCLUSION

Excess molar volumes and viscosity deviations for mixtures of cyclohexanone and 2-alkanols were obtained from experimental results and fitted by the Redlich−Kister type equation to derive the coefficients and estimate the standard error. For mixtures of cyclohexanone with used 2-alkanols, V_m^E is positive, and $\Delta\eta$ is negative over the entire range of mole fraction. It has been concluded that an increase in chain length of the 2-alkanol causes a greater deviation of the mixtures from ideal mixing behavior. The obtained excess quantities show that the alcohol chain length is a determining factor conditioning the excess thermodynamic properties of the binary mixtures.

ASSOCIATED CONTENT

Supporting Information

Excess molar volumes, partial molar volumes, and viscosity deviations for the mixtures of cyclohexanone and 2-alkanol. This material is available free of charge via the Internet at http://pubs.acs.org.

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