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Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory

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Ⓢ *Supporting Information*

ABSTRACT: The present study reports the densities and viscosities of mixing at various temperatures [(293.15 to 323.15) K] for mixtures composed of ethyl formate and 2-alkanols (from 2-propanol to 2-pentanol). From these measurements, excess molar volumes V_m^E and viscosity deviations $\Delta\eta$ were calculated. These results were fitted to Redlich−Kister type polynomials. Positive excess molar volumes and negative viscosity deviations for studied mixtures indicate that no strong specific interactions occur in the mixtures. The data of viscosities have been used to study the performance of two viscosity models. The evaluated models are friction theory and free volume theory. Overall two models can describe the fluid viscosity with good accuracy. Results show that the performance of friction theory for correlating the viscosities is more satisfactory.
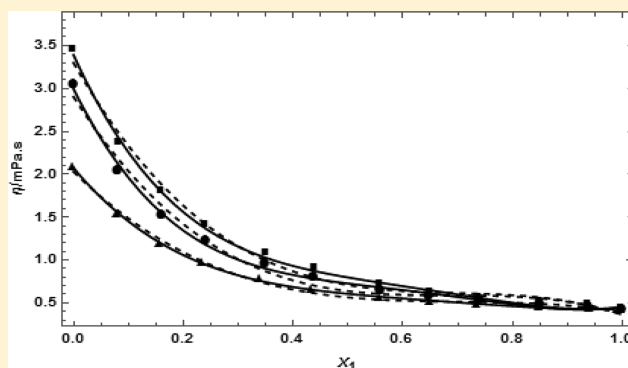
INTRODUCTION

Excess and deviation quantities are of great importance in the solution thermodynamics as they provide information about the molecular interactions and macroscopic behavior of fluid mixtures. Determination of these quantities can provide significant thermodynamic data for development and design of the chemical engineering process and also an help to clarify the structure of solutions. Alkyl formates are a group of esters whose behavior requires specific analysis because they form intermolecular associations by means of hydrogen bridges and may even exist as stable dimmers.[1] Nonaqueous organic electrolyte solutions play a major role in determining cell performance, operating temperature and shelf life of lithium batteries. Ethyl formate with properties such as low viscosity, low melting points, and high solubility is a suitable solvent for lithium salts. Mixed solvents containing these components show high conductivities and stability and possess excellent temperature performance.[2] Also ethyl formate is an important material in the manufacturing processes of flavor and fragrance industries. The most common mixed components with ethylformate in these processes are alcohols.[3] A survey in the scientific literature shows that few data have been published for the excess molar volumes and viscosity deviations of mixtures containing ethyl formate and 2-alkanols. Data available from the literature, concerning deviations from ideality for this kind of mixture, mainly deal with excess molar volumes of ethyl formate and 1-alkanols, excess enthalpy of ethyl formate +1-alkanols or 1-alkans, and excess enthalpy of ethyl formate with 1-alkanols and 2-alkanols.[4−6] Because of the properties of the HCOO group, it is of great interest to study the consequences of interactions between ethyl formate and 2-alkanols, which are strongly associated by hydrogen bridging. The goal of the present work is 2-fold: on one side, as a part of our systematic studies on the thermodynamic and transport properties of compounds composing the mixtures containing 2-alkanols,[7−9] we reported here the densities, viscosities, excess molar volumes, and viscosity deviations of mixing for the binary mixtures of ethyl formate + 2-alkanols at various temperatures. The obtained results will be used to analyze the effect of carbon chain length of alkanols on their interaction with the ester and also to see the influence of temperature upon the excess molar volumes and viscosity deviations. On the other side, we intend to apply the friction theory and free volume theory for the description of the viscosity of pure materials and binary mixtures. Mentioned theories provided satisfactory results for the modeling of the viscosities over the wide ranges of temperatures and pressures for binary systems containing water + 1-alkkanols, pure alkanes, *n*-alkane + *n*-alkane, and pure alcohols.[10−14]

EXPERIMENTAL SECTION

Ethyl formate, 2-propanol, 2-butanol, and 2-pentanol were supplied by Merck with the mass purity > 0.99, and used with no further purification. Reagents employed in present work are included in Table 1. In Table 2, we compared the measured densities and viscosities at *T* = 298.15 K with values available in the literature.[15,16]

