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Thermophysical Properties of Mixtures of Tetrahydropyran with Chlorobutanes

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Densities and absolute viscosities for the binary mixtures containing tetrahydropyran and isomeric chlorobutanes have been determined at 298.15 and 313.15 K at atmospheric pressure. From the densities, excess molar volumes were calculated. On the other hand, excess volumes and absolute viscosities have been correlated using the Peng–Robinson–Stryjek–Vera (PRSV) equation of state and the Lee model, respectively.

KEY WORDS: cubic equation of state; density; excess volume; isomeric chlorobutanes; tetrahydropyran; viscosity.

1. INTRODUCTION

Here, we report the volumetric and viscosity behavior of liquid mixtures containing tetrahydropyran and isomeric chlorobutanes (1-chlorobutane, 2-chlorobutane, 2-methyl-1-chloropropane or 2-methyl-2-chloropropane) at 298.15 and 313.15 K. This work follows our study of liquid mixtures containing cyclic ethers (2-methyl-tetrahydrofuran, 1,3-dioxolane, 1,4-dioxane) and chloroalkanes [1–7]; the behavior of these kinds of mixtures is mainly influenced by the existence of a Cl-O specific interaction.

On the other hand, we have tested the reliability of cubic equations of state together with suitable mixing rules to correlate thermophysical properties of mixtures [8, 9]. We have employed the Peng–Robinson–Stryjek–Vera (PRSV) equation [10, 11] together with some classical two-parameter mixing rules to correlate the excess volumes and the Lee model [12] that combines Eyring's viscosity model with cubic equation of states to correlate the viscosities.

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2. EXPERIMENTAL

The liquids used were 1-chlorobutane, 2-methyl-2-chloropropane, and 2-chlorobutane (better than 99%) provided by Aldrich, 2-methyl-1-chloropropane (better than 99%) obtained from Fluka, and tetrahydropyran (better than 99%) obtained from Acros. No additional purification has been carried out. The physical properties of the components, density and viscosity, appear together with literature values [13–16] in Table I.

Densities, ρ, were measured using an Anton Paar DMA-58 vibrating tube densimeter internally thermostated within ±0.01 K. The apparatus was calibrated with deionized doubly-distilled water and dry air. The precision of the density measurements is $\pm 5 \times 10^{-6}\ \text{g}\cdot\text{cm}^{-3}$, and the uncertainty of these measurements after proper calibration is $\pm 1 \times 10^{-3}\ \text{g}\cdot\text{cm}^{-3}$.

Kinematic viscosities, ν, were determined using an Ubbelohde viscometer with a Schoot-Geräte automatic measuring unit model AVS-440. The temperature was kept constant within ±0.01 K by means of a Schoot-Geräte thermostat. The viscometer was calibrated with deionized doubly distilled water. The uncertainty of the time flow measurements was ±0.01 s, and the corresponding uncertainty in the kinematic viscosity was $\pm 1 \times 10^{-4}\ \text{mm}^2\cdot\text{s}^{-1}$. Kinetic energy corrections were applied to the experimental data. From the density and kinematic viscosity, the absolute viscosity, η, can be obtained: $\eta = \rho\nu$; the estimated uncertainty in the absolute viscosity was $\pm 1 \times 10^{-4}$ mPa·s.

3. RESULTS AND DISCUSSION

Excess volumes, V^{E}, were calculated from the density of the mixture, ρ, densities, ρ_{i}, and molar masses, M_{i}, of the pure components, and the corresponding molar fractions, x_{i}, by using the following equation:

Table I. Densities, ρ, and Absolute Viscosities, η, of Pure Components at 298.15 K and Comparison with Literature Data

	ρ (g·cm^{-3})		η (mPa·s)	
Compound	Exptl.	Lit.	Exptl.	Lit.
Tetrahydropyran	0.87881	0.87916 [13]	0.7997	0.764 [15]
1-Chlorobutane	0.88069	0.88095 [14]	0.4212	0.427 [16]
2-Chlorobutane	0.86737	0.8671 [14]	0.3938	
2-Methyl-1-chloropropane	0.87113	0.8719 [14]	0.4295	0.431 [16]
2-Methyl-2-chloropropane	0.83645	0.8361 [14]	0.4751	

$$V^E = x_1\left(\frac{M_1}{\rho}-\frac{M_1}{\rho_1}\right)+x_2\left(\frac{M_2}{\rho}-\frac{M_2}{\rho_2}\right). \tag{1}$$

The measured densities and calculated excess volumes are given in Table II; excess molar volumes are also graphically represented in Figs. 1 and 2. The measured kinematic viscosities, ν, and absolute viscosities, η, are given in Table III; absolute viscosities are represented in Figs. 3 and 4.

