Thermodynamic Properties on Mixing for Hexane + Cyclohexane + 1-Octanol at 298.15 K

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Density, speed of sound, isentropic compressibility, and refractive index have been measured for the ternary mixture hexane + cyclohexane + 1-octanol at 298.15 K and at atmospheric pressure. From these data, excess molar volumes and excess isentropic compressibilities have been calculated. The results were fitted by means of different polynomial expressions. Several empirical methods for predicting ternary derived properties from binary data were tested. The Nitta−Chao group contribution model was applied to predict the excess molar volume for this mixture.

Introduction

In a previous paper,[1] experimental mixing properties were reported for the ternary mixture hexane + cyclohexane + 1-butanol at 298.15 K. Continuing our research on theoretical and experimental studies of thermophysical properties of nonelectrolite ternary mixtures containing alkane−cycloalkane−alkanol, in this paper, experimental measurements of density, refractive index, and speed of sound for the ternary mixture hexane + cyclohexane + 1-octanol at 298.15 K and atmospheric pressure are reported. The polynomial equation proposed by Redlich and Kister[2] was used to correlate experimental values for the binary mixtures. The equations proposed by Cibulka[3] and Nagata and Tamura[4] were applied to correlate the ternary contribution to the magnitudes. Ternary magnitudes were also correlated using two equations introduced in an earlier work.[5]

The measured values have also been used to test several empirical predictive methods compiled in Piñeiro et al.,[6] which are used to estimate multicomponent properties from the corresponding magnitude of the binary mixtures involved. The experimental excess molar volumes were compared with the predictions obtained using the Nitta et al.[7] group contribution model, based on the Carnahan and Starling[8] hard-sphere equation of state, and the model was found to describe, in a qualitative way, the variation of the magnitude of the excess molar volume with the length of alkanol chain.

Experimental Section

Substances employed were supplied by Merck. The mole fraction purities were better than 0.99 for hexane and 1-octanol and better than 0.995 for cyclohexane. Chemicals were kept in an argon (N-55) atmosphere, degassed ultrasonically, and dried on molecular sieves (Sigma, type 0.4 nm). Mixtures were prepared by mass using a Mettler AE-240 balance, with an accuracy of $\pm 10^{-4}$ g. Precautions were taken during sample preparation, such as weighing liquids in increasing order of volatility and reducing to a minimum the vapor space in the vessels, to avoid losses by evaporation during manipulation and possible errors in mole fraction calculations.

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Table 1. Comparison of Experimental Densities, ρ, Speeds of Sound, u, and Refractive Indices, n_D, with Literature Data for Pure Liquids at 298.15 K

	ρ (g cm^{-3})		u (m s^{-1})		n_D	
compound	expt	lit	expt	lit	expt	lit
cyclohexane	0.7738	0.77389[a]	1254.1	1254[c]	1.42359	1.42354[a]
		0.77378[b]		1254.4[d]		1.4235[e]
hexane	0.6553	0.65481[a]	1078.0	1077[h]	1.37242	1.37226[a]
		0.6552[f]		1077.7[i]		1.37236[j]
1-octanol	0.8215	0.8223[a]	1347.9	1348[h]	1.42765	1.4276[a]
		0.82159[g]				1.42747[h]

[a] Reference 9. [b] Reference 10. [c] Reference 11. [d] Reference 12. [e] Reference 13. [f] Reference 14. [g] Reference 15. [h] Reference 16. [i] Reference 17. [j] Reference 18.

Experimental values of density, speed of sound, and refractive index for the pure liquids at 298.15 K were compared with those found in the literature and were found to be in fairly good agreement, as shown in Table 1.