Density and viscosity measurements of all the pure compounds and binary mixtures at different temperatures were

Table 1. Sample Description Table

chemical name	source	initial mass fraction purity
ethylformate	Merck	> 0.99
2-propanol	Merck	0.997
2-butanol	Merck	0.995
2-pentanol	Merck	0.995

Table 2. Densities, ρ, and Viscosities, η, of Pure Components at T = 298.15 K and P = 0.1 MPa

chemical name	$\rho/(\text{g·cm}^{-3})$		$\eta/(\text{mPa·s})$	
	exptl.	lit.	exptl.	lit.
ethyl formate	0.9101	0.91018[a]	0.38	0.41[b]
		0.91024[a]		0.39[b]
2-propanol	0.7811	0.78121[a]	2.08	2.05[b]
		0.7811[a]		2.047[b]
2-butanol	0.8027	0.80291[a]	3.04	2.99[b]
		0.8031[a]		3.117[b]
2-pentanol	0.8053	0.80514[a]	3.44	3.41[b]
		0.80542[a]		3.47[b]
		0.81019[a]		3.98[b]

[a]Reference 15. [b]Reference 16.

performed by using a fully automated SVM 3000 Anton-Paar rotational Stabinger viscometer. The viscometer is based on a modified Couette principle with a rapidly rotating outer tube and an inner measuring bob which rotates more slowly. Uncertainty for density measurements is $\pm\ 1\cdot10^{-4}$ g·cm^{-3} and for viscosity measurements is $\pm$ 0.01. The mixtures were prepared just before use by mass on an electronic balance (Mettler AE 163, Switzerland) accurate to 0.01 mg and kept in airtight stoppered glass bottles to avoid evaporation. Three to five sets of readings were taken for each sample. The maximum estimated uncertainty in the mole fractions is $1\cdot10^{-4}$.

■ RESULTS AND DISCUSSION

Densities and Excess Molar Volumes. Excess molar volumes, V_m^E were calculated from densities of pure liquids and mixtures by use of the following equation:

$$V_m^E = \sum_{i=1}^{N} x_i M_i (\rho^{-1} - \rho_i^{-1}) \tag{1}$$

where ρ_i is the density of pure component i, ρ is the density of the mixture, 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. Densities of binary mixtures decrease with increase of temperature. Also with increase of carbon chain length, values of densities are increased. Changes of densities with temperature for binary mixtures are graphically shown in the SI file. Moreover densities of ethyl formate + 2-propanol and 2-butanol at T = 298.15 K are compared with values of ref 17, and results are presented graphically in the SI file. Results are in good agreement. Standard uncertainty for excess molar volume is $\pm\ 1\cdot10^{-3}$ cm^3·mol^{-1}. Values of excess molar volumes are presented in SI, Table S1. Excess molar volumes for binary mixtures of ethyl formate + 2-alkanols at T = 298.15 K are shown in Figure 1. Values of densities are listed in Table 3. The V_m^E values have been fitted to the following type of Redlich−Kister polynomial[18]
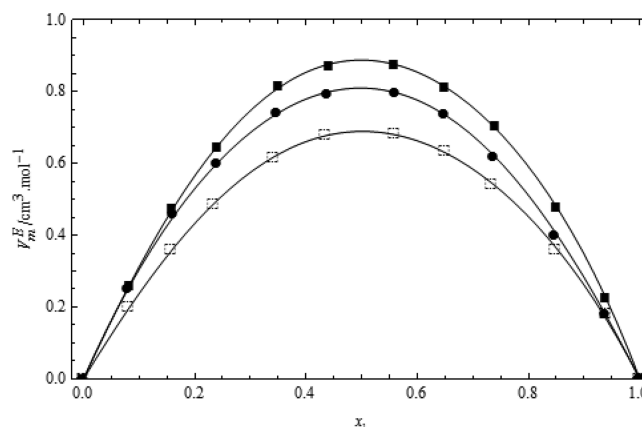

Figure 1. Excess molar volumes V_m^E vs mole fraction of ethyl formate for binary mixtures of ethyl formate with (□) 2-propanol, (●) 2-butanol, and (■) 2-pentanol at T = 298.15 K. Solid curves are Redlich−Kister equation.