The excess molar volumes are negative over the whole composition range, and they became more negative when the temperature increases; this effect is more marked for the tetrahydropyran + 1-chlorobutane mixture. The volumetric behavior of the mixtures containing 2-chlorobutane and 2-methyl-1-chloropropane is very similar. V^{E} values for these mixtures are intermediate between those determined for the mixtures tetrahydropyran + 1-chlorobutane and tetrahydropyran + 2-methyl-2-chloropropane, where the V^{E} values for the latter mixtures are the largest ones in absolute value.

The results obtained, that is, negative V^{E} values reflect the existence of a specific interaction among the mixed molecules that is established between the lone pair of electrons of the oxygen atom in the cyclic ether and the chlorine atom of chlorobutanes.

4. CEOS CORRELATION

We have chosen the PRSV cubic equation of state to correlate excess volumes.

$$P = \frac{RT}{\overline{V}-b} - \frac{a(T)}{\overline{V}\left(\overline{V}+b\right)+b\left(\overline{V}-b\right)}, \tag{2}$$

where P, T, and $\overline{V}$ denote the pressure, temperature, and molar volume, respectively, and R is the universal gas constant.

For pure component i, the parameter a, copressure parameter, and parameter b, covolume parameter, are given by the following equations:

$$a_i(T) = 0.457235\frac{(RT_{\mathrm{c}i})^2}{P_{\mathrm{c}i}}\left[1+m_i\left(1-T_{\mathrm{r}i}^{1/2}\right)\right]^2 \tag{3}$$

$$m_i = k_{\mathrm{o}i} + k_{1i}\left(1-T_{\mathrm{r}i}^{1/2}\right)(0.7-T_{\mathrm{r}i}) \tag{4}$$

$$k_{\mathrm{o}i} = 0.378893 + 1.4897153\omega_i - 0.1713848\omega_i^2 + 0.0196554\omega_i^3 \tag{5}$$

Table II. Densities, ρ, and Excess Molar Volumes, V^E, of Tetrahydropyran (1) + Isomeric Chlorobutanes (2)

x_1	ρ (g·cm^{-3})	V^E (cm^3·mol^{-1})	x_1	ρ (g·cm^{-3})	V^E (cm^3·mol^{-1})
Tetrahydropyran (1) + 1-chlorobutane (2) at 298.15 K					
0.0000	0.88069		0.5948	0.88006	−0.052
0.0521	0.88067	−0.009	0.6610	0.87987	−0.045
0.1006	0.88066	−0.017	0.7893	0.87949	−0.030
0.1949	0.88062	−0.033	0.9203	0.87907	−0.011
0.2549	0.88059	−0.042	0.9666	0.87891	−0.004
0.3774	0.88048	−0.055	1.0000	0.87881	
0.5035	0.88026	−0.056			
Tetrahydropyran (1) + 2-chlorobutane (2) at 298.15 K					
0.0000	0.86737		0.5971	0.87542	−0.167
0.0453	0.86805	−0.021	0.7181	0.87672	−0.152
0.1136	0.86906	−0.056	0.7924	0.87746	−0.135
0.1929	0.87026	−0.097	0.8967	0.87836	−0.093
0.3014	0.87180	−0.139	0.9249	0.87855	−0.075
0.3888	0.87295	−0.159	1.0000	0.87881	
0.4968	0.87428	−0.170			
Tetrahydropyran (1) + 2-methyl-1-chloropropane (2) at 298.15 K					
0.0000	0.87113		0.6273	0.87723	−0.165
0.0480	0.87169	−0.027	0.6897	0.87763	−0.153
0.1084	0.87239	−0.059	0.8111	0.87826	−0.113
0.2120	0.87353	−0.104	0.9088	0.87868	−0.070
0.2900	0.87438	−0.136	0.9520	0.87879	−0.042
0.3951	0.87537	−0.159	1.0000	0.87881	
0.5062	0.87630	−0.167			
Tetrahydropyran (1) + 2-methyl-2-chloropropane (2) at 298.15 K					
0.0000	0.83645		0.6107	0.86498	−0.464
0.0324	0.83808	−0.054	0.6483	0.86646	−0.443
0.1086	0.84207	−0.194	0.8093	0.87239	−0.286
0.2097	0.84711	−0.331	0.8606	0.87422	−0.224
0.2891	0.85105	−0.426	0.9540	0.87725	−0.071
0.4276	0.85741	−0.502	1.0000	0.87881	
0.4960	0.86032	−0.503			
Tetrahydropyran (1) + 1-chlorobutane (2) at 313.15 K					
0.0000	0.86382		0.6026	0.86459	−0.102
0.0348	0.86398	−0.020	0.7085	0.86452	−0.095
0.0899	0.86419	−0.047	0.8006	0.86445	−0.088
0.1717	0.86439	−0.073	0.8990	0.86422	−0.062
0.2933	0.86454	−0.093	0.9724	0.86388	−0.024
0.4130	0.86460	−0.101	1.0000	0.86367	
0.4926	0.86461	−0.103			
0.0000	0.85013		0.5947	0.85958	−0.203
0.0525	0.85111	−0.042	0.7116	0.86103	−0.180
0.1035	0.85202	−0.075	0.8090	0.86210	−0.142
0.1947	0.85359	−0.126	0.8917	0.86290	−0.095