Density and speed of sound were measured at 298.15 K with an Anton Paar DSA-48 densimeter and sound analyzer, with a precision of $\pm(5 \times 10^{-5})$ g cm^{-3} and $\pm 10^{-1}$ m s^{-1}, respectively. Both measuring cells are thermostated with the same solid-state thermostat, with a temperature stability of $\pm 10^{-2}$ K. The refractive index was measured by an automatic refractometer ABBEMAT-HP Dr. Kernchen, with a precision of $\pm 10^{-5}$. The refractometer was thermostated with a Polyscience controller bath model 9510 with a temperature stability of $\pm 10^{-2}$ K. Apparatus calibration was performed periodically using ambient air and Millipore-quality water. Additional information about the experimental technique was provided in a previous work.[1]

Results and Discussion

Densities ρ, speeds of sound u, isentropic compressibilities κ_S [calculated by means of the Laplace equation ($\kappa_S = \rho^{-1}u^{-2}$)], and refractive indices n_D are listed in Tables 2−4 for the binary mixtures and in Table 5 for the ternary mixture. Excess magnitudes, excess molar volumes, V^E, and

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Table 2. Densities, ρ, Speeds of Sound, u, Isentropic Compressibilities, κ_S, Excess Molar Volumes, V^E, and Excess Isentropic Compressibilities, κ_S^E, at 298.15 K for Hexane (1) + 1-Octanol (2)

x_1	ρ / g cm^{-3}	u / m s^{-1}	κ_S / TPa^{-1}	V^E / cm^3 mol^{-1}	κ_S^E / TPa^{-1}
0.0541	0.8145	1334.3	690	−0.102	−14
0.0997	0.8084	1322.3	707	−0.170	−26
0.2019	0.7943	1294.4	751	−0.314	−47
0.3102	0.7784	1263.1	805	−0.396	−63
0.3460	0.7730	1252.4	825	−0.423	−67
0.4039	0.7640	1235.6	857	−0.445	−73
0.5016	0.7482	1207.2	917	−0.450	−77
0.6028	0.7310	1177.8	986	−0.414	−74
0.7069	0.7124	1148.8	1064	−0.335	−65
0.8065	0.6938	1121.6	1149	−0.239	−47
0.8539	0.6846	1109.5	1187	−0.175	−36
0.9030	0.6749	1097.4	1230	−0.108	−24
0.9498	0.6655	1086.1	1274	−0.049	−9

Table 3. Refractive Indices, n_D, at 298.15 K for Hexane (1) + 1-Octanol (2)

x_1	n_D
0.0984	1.42363
0.1950	1.41953
0.2987	1.41496
0.4080	1.40951
0.4525	1.40730
0.5068	1.40443
0.5543	1.40181
0.6057	1.39877
0.6581	1.39556
0.7051	1.39258
0.8067	1.38588
0.9070	1.37902

Table 4. Densities, ρ, Speeds of Sound, u, Isentropic Compressibilities, κ_S, Refractive indices, n_D, Excess Molar Volumes, V^E, and Excess Isentropic Compressibilities, κ_S^E, at 298.15 K for Cyclohexane (1) + 1-Octanol (2)

x_1	ρ / g cm^{-3}	u / m s^{-1}	κ_S / TPa^{-1}	n_D	V^E / cm^3 mol^{-1}	κ_S^E / TPa^{-1}
0.0474	0.8196	1342.3	677	1.42733	0.062	0
0.0944	0.8177	1336.3	685	1.42701	0.116	0
0.1962	0.8135	1323.8	701	1.42630	0.211	0
0.3009	0.8089	1310.5	720	1.42562	0.306	1
0.4013	0.8042	1297.6	738	1.42500	0.392	3
0.4984	0.7995	1285.7	757	1.42443	0.446	5
0.5495	0.7970	1279.5	766	1.42417	0.456	6
0.5988	0.7945	1274.0	775	1.42393	0.465	7
0.6528	0.7917	1267.8	786	1.42367	0.466	9
0.7052	0.7890	1262.3	795	1.42345	0.447	10
0.8035	0.7838	1254.9	810	1.42315	0.383	10
0.9032	0.7786	1250.1	822	1.42308	0.240	9
0.9523	0.7760	1249.8	825	1.42325	0.149	7

excess isentropic compressibilities, κ_S^E, were calculated using the following equation:

$$Q^E = Q - Q^{id} \quad (1)$$

where Q is either V/(cm^3 mol^{-1}) or κ_S/(TPa^{-1}). The molar volume for an ideal mixture was calculated using the expression

$$V^{id} = \sum_{i=1}^{n} x_i V_i = \sum_{i=1}^{n} x_i M_i / \rho_i \quad (2)$$

where x_i, M_i, and ρ_i represent the mole fraction, molar mass, and density, respectively, of component i in the mixture and n is the number of components in the mixture. The isentropic compressibility for an ideal mixture was