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

where $Y^E \equiv V_m^E$ or $\Delta\eta$ and x_1 is the mole fraction of ethyl formate. Coefficients A_k were determined by the least-squares method. Standard deviations were obtained by this equation:

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

where Y and Y_{cal} are the experimental and calculated data respectively, n is the total number of experimental points, and p is the number of parameters of eq 2. Adjustable parameters of eq 2 are listed in Table S2 together with the standard deviations.

Excess molar volumes, V_m^E, is positive for all studied mixtures and increase with increase of alkanols chain length. The positive values of V_m^E indicate a preference of the dissociation of the homomolecular interactions (hydrogen bonds in alcohols and dipole−dipole interactions in both components) rather than volume contracting contributions due to the promotion of new heteromolecular interactions such as hydrogen bond between the C=O group of ethyl formate and OH group of 2-alkanol (C=O···H−O). Similar results for positive excess molar volumes and interacting forces in the mixtures of ethylformate and n-alkanols are reported elsewhere.[4] The rise of the V_m^E values with the molecular size of 2-alkanols may be closely connected with the increasing difficulty to produce heteromolecular interactions when the aliphatic chain of alcohol is increased. These results suggest the weak heteromolecular interactions. Increase of the temperature reduces the values of excess molar volumes.

Dynamic Viscosities. The viscosity deviation can be calculated as

$$\Delta\eta = \eta - x_1\eta_1 - x_2\eta_2 \tag{4}$$

where η is the viscosity of mixture and η_1 and η_2 are pure components viscosity. Viscosity deviations for the mixtures of ethyl formate +2-alkanols were fitted by Redlich−Kister polynomial and results at T = 298.15 K are presented in Figure 2. Values of viscosities and viscosity deviations are reported in Table 3 and SI, Table S1 respectively. Viscosities for binary mixtures increase with increase of chain length and decrease with rise of temperature. Plot of change of viscosities with

temperature for binary mixtures are shown in the SI file. The $\Delta\eta$ values for all binary systems are negative over the entire range of compositions and decrease in absolute value with increase of temperature. Also for all studied mixtures, $\Delta\eta$ increases in absolute value when the carbon chain length of 2-alkanols rises. Negative values of $\Delta\eta$ indicate that interactions

Table 3. Densities, ρ, and Viscosities, η, for the binary Mixtures at Various Temperatures and Pressure $p = 0.1$ MPa^{a}