Table II. (*Continued*)

x_1	ρ (g·cm^{-3})	V^E (cm^3·mol^{-1})	x_1	ρ (g·cm^{-3})	V^E (cm^3·mol^{-1})
Tetrahydropyran (1) + 2-chlorobutane (2) at 313.15 K					
0.3042	0.85540	−0.173	0.9599	0.86345	−0.043
0.4091	0.85700	−0.198	1.0000	0.86367	
0.5025	0.85835	−0.208			
Tetrahydropyran (1) + 2-methyl-1-chloropropane (2) at 313.15 K					
0.0000	0.85351		0.6079	0.86119	−0.205
0.0432	0.85417	−0.032	0.7238	0.86224	−0.184
0.0934	0.85493	−0.068	0.7895	0.86278	−0.164
0.1923	0.85635	−0.127	0.8874	0.86342	−0.115
0.3025	0.85783	−0.176	0.9463	0.86368	−0.070
0.4060	0.85908	−0.201	1.0000	0.86367	
0.5018	0.86014	−0.211			
Tetrahydropyran (1) + 2-methyl-2-chloropropane (2) at 313.15 K					
0.0000	0.81831		0.6093	0.84916	−0.567
0.0584	0.82170	−0.142	0.7052	0.85315	−0.495
0.0875	0.82335	−0.205	0.7988	0.85689	−0.394
0.1943	0.82915	−0.385	0.9097	0.86095	−0.219
0.3028	0.83483	−0.518	0.9614	0.86264	−0.110
0.4249	0.84083	−0.591	1.0000	0.86367	
0.4929	0.84399	−0.599			

$$b_i = 0.077796 \frac{RT_{ci}}{P_{ci}}. \tag{6}$$

Subscripts c and r denote critical and reduced values, respectively, ω_i is the acentric factor of pure component i, and k_{1i} is a pure component adjustable parameter [17]. The critical properties were either taken from the literature [14, 18] or calculated using a group contribution method [19]. In Table IV the pure compound parameters are reported.

The parameters a and b for the mixture are obtained from the following two-parameter mixing rules [20, 21]:

$$a = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (a_i a_j)^{1/2} \left(1 - k_{ij}\right) \tag{7}$$

$$b = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j \left(\frac{b_i + b_j}{2}\right) \left(1 - m_{ij}\right), \tag{8}$$

where k_{ij} and m_{ij} are adjustable parameters. Estimation of these parameters was based on minimization using the Marquardt algorithm [22] of the following objective function:

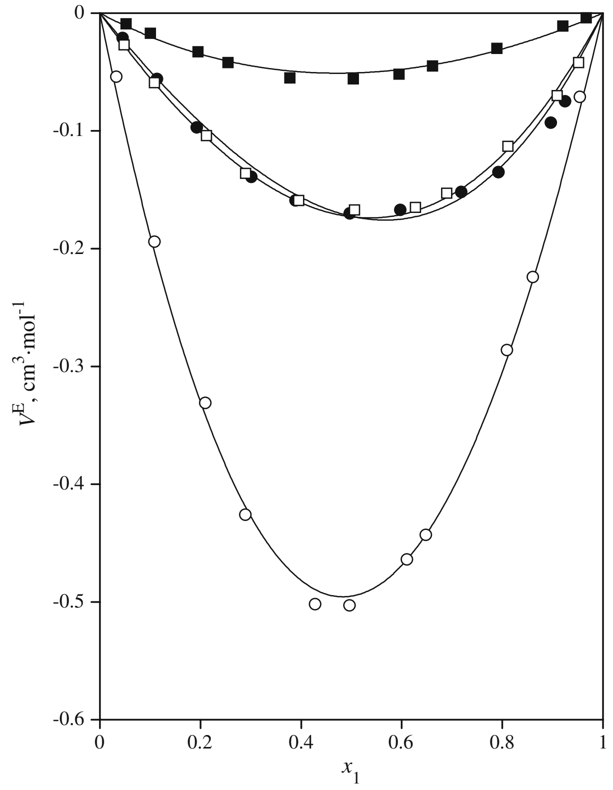

Fig. 1. Excess molar volumes, V^E, at 298.15 K for tetrahydropyran (1) with isomeric chlorobutanes (2): (■) 1-chlorobutane; (●) 2-chlorobutane; (□) 2-methyl-1-chloropropane; (○) 2-methyl-2-chloropropane; (—) PRSV–CEOS.

$$F = \sum_{i=1}^{n} \left(V^E_{\text{exptl}} - V^E_{\text{CEOS}} \right)_i^2 \tag{9}$$

These parameters are given for each mixture in Table V together with the corresponding root-mean-square deviations, RMSD, between correlated and experimental values of the excess molar volume. In Figs. 1 and 2 the experimental and correlated V^E values are compared. Results show that the PRSV–CEOS correlates satisfactorily the experimental V^E values; the worst correlation is for the mixture tetrahydropyran with 2-methyl-2-chloropropane.

The absolute viscosities have been correlated using the Lee model; this model combines Eyring's absolute rate theory [23] with the use of an equation of state in order to calculate the excess Gibbs function of the mixture.

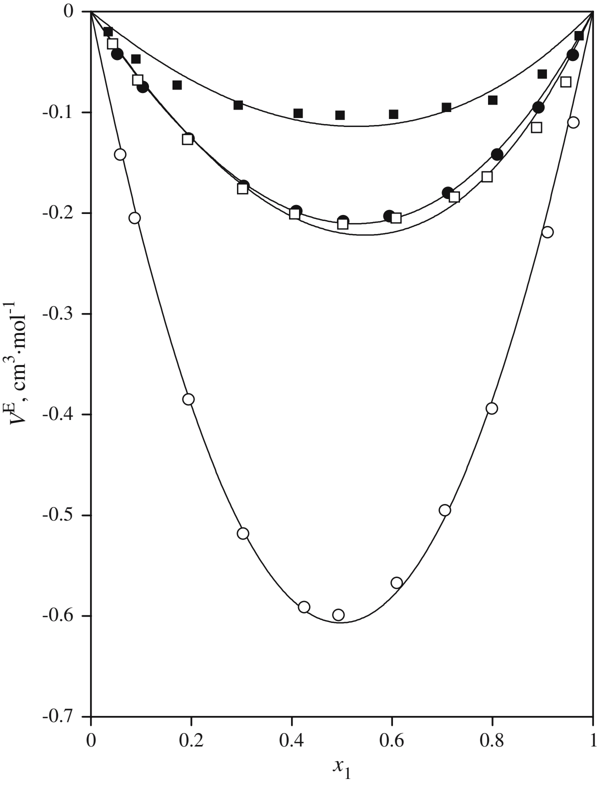

Fig. 2. Excess molar volumes, V^E, at 313.15 K for tetrahydropyran (1) with isomeric chlorobutanes (2): (■) 1-chlorobutane; (●) 2-chlorobutane; (□) 2-methyl-1-chloropropane; (○) 2-methyl-2-chloropropane; (—) PRSV–CEOS.

According to Eyring's theory, the viscosity of a liquid can be evaluated using

$$\eta = \frac{N_A h}{\overline{V}} \exp\left(\frac{\Delta G^*}{RT}\right), \tag{10}$$

where N_A is Avogadro's number, h is Planck's constant, $\overline{V}$ is the molar volume, and ΔG^* is the activation Gibbs function of viscous flow.