Table 5. Densities, ρ, Speeds of Sound, u, Isentropic Compressibilities, κ_S, Refractive Indices, n_D, Excess Molar Volumes, V^E, and Excess Isentropic Compressibilities, κ_S^E, at 298 .15 K for Hexane (1) + Cyclohexane (2) + 1-Octanol (3)

x_1	x_2	ρ / g cm^{-3}	u / m s^{-1}	κ_S / TPa^{-1}	n_D	V^E / cm^3 mol^{-1}	κ_S^E / TPa^{-1}
0.0481	0.0481	0.8133	1329.4	696	1.42530	−0.037	−12
0.0483	0.9042	0.7690	1238.2	848	1.42024	0.189	2
0.0986	0.0965	0.8042	1309.3	725	1.42269	−0.053	−24
0.0972	0.1985	0.7995	1296.4	744	1.42190	0.073	−22
0.0989	0.2996	0.7941	1282.4	766	1.42095	0.183	−19
0.0981	0.4009	0.7888	1269.2	787	1.42014	0.278	−16
0.0985	0.5009	0.7832	1256.6	809	1.41917	0.335	−12
0.0982	0.6067	0.7771	1244.8	830	1.41839	0.370	−8
0.0992	0.7052	0.7710	1235.3	850	1.41777	0.353	−5
0.0970	0.8063	0.7653	1229.4	864	1.41747	0.268	−3
0.2001	0.0977	0.7895	1280.9	772	1.41833	−0.172	−43
0.1998	0.1984	0.7840	1266.9	795	1.41718	−0.030	−40
0.2001	0.3009	0.7780	1252.5	819	1.41590	0.097	−35
0.1985	0.4001	0.7722	1239.9	842	1.41486	0.202	−29
0.1997	0.4988	0.7657	1227.6	867	1.41376	0.271	−24
0.1993	0.6043	0.7589	1216.9	890	1.41266	0.281	−19
0.1979	0.7031	0.7524	1209.4	909	1.41178	0.258	−14
0.3020	0.0997	0.7738	1250.8	826	1.41322	−0.235	−57
0.3025	0.1984	0.7676	1236.6	852	1.41179	−0.090	−51
0.3024	0.2998	0.7609	1222.6	879	1.41060	0.058	−44
0.3013	0.4039	0.7540	1209.7	906	1.40897	0.151	−36
0.2991	0.5030	0.7473	1199.5	930	1.40794	0.213	−29
0.3012	0.6009	0.7396	1190.4	954	1.40639	0.225	−23
0.4090	0.0968	0.7568	1219.8	888	1.40786	−0.278	−65
0.4065	0.1962	0.7502	1206.6	916	1.40619	−0.105	−57
0.4041	0.3006	0.7430	1193.4	945	1.40458	0.029	−47
0.4031	0.4008	0.7355	1182.1	973	1.40303	0.124	−38
0.4000	0.5025	0.7279	1173.2	998	1.40153	0.188	−29
0.5062	0.0959	0.7404	1191.7	951	1.40246	−0.270	−67
0.5044	0.1992	0.7327	1178.3	983	1.40040	−0.098	−56
0.5027	0.2989	0.7249	1166.4	1014	1.39855	0.038	−44
0.5018	0.4002	0.7165	1156.4	1044	1.39680	0.120	−33
0.6053	0.1014	0.7223	1163.0	1023	1.39660	−0.212	−61
0.6067	0.1985	0.7138	1150.4	1058	1.39417	−0.065	−48
0.6046	0.2998	0.7051	1140.2	1091	1.39199	0.064	−34
0.7042	0.1012	0.7039	1136.2	1101	1.39002	−0.147	−49
0.7042	0.1994	0.6947	1124.9	1137	1.38764	0.007	−32
0.8081	0.0966	0.6841	1110.0	1186	1.38325	−0.062	−28
0.9031	0.0490	0.6698	1092.4	1251	1.37792	−0.025	−13