			ethyl formate + 2-propanol				
			$\rho/(\text{g·cm}^{-3})$				
x_1	$T/K = 293.15$	$T/K = 298.15$	$T/K = 303.15$	$T/K = 308.15$	$T/K = 313.15$	$T/K = 318.15$	$T/K = 323.15$
0	0.7854	0.7811	0.7768	0.7724	0.7680	0.7634	0.7588
0.0814	0.7954	0.7907	0.7861	0.7814	0.7766	0.7718	0.7667
0.1589	0.8048	0.7999	0.7950	0.7901	0.7851	0.7801	0.7748
0.2351	0.8140	0.8088	0.8038	0.7988	0.7936	0.7883	0.7828
0.3413	0.8268	0.8215	0.8162	0.8110	0.8057	0.8000	0.7944
0.4351	0.8383	0.8328	0.8274	0.8220	0.8165	0.8105	0.8048
0.5587	0.8539	0.8482	0.8425	0.8368	0.8311	0.8247	0.8186
0.6507	0.8657	0.8599	0.8540	0.8480	0.8421	0.8354	0.8292
0.7349	0.8771	0.8710	0.8650	0.8586	0.8524	0.8456	0.8391
0.8498	0.8935	0.8872	0.8808	0.8741	0.8676	0.8604	0.8538
0.9394	0.9071	0.9006	0.8940	0.8873	0.8808	0.8735	0.8667
1	0.9166	0.9101	0.9036	0.8971	0.8905	0.8830	0.8760
			$\eta/(\text{mPa·s})$				
0	2.42	2.08	1.80	1.56	1.36	1.19	1.05
0.0814	1.77	1.53	1.35	1.19	1.05	0.92	0.81
0.1589	1.33	1.18	1.06	0.95	0.85	0.75	0.67
0.2351	1.06	0.95	0.87	0.79	0.71	0.64	0.57
0.3413	0.82	0.76	0.70	0.65	0.59	0.54	0.49
0.4351	0.68	0.64	0.59	0.56	0.52	0.48	0.44
0.5587	0.57	0.54	0.51	0.48	0.45	0.42	0.38
0.6507	0.52	0.49	0.46	0.44	0.41	0.39	0.36
0.7349	0.48	0.46	0.43	0.41	0.39	0.36	0.33
0.8498	0.44	0.42	0.40	0.38	0.36	0.34	0.31
0.9394	0.42	0.40	0.38	0.36	0.34	0.32	0.30
1	0.402	0.38	0.36	0.345	0.328	0.31	0.29
			ethyl formate + 2-butanol				
			$\rho/(\text{g·cm}^{-3})$				
x_1	$T/K = 293.15$	$T/K = 298.15$	$T/K = 303.15$	$T/K = 308.15$	$T/K = 313.15$	$T/K = 318.15$	$T/K = 323.15$
0	0.8067	0.8027	0.7984	0.7941	0.7898	0.7852	0.7806
0.0818	0.8130	0.8088	0.8042	0.7996	0.7951	0.7903	0.7854
0.1617	0.8195	0.8149	0.8102	0.8055	0.8007	0.7957	0.7906
0.2415	0.8263	0.8215	0.8166	0.8118	0.8068	0.8015	0.7963
0.3497	0.8362	0.8311	0.8261	0.8209	0.8158	0.8102	0.8048
0.4398	0.8452	0.8399	0.8346	0.8293	0.8240	0.8181	0.8125
0.5611	0.8582	0.8527	0.8471	0.8415	0.8359	0.8297	0.8238
0.6500	0.8685	0.8628	0.8571	0.8513	0.8454	0.8390	0.8328
0.7399	0.8798	0.8738	0.8679	0.8620	0.8559	0.8492	0.8429
0.8500	0.8946	0.8884	0.8822	0.8760	0.8698	0.8628	0.8562
0.9396	0.9075	0.9012	0.8948	0.8883	0.8818	0.8745	0.8679
1	0.9166	0.9101	0.9036	0.8971	0.8905	0.8830	0.8760
			$\eta/(\text{mPa·s})$				
0	3.67	3.04	2.54	2.13	1.80	1.54	1.33
0.0818	2.41	2.03	1.74	1.50	1.30	1.13	1.00
0.1617	1.74	1.51	1.32	1.17	1.02	0.90	0.82
0.2415	1.35	1.20	1.07	0.96	0.85	0.77	0.72
0.3497	1.04	0.94	0.84	0.77	0.71	0.65	0.61
0.4398	0.86	0.78	0.71	0.66	0.61	0.57	0.55
0.5611	0.69	0.62	0.58	0.55	0.51	0.48	0.47
0.6500	0.59	0.55	0.51	0.49	0.46	0.43	0.42
0.7399	0.53	0.50	0.47	0.45	0.42	0.39	0.38
0.8500	0.48	0.45	0.43	0.41	0.39	0.36	0.35
0.9396	0.44	0.42	0.40	0.38	0.36	0.34	0.32
1	0.402	0.38	0.36	0.345	0.328	0.31	0.29