For a mixture, ΔG^* is given by

$$\Delta G^* = \sum_{i=1}^{n} x_i \Delta G_i^* + \Delta G^{*E}, \tag{11}$$

Table III. Kinematic Viscosities, ν, and Absolute Viscosities, η, of Tetrahydropyran (1) + Isomeric Chlorobutanes (2)

x_1	ν ($mm \cdot s^{-1}$)	η (mPa·s)	x_1	ν ($mm \cdot s^{-1}$)	η (mPa·s)
Tetrahydropyran (1) + 1-chlorobutane (2) at 298.15 K					
0.0000	0.4783	0.4212	0.6038	0.6685	0.5883
0.0243	0.4835	0.4258	0.7064	0.7176	0.6313
0.1039	0.5023	0.4424	0.7994	0.7682	0.6756
0.2058	0.5293	0.4661	0.9058	0.8374	0.7362
0.3070	0.5590	0.4922	0.9498	0.8698	0.7645
0.3984	0.5888	0.5184	1.0000	0.9100	0.7997
0.5077	0.6296	0.5542			
Tetrahydropyran (1) + 2-chlorobutane (2) at 298.15 K					
0.0000	0.4540	0.3938	0.6122	0.6620	0.5796
0.0605	0.4657	0.4044	0.7108	0.7136	0.6256
0.1166	0.4805	0.4176	0.8059	0.7687	0.6747
0.2131	0.5081	0.4423	0.9023	0.8336	0.7323
0.3174	0.5425	0.4731	0.9549	0.8729	0.7671
0.4088	0.5751	0.5022	1.0000	0.9100	0.7997
0.4994	0.6111	0.5343			
Tetrahydropyran (1) + 2-methyl-1-chloropropane (2) at 298.15 K					
0.0000	0.4930	0.4295	0.5950	0.6816	0.5978
0.0540	0.5063	0.4415	0.6954	0.7270	0.6380
0.1069	0.5193	0.4532	0.8028	0.7826	0.6872
0.2033	0.5457	0.4769	0.9066	0.8464	0.7436
0.3110	0.5776	0.5053	0.9578	0.8797	0.7730
0.4126	0.6112	0.5352	1.0000	0.9100	0.7997
0.5040	0.6445	0.5648			
Tetrahydropyran (1) + 2-methyl-2-chloropropane (2) at 298.15 K					
0.0000	0.5680	0.4751	0.6155	0.7540	0.6524
0.0614	0.5840	0.4903	0.7156	0.7908	0.6872
0.1075	0.5961	0.5019	0.8277	0.8349	0.7289
0.2173	0.6274	0.5317	0.9097	0.8699	0.7619
0.3205	0.6570	0.5601	0.9547	0.8894	0.7803
0.4200	0.6879	0.5896	1.0000	0.9100	0.7997
0.5176	0.7198	0.6199			
Tetrahydropyran (1) + 1-chlorobutane (2) at 313.15 K					
0.0000	0.4214	0.3640	0.6038	0.5717	0.4943
0.0243	0.4276	0.3694	0.7064	0.6101	0.5274
0.1039	0.4418	0.3818	0.7994	0.6489	0.5609
0.2058	0.4629	0.4002	0.9058	0.7010	0.6058
0.3070	0.4855	0.4197	0.9498	0.7250	0.6264
0.3984	0.5090	0.4401	1.0000	0.7571	0.6539
0.5077	0.5404	0.4672			

Table III. (*Continued*)