evaluated using the expression suggested by Benson and Kiyohara[19] as follows:

$$\kappa_S^{id} = \sum_{i=1}^{n} \phi_i(\kappa_{S,i} + TV_i\alpha_i^2/C_{p,i}) - T(\sum_{i=1}^{n} x_i V_i)(\sum_{i=1}^{n} \phi_i\alpha_i)^2/\sum_{i=1}^{n} x_i C_{p,i} \quad (3)$$

In this equation, n is the number of components in the mixture; ϕ_i is the volume fraction of component i in the mixture, stated in terms of the unmixed compounds; x_i is the corresponding mole fraction; T is the temperature; and $\kappa_{s,i}$, $V_{m,i}$, α_i, and $C_{p,i}$ are the isentropic compressibility, molar volume, cubic expansion coefficient, and molar heat capacity, respectively, of component i. The values of α_i and $C_{p,i}$ were obtained from the literature.[20] From the κ_S data for the binary mixture hexane + cyclohexane reported in a previous work[1], excess isentropic compressibilities were calculated. These calculated values, V^E and κ_S^E, at 298.15 K are also reported in Tables 2−4 for the binary mixtures and in Table 5 for the ternary mixture.

Excess magnitudes of the binary systems were correlated using the Redlich and Kister[2] expression

$$Q_{ij}^E = x_i x_j \sum_{p=0}^{m} A_p(2x_i - 1)^p \quad (4)$$

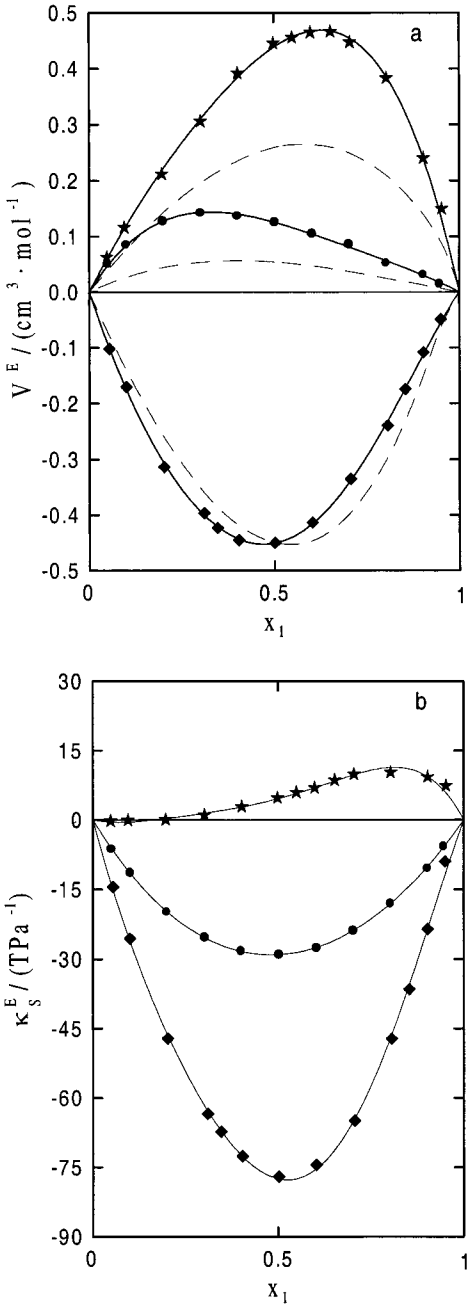

Figure 1. (a) V^E (cm^3 mol^{-1}) and (b) κ_S^E (TPa^{-1}) at 298.15 K for ●, hexane (1) + cyclohexane (2); ◆, hexane (1) + 1-octanol (2); ★, cyclohexane (1) + 1-octanol (2); —, eq 4; – –, Nitta–Chao model prediction.