C

Table 3. continued

	ethyl formate + 2-pentanol						
	$\rho/(\text{g·cm}^{-3})$						
x_1	$T/\text{K} = 293.15$	$T/\text{K} = 298.15$	$T/\text{K} = 303.15$	$T/\text{K} = 308.15$	$T/\text{K} = 313.15$	$T/\text{K} = 318.15$	$T/\text{K} = 323.15$
0	0.8093	0.8053	0.8012	0.7970	0.7927	0.7884	0.7840
0.0826	0.8144	0.8103	0.8060	0.8017	0.7973	0.7929	0.7883
0.1603	0.8196	0.8154	0.8110	0.8065	0.8020	0.7974	0.7926
0.2396	0.8254	0.8210	0.8165	0.8118	0.8072	0.8023	0.7973
0.3504	0.8345	0.8297	0.8250	0.8200	0.8152	0.8099	0.8047
0.4402	0.8426	0.8376	0.8326	0.8275	0.8224	0.8169	0.8114
0.5595	0.8547	0.8494	0.8440	0.8387	0.8332	0.8273	0.8215
0.6497	0.8650	0.8594	0.8537	0.8481	0.8424	0.8362	0.8302
0.7400	0.8764	0.8704	0.8646	0.8587	0.8529	0.8462	0.8399
0.8501	0.8920	0.8857	0.8796	0.8734	0.8672	0.8602	0.8536
0.9381	0.9060	0.8994	0.8930	0.8867	0.8802	0.8728	0.8660
1	0.9166	0.9101	0.9036	0.8971	0.8905	0.8830	0.8760
	$\eta/(\text{mPa·s})$						
0	3.97	3.44	2.94	2.48	2.04	1.65	1.29
0.0826	2.84	2.50	2.20	1.90	1.60	1.32	1.06
0.1603	2.16	1.96	1.74	1.53	1.30	1.06	0.84
0.2396	1.73	1.57	1.40	1.23	1.05	0.89	0.70
0.3504	1.34	1.23	1.11	0.98	0.86	0.73	0.59
0.4402	1.12	1.02	0.93	0.84	0.75	0.64	0.53
0.5595	0.91	0.85	0.77	0.70	0.63	0.54	0.45
0.6497	0.78	0.73	0.67	0.60	0.54	0.47	0.40
0.7400	0.65	0.60	0.57	0.52	0.46	0.41	0.36
0.8501	0.52	0.49	0.46	0.43	0.40	0.36	0.33
0.9381	0.45	0.43	0.41	0.39	0.36	0.33	0.31
1	0.402	0.38	0.36	0.345	0.328	0.31	0.29

[a]x_1 is the mole fraction of ethyl formate in the (ethyl formate + 2-alkanol) solutions. Standard uncertainties u are $u(T) = 0.01$ K, $u(x) = 0.0001$, $u(p) = 10$ kPa, the combined expanded uncertainty $U_c(\rho) = 2\cdot10^{-4}$ g·cm^{-3} (0.95 level of confidence) and for viscosity the relative combined expanded uncertainty $U_r(\eta) = 0.02$ (0.95 level of confidence).
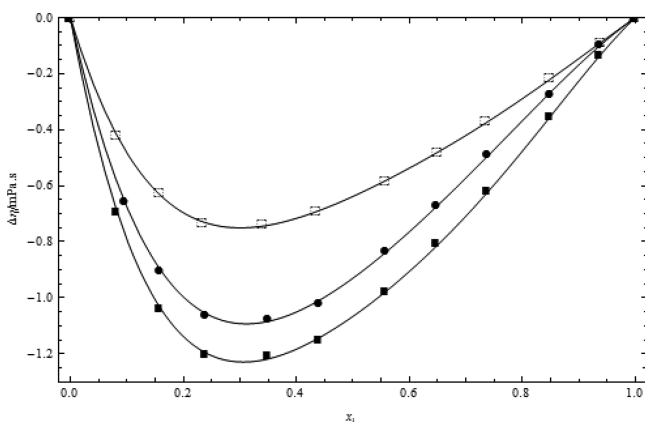

Figure 2. Viscosity deviations $\Delta\eta$ vs mole fraction of ethyl formate for binary mixtures of ethyl formate with (□) 2-propanol, (●) 2-butanol, and (■) 2-pentanol at $T = 298.15$ K. Solid curves are the Redlich–Kister equation.

are weak and dispersion forces are dominant. It is notable that positive excess molar volumes for studied mixtures, which are in good agreement with the negative viscosity deviations, indicate that no strong specific interactions occur in the mixtures.

Friction Theory. In this work, the friction theory[12] coupled with the Peng–Robinson–Stryjek–Vera[19] equation of state (PRSV EOS) has been extended to evaluate the viscosities of pure materials and binary mixtures. In the friction theory total

viscosity η is separated in two terms; a dilute gas viscosity term η_0 and a term arising from the friction between layers η_f

$$\eta = \eta_0 + \eta_f \tag{5}$$

The dilute gas viscosity η_0 is defined as the viscosity at the zero density limits, while the other term η_f can be expressed as follows:

$$\eta_f = \kappa_r p_r + \kappa_a p_a + \kappa_{rr} p_r^2 \tag{6}$$

where κ_a, κ_r, and κ_{rr} are the temperature dependent friction coefficients and p_a and p_r are the van der Waals attractive and repulsive pressure terms of the fluid. In this work PRSV EOS was used to calculate the viscosities of pure alcohols and ethyl formate. The entire EOS required parameters are taken from the Reference.[20] The dilute gas viscosity is calculated by proposed model of Chung et al.[21] and is given by