x_1	ν (mm·s^{-1})	η (mPa·s)	x_1	ν (mm·s^{-1})	η (mPa·s)
Tetrahydropyran (1) + 2-chlorobutane (2) at 313.15 K					
0.0000	0.3965	0.3371	0.6122	0.5656	0.4863
0.0605	0.4093	0.3484	0.7108	0.6059	0.5217
0.1166	0.4220	0.3596	0.8059	0.6485	0.5590
0.2131	0.4454	0.3803	0.9023	0.6975	0.6019
0.3174	0.4720	0.4039	0.9549	0.7280	0.6285
0.4088	0.4971	0.4260	1.0000	0.7571	0.6539
0.4994	0.5253	0.4509			
Tetrahydropyran (1) + 2-methyl-1-chloropropane (2) at 313.15 K					
0.0000	0.4292	0.3664	0.5950	0.5796	0.4991
0.0540	0.4398	0.3757	0.6954	0.6156	0.5307
0.1069	0.4509	0.3856	0.8028	0.6605	0.5699
0.2033	0.4718	0.4041	0.9066	0.7068	0.6103
0.3110	0.4967	0.4262	0.9578	0.7332	0.6332
0.4126	0.5231	0.4494	1.0000	0.7571	0.6539
0.5040	0.5502	0.4733			
Tetrahydropyran (1) + 2-methyl-2-chloropropane (2) at 313.15 K					
0.0000	0.4775	0.3907	0.6359	0.6363	0.5410
0.0451	0.4872	0.3999	0.7056	0.6575	0.5610
0.0887	0.4969	0.4091	0.7960	0.6859	0.5877
0.1978	0.5209	0.4320	0.9063	0.7230	0.6224
0.3053	0.5466	0.4564	0.9526	0.7397	0.6379
0.3972	0.5699	0.4784	1.0000	0.7571	0.6539
0.5024	0.5985	0.5054			

where ΔG^{*E} is the excess activation Gibbs function of viscous flow that is related with the excess Gibbs function of the mixture by means of the following equation:

$$\Delta G^{*E} = (\sigma_0 + \sigma_1 x_1)\, G^E, \tag{12}$$

where σ_0 and σ_1 are adjustable parameters.

The excess Gibbs function of the mixture can be calculated as follows:

$$G^E = RT \sum_{i=1}^{n} x_i (ln\hat{\phi}_i - ln\phi_i), \tag{13}$$

where the fugacity coefficients of the components in the pure state, ϕ_i, and in the mixture, $\hat{\phi}_i$, are calculated using an equation of state. In our case we have employed the PRSV–EOS together with the mixing rules and the correlating parameters previously used in the excess-volume calculations.

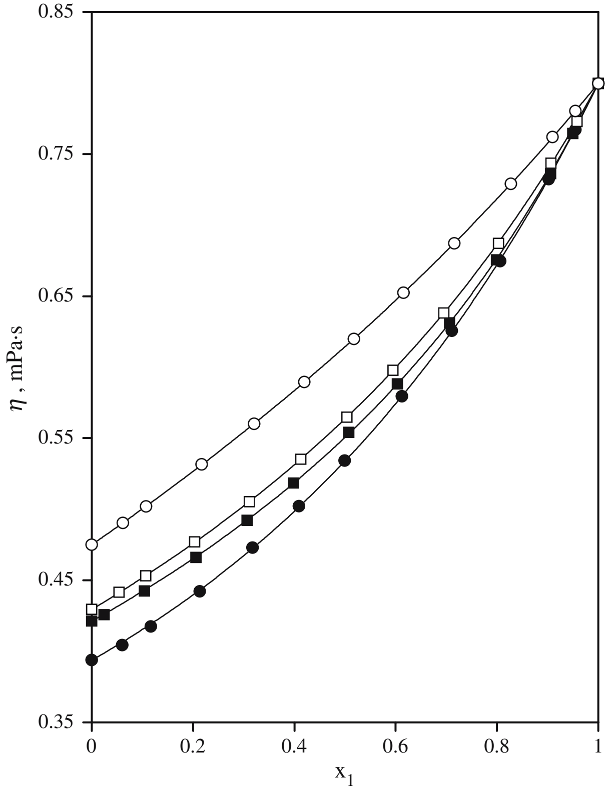

Fig. 3. Absolute viscosities, η, at 298.15 K for tetrahydropyran (1) with isomeric chlorobutanes (2): (■) 1-chlorobutane; (●) 2-chlorobutane; (□) 2-methyl-1-chloropropane; (○) 2-methyl-2-chloropropane; (—) Lee model.

The parameters σ_0 and σ_1 have been obtained by minimizing the following objective function:

$$F = \sum_{i=1}^{n} \left(\eta_{\text{exptl}} - \eta_{\text{CEOS}}\right)_i^2 \tag{14}$$

In Table V these parameters for each mixture are reported together with the corresponding *RMSD*. The graphical comparison between correlated and experimental η values is shown in Figs. 3 and 4. It can be pointed out that the results provided by the Lee model are excellent.