where x_i and x_j are the mole fractions of the components and A_p represents the adjustable fitting parameters. An unweighted least-squares method was used to calculate these parameters. The number of parameters, m, was determined using the optimization F-test.[21] Figure 1 shows the experimental values of V^E and κ_S^E plotted against the molar fraction of the most volatile component of the binary mixture, as well as the corresponding Redlich–Kister fitting curves. In Figure 2, the experimental values of the excess molar volumes for the binary mixture hexane + 1-octanol are compared with the literature data.

The ternary mixture derived properties were correlated using the equation

$$Q^E_{123} = Q^E_{12} + Q^E_{13} + Q^E_{23} + x_1x_2x_3\Delta_{123} \qquad (5)$$

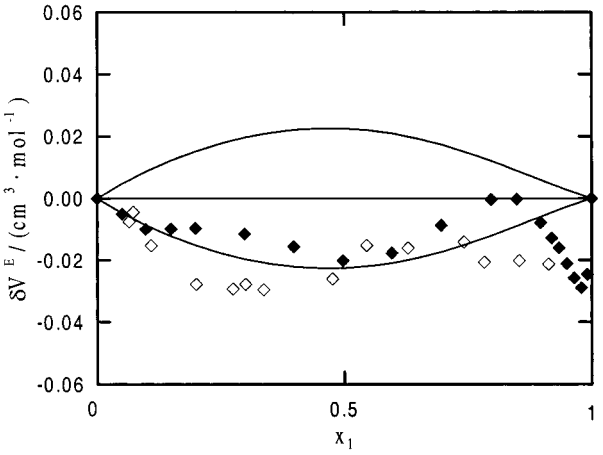

Figure 2. Deviations δV^E for hexane (1) + 1-octanol (2) at 298.15 K (experimental values are shown through the zero value line, and the plotted solid line represents a 5% deviation of V^E) and literature values from ◆, Heintz et al.;[15] ◇, Iglesias et al.[14]

Table 6. Parameters A_p and B_i of Equations 4 and 6, Respectively, and Standard Deviations s

	A_0	A_1	A_2	A_3	s
hexane (1) + cyclohexane (2)[a]					
V^E (cm^3 mol^{-1})	0.502	−0.368	0.208	–	0.003
κ_S^E (TPa^{-1})	−116.2	7.9	−8.0	–	0.1
hexane (1) + 1-octanol (2)					
V^E (cm^3 mol^{-1})	−1.803	0.254	0.285	0.258	0.005
κ_S^E (TPa^{-1})	−310	−35	46	77	1
cyclohexane (1) + 1-octanol (2)					
V^E (cm^3 mol^{-1})	1.755	0.875	0.433	-	0.008
κ_S^E (TPa^{-1})	18.4	41.8	50.1	43.2	0.7

	B_0	B_1	B_2	s
hexane (1) + cyclohexane (2) + 1-octanol (3)				
V^E (cm^3 mol^{-1})	−0.917	2.411	2.431	0.007
κ_S^E (TPa^{-1})	−192	403	405	1

[a] Reference 1.

where Q^E_{ij} is the binary contribution for each ij binary mixture; $x_3 = 1 - x_1 - x_2$; and $x_1x_2x_3\Delta_{123}$ is the ternary contribution, which was correlated using the expression suggested by Cibulka[3]

$$\Delta_{123} = B_0 + B_1x_1 + B_2x_2 \qquad (6)$$

and the one proposed by Nagata and Tamura.[4]

$$\frac{\Delta_{123}}{RT} = C_0 - C_1x_1 - C_2x_2 - C_3x_1^2 - C_4x_2^2 - C_5x_1x_2 - C_6x_1^3 - C_7x_2^3 - C_8x_1^2x_2 \qquad (7)$$