$$\eta_0 = 40.785 \frac{\sqrt{M_W T}}{v_c^{2/3}\Omega^*}F_c \tag{7}$$

where T is the absolute temperature, v_c is the critical volume, M_w is the molecular weight, and Ω^* is the reduced collision integral. Empirical expression for the F_c factor is defined as

$$F_c = 1 - 0.275\omega + 0.059035\mu_r^4 + \chi \tag{8}$$

where ω is the acentric factor, χ is a correction factor for the influence of hydrogen bonds, and μ_r is the dipole moment in Debye.

Regarding the temperature dependency of the friction constants, an exponential dependency of the following form was applied:[22]

$$\kappa_r = (a_1 \exp(\Gamma - 1) + a_2(\exp(2(\Gamma - 1)) - 1)$$
$$+ a_3(\exp(3(\Gamma - 1)) - 1))/P_c$$

$$\kappa_r = (b_1 \exp(\Gamma - 1) + b_2(\exp(2(\Gamma - 1)) - 1)$$
$$+ b_3(\exp(3(\Gamma - 1)) - 1))/P_c$$

$$\kappa_r = (c_4(\exp(4\Gamma) - 1)/P_c^2 \tag{9}$$

where

$$\Gamma = \frac{T_c}{T} \tag{10}$$

T_c is the critical temperature. Thus, for each pure substance, the corresponding model consists of seven adjustable parameters. Adjustable parameters in eq 9 have been estimated by a least-squares fit for the PRSV f-theory model and the results are given in Table S3 along with the obtained overall AAD (absolute average deviation).

For mixtures the dilute gas limit mixture contribution can be calculated using the following mixing rule:

$$\eta_0 = \exp\left[\sum_{i=1}^{n} x_i \ln(\eta_{0,i})\right] \tag{11}$$

where x_i is the mole fraction of compound "i" in the mixture. The mixing rules for the friction coefficients are given by

$$\kappa_r = \sum_{i=1}^{n} z_i \kappa_{r,i} \tag{12}$$

$$\kappa_a = \sum_{i=1}^{n} z_i \kappa_{a,i} \tag{13}$$

$$\kappa_{rr} = \sum_{i=1}^{n} z_i \kappa_{rr,i} \tag{14}$$

For the friction coefficients mixing rules, a mass weighted fraction z_i is estimated using the relation

$$z_i = \frac{x_i}{M_i^{\varepsilon} \hat{M}} \tag{15}$$

$$\hat{M} = \sum_{i=1}^{n} \frac{x_i}{M_i^{\varepsilon}} \tag{16}$$

where M_i is the molar mass of compound i, n is the number of components, and ε is an adjustable parameter to enhance the accuracy of the results. For the studied systems the best results were obtained by using $\varepsilon = 0.064$. In the PRSV EOS the regular van der Waals mixing rules have been used with a binary interaction parameter $\kappa_{ij} = 0.048$ optimized against the viscosity data. PRSV equation yields an accurate representation of viscosity data that are within the uncertainty error. Also previously have been reported[7,8] that this model can reproduce the viscosities of pure materials and binary mixtures successfully. It should be stressed that a successful viscosity modeling scheme requires that the used EOS is capable of describing the right phase behavior for the studied mixtures.

Free Volume Theory. Free volume theory[10,11] expresses the viscosity of a system as a sum of two contributions; dilute gas term η_0 and a dense-state correction term $\Delta\eta$

$$\eta = \eta_0 + \Delta\eta \tag{17}$$

The dilute gas term is similar to friction theory and calculated by eqs 7 and 8. The dense-state term is calculated using a generalized dumbbell model

$$\Delta\eta = 10^{-14} \rho N_a \zeta L^2 \tag{18}$$

where ρ is the density, N_a is Avogadro's number, and ζ is the friction coefficient. From the other side, the viscosity is dependent on free spaces among the molecules defined as a free volume fraction f_V through an exponential relation[23]

$$\Delta\eta = A \exp\left(\frac{B}{f_V}\right) \tag{19}$$

The combination of eqs 18 and 19 leads to the following equation:

$$\Delta\eta = 10^{-14} \rho N_a \zeta_0 \exp\left(\frac{B}{f_V}\right) \tag{20}$$