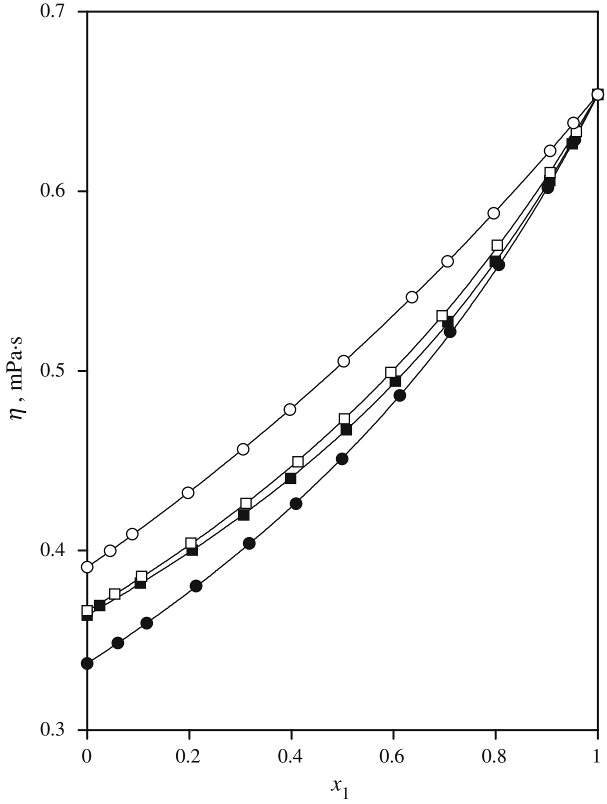

Fig. 4. Absolute viscosities, η, at 313.15 K for tetrahydropyran (1) with isomeric chlorobutanes (2): (■) 1-chlorobutane; (●) 2-chlorobutane; (□) 2-methyl-1-chloropropane; (○) 2-methyl-2-chloropropane; (—) Lee model.

Table IV. Critical Temperature, T_c, and Critical Pressure, P_c, Acentric Factor, ω, and Adjustable Parameter, k_1, of the Pure Compounds

Compound	T_c (K)	P_c (bar)	ω	k_1
Tetrahydropyran [14]	572.2	47.7	0.2205	0.0458
1-Chlorobutane [14]	542.2	36.85	0.2166	0.1843
2-Chlorobutane [18]	520.6	36.8	0.267	0.0003
2-Methyl-1-chloropropane [19]	517.3	35.62	0.2895	−0.0088
2-Methyl-2-chloropropane [19]	501.2	38.36	0.2273	0.0445

Table V. Adjustable Parameters for PRSV-EOS and Lee Model Together with the Corresponding Root-Mean-Square Deviations

Function	T (K)	A	B	$RMSD$
	Tetrahydropyran (1) + 1-chlorobutane (2)			
V^E ($cm^3 \cdot mol^{-1}$)[a]	298.15	−0.0115	−0.0012	0.003
	313.15	0.0102	0.0035	0.010
η (mPa·s)[b]	298.15	3.7255	1.7387	0.0005
	313.15	−0.5436	−0.3159	0.0007
	Tetrahydropyran (1) + 2-chlorobutane (2)			
V^E ($cm^3 \cdot mol^{-1}$)	298.15	0.0338	0.0074	0.008
	313.15	0.0152	0.0044	0.004
η (mPa·s)	298.15	−0.3210	0.0310	0.0010
	313.15	−0.3370	−0.2173	0.0005
	Tetrahydropyran (1) + 2-methyl-1-chloropropane (2)			
V^E ($cm^3 \cdot mol^{-1}$)	298.15	0.0176	0.0045	0.004
	313.15	0.0245	0.0065	0.009
η (mPa·s)	298.15	−0.2860	−0.1087	0.0003
	313.15	−0.2470	−0.0570	0.0005
	Tetrahydropyran (1) + 2-methyl-2-chloropropane (2)			
V^E ($cm^3 \cdot mol^{-1}$)	298.15	0.0009	0.0039	0.008
	313.15	0.0139	0.0072	0.011
η (mPa·s)	298.15	−0.1159	−0.1400	0.0002
	313.15	−0.0717	−0.0226	0.0002

[a] $A = k_{12}$, $B = m_{12}$.
[b] $A = \sigma_0$, $B = \sigma_1$.

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