Ternary excess magnitudes have been also correlated using the following expressions introduced in an earlier work:[5]

$$Q^E_{123} = D_1x_1x_2 + D_2x_2x_3 + D_3x_3x_1 + D_4x_1^2x_2 + D_5x_2^2x_3 + D_6x_3^2x_1 \qquad (8)$$

$$Q^E_{123} = E_1x_1x_2 + E_2x_2x_3 + E_3x_3x_1 + E_4x_1^2x_2 + E_5x_2^2x_3 + E_6x_3^2x_1 + E_7x_1^3x_2 + E_8x_2^3x_3 + E_9x_3^3x_1 \qquad (9)$$

The parameters A_p and B_i of eqs 4 and 6 and corresponding standard deviations are given in Table 6. Table 7 presents a comparison among the standard deviations obtained with the different correlation equations applied.

Table 7. Comparison of the Standard Deviations, *s*, Obtained with Correlation Equations Applied

	s [V^E (cm^3 mol^{-1})]	s [κ_S^E (TPa^{-1})]
eq 6	0.007	1
eq 7	0.007	0.8
eq 8	0.02	1
eq 9	0.006	0.6

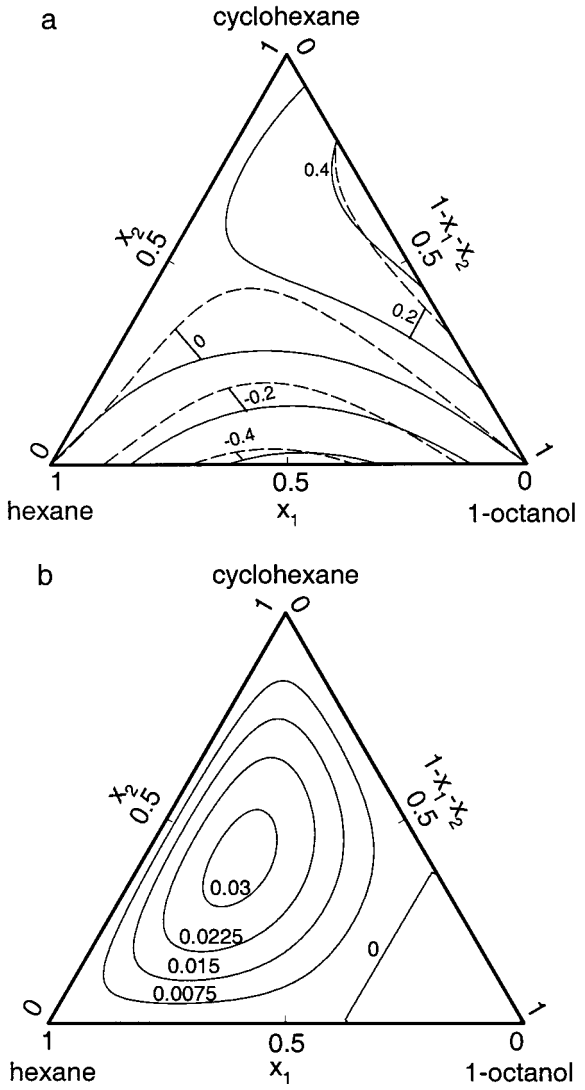

Figure 3. Isolines of (a) V^E(cm^3 mol^{-1}), (b) ternary contribution (cm^3 mol^{-1}) for hexane (1) + cyclohexane (2) + 1-octanol (3); —, eq 6; — —, Nitta–Chao model prediction.