ζ_0 is a friction coefficient related to the diffusion process and the mobility of the molecule, L^2 is an average quadratic length related to the size of the molecule, and B is a parameter related to the free-volume overlap among the molecules.[24] The ζ_0 friction coefficient is related to the energy of dissipation E by the expression

$$\zeta_0 = 10^{10} \frac{E}{N_a b_f} \left(\frac{10^{-3} M_W}{3RT}\right)^{0.5} \tag{21}$$

where b_f is the dissipation length of the energy E. Combination of eqs 19 to 21 provides a final expression that reads

$$\Delta\eta = L_V(0.1P + 10^{-4}\alpha\rho^2 M_W)$$
$$\times \sqrt{\frac{10^{-3} M_W}{3RT}} \exp\left[B\left(\frac{10^3 P + \alpha\rho^2 M_W}{\rho RT}\right)^{1.5}\right] \tag{22}$$

or in an equivalent condensed free-volume-dependent expression

$$\Delta\eta = 10^{-4} \rho L_V \sqrt{\frac{10^{-3} RT M_W}{3}} f_V^{-2/3} \exp\left[\frac{B}{f_V}\right] \tag{23}$$

The approach includes three adjustable parameters related to the structural and energetic properties of the fluid: L_V, α, and B. The extension to mixtures depends on the evaluation of these three parameters for mixtures. In the present study a linear compositional mixing rule for the three viscosity parameters was applied.

$$Y_{mix} = \sum_{i=1}^{n} Y_i x_i \tag{24}$$

It is important to notice that no binary adjustable parameters are used for the viscosity treatment of mixtures. Adjustable parameters of pure materials are listed in SI, Table S4 along with AAD. For 2-alkanols the barrier energy parameter α increases with the molecular weight. Conversely, the B

parameter decreases with the molecular weight. Finally the L_v parameter also decreases, with increase of molecular weight. Correlated viscosities by this model are satisfactory and maximum obtained AAD is 4 %. Comparison of results of free volume theory and friction model reveals that viscosity values obtained by the friction theory are more precise. This may be due to the fact that regressed parameters of this theory from experimental data are more than free volume theory and also the free volume theory has not the binary adjustable parameters for mixtures. Comparison of viscosities of two model at T = 298.15 K are shown in Figure 3.
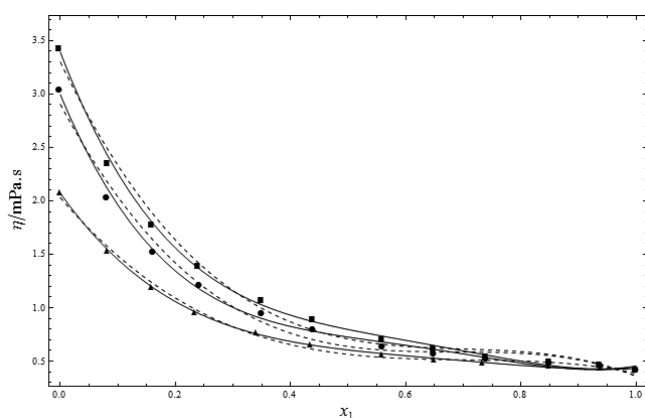

Figure 3. Experimental and calculated viscosities of ethyl formate with (◤) 2-propanol, (●) 2-butanol, and (■) 2-pentanol at T = 298.15 K. (—) Friction theory, (----) free volume theory.

CONCLUSIONS

This paper reports the densities and viscosities for binary mixtures of ethyl formate and 2-alkanols. Excess molar volumes and viscosity deviations were calculated from experimental data. Excess molar volumes are positive and viscosity deviations are negative over the whole composition range. This behavior is representative of systems where dispersion forces are predominant and do not take place in the formation of strong heteromolecular complexes. Free volume theory and friction theory have been applied for calculation of transport properties of pure materials and binary mixtures. The mentioned models give good agreement over the whole temperature range of interest. However, the power of the free volume theory to reproduce the viscosities is weaker than friction theory.

ASSOCIATED CONTENT

ⓢ Supporting Information

Excess molar volumes, viscosity deviations, and other useful data for the present paper. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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