Isolines of V^E and κ_S^E and their corresponding ternary contribution have been plotted in Figures 3 and 5, respectively. It can be seen in Figure 3a that the ternary mixture presents an isoline of ideal behavior. The maximum of the excess molar volume is located on the binary cyclohexane + 1-octanol, shifted to high cyclohexane concentration. The expansive region in the ternary diagram can probably be ascribed to the inefficient packing in the mixtures of these components as a result of their incompatible structures, cyclohexane with an arm-chair structure and hexane and 1-octanol flexible-chain structures. For the mixture hexane + 1-octanol, packing effects are more relevant than energetic effects, as excess enthalpies for this mixture show positive values (Brown et al.[22]) whereas excess molar volumes are negative. This may explain why ternary excess molar volumes present a contractive region close to the binary hexane + 1-octanol. Excess isentropic compressibilities show a trend similar to that of the excess molar volumes for hexane + 1-octanol and for cyclohexane + 1-octanol and an opposite to that of hexane + cyclohexane (Figure 1b). The ternary contributions to the magnitudes studied are negligible (Figures 3b and 5b), so three-body effects in the mixture can be neglected.

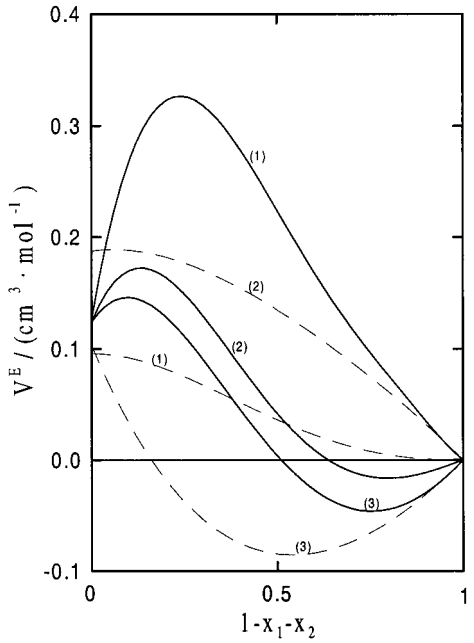

Figure 4. V^E (cm^3 mol^{-1}) at 298.15 K in a pseudobinary representation at equimolar concentration of hexane + cyclohexane, plotted against concentration of 1-octanol for (1) *n*-hexane + cyclohexane + 1-butanol (Mascato et al.[1]); (2) hexane + cyclohexane + 1-hexanol (Menaut et al.[10]); (3) hexane + cyclohexane + 1-octanol; — —, Nitta–Chao model prediction.

Estimation Methods

Several empirical equations compiled in Piñeiro et al.[6] have been applied to predict derived properties of ternary mixtures from the experimental data for the binaries involved. Lower deviations will be obtained for those excess magnitudes for which the ternary contribution is not as important (Figures 3b and 5b). These equations are asymmetric when the numerical predictions depend on the arbitrary designation of component numbering and symmetric in the opposite case. The equations of Kohler, Jacob–Fitzner, Colinet, and Knobeloch–Schwartz are symmetric, whereas those of Tsao–Smith, Toop, Scatchard, Mathieson–Thynne and Hillert are asymmetric. The root-mean-square deviations between experimental and estimated values are shown in Table 8, where both symmetric and asymmetric equations perform the same for both magnitudes. Moreover, the results obtained with asymmetric equations do not show a clear dependence on the ordering of the components in the mixture.

The group contribution model of Nitta et al.[7] was applied to predict the excess molar volumes, using the parameters calculated by Nitta et al.,[7] Koukios et al.,[23] Fernandez et al.,[24] and Piñeiro,[25] giving root-mean-square deviations of 0.06 cm^3 mol^{-1}, 0.04 cm^3 mol^{-1}, and 0.15 cm^3 mol^{-1} for the binaries hexane + cyclohexane, hexane + 1-octanol, and cyclohexane + 1-octanol, respectively, and 0.12 cm^3 mol^{-1} for the ternary mixture. Figures 1a and 3a display the experimental values for the binary and ternary mixtures, respectively, as well as the Nitta–Chao prediction. Figure 4, shows the excess molar volumes for the ternary mixtures

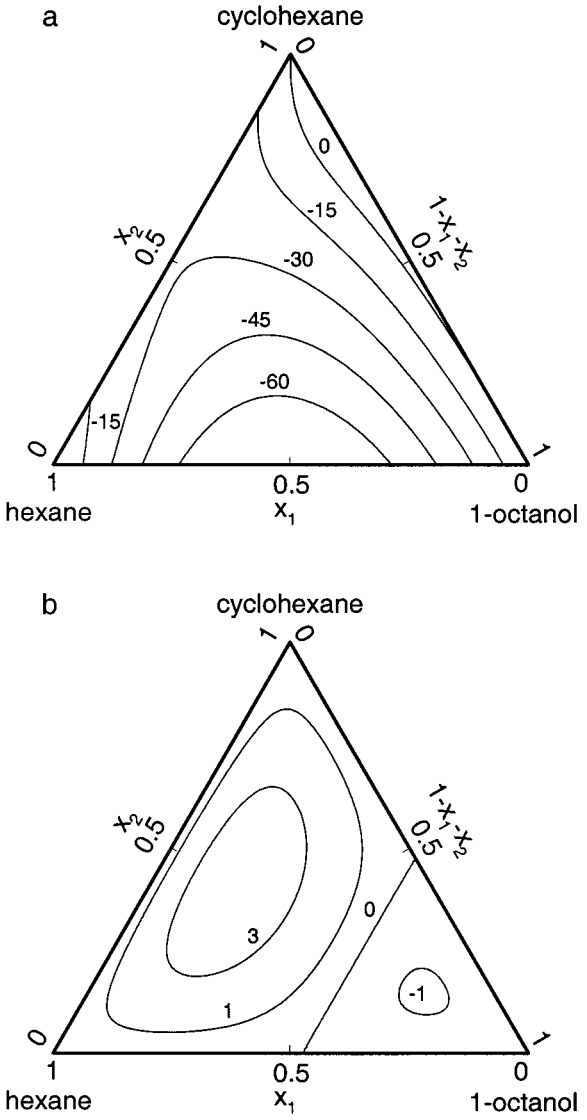

Figure 5. Isolines of (a) κ_S^E (TPa^{-1}), (b) ternary contribution (TPa^{-1}) for hexane (1) + cyclohexane (2) + 1-octanol (3); —, eq 6.

Table 8. Root-Mean-Square Deviations of Experimental Results from Prediction Results for Different Empirical Equations

	$\sigma[V^E/(\text{cm}^3\ \text{mol}^{-1})]$			$\sigma[\kappa_S^E/(\text{TPa}^{-1})]$		
Kohler		0.01			2	
Jacob−Fitzner		0.02			2	
Colinet		0.01			2	
Knobeloch−Schwartz		0.03			10	
Tsao−Smith	0.06[a]	0.1[b]	0.04[c]	1[a]	14[b]	5[c]
Toop	0.01[a]	0.04[b]	0.02[c]	2[a]	3[b]	1[c]
Scatchard	0.02[a]	0.04[b]	0.02[c]	2[a]	3[b]	1[c]
Mathieson−Thynne	0.02[a]	0.03[b]	0.01[c]	2[a]	3[b]	2[c]
Hillert	0.01[a]	0.04[b]	0.02[c]	2[a]	3[b]	1[c]

[a] Hexane is the asymmetric component in the equation. [b] Cyclohexane is the asymmetric component in the equation. [c] 1-Octanol is the asymmetric component in the equation.

(1) hexane + cyclohexane + 1-butanol (Mascato et al.[1]), (2) hexane + cyclohexane + 1-hexanol (Menaut et al.[10]), and (3) hexane + cyclohexane + 1-octanol in a pseudobinary representation at equimolar concentration of hexane + cyclohexane for the ternary mixture, together with Nitta−Chao prediction. The model predicts qualitatively the value of the magnitude and its variation with the length of the alkanol chain. For mixture 3, the model is able to predict the change in the sign of the excess molar volume, but as a whole, quantitative predictions are not as good as would be desirable. From this representation, information about the behavior of the excess molar volume when the length of the alcohol chain increases can be obtained. As can be seen in Figure 4, excess molar volume decreases with increasing the alcohol chain.

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