Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether

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From experimental data (densities, speeds of sound, and refractive indices) over the temperature range (283.15 to 313.15) K for the binary mixtures formed by an isomer of chlorobutane (1-chlorobutane, 2-chlorobutane, 2-methyl-1-chloropropane, or 2-methyl-2-chloropropane) plus diisopropyl ether, the following properties have been calculated: excess volumes, excess isentropic compressibilities, and refractive index deviations. The excess properties and deviations were fitted using the Redlich−Kister polynomial equation. The excess volumes and excess isentropic compressibilities for the four systems are all negative over both the composition and temperature ranges, whereas the refractive index deviations are always positive.

Introduction

Over past years, many researchers have directed their attention to ethers, particularly diisopropyl ether, because of their applications as additives in fuels.[1−4] This interest overlaps in part with the objectives of our research line, which is devoted to the thermophysical characterization of multicomponent liquid systems involving oxygenated organic compounds mixed with haloalkanes or other organic solvents.[5−10] Specifically, we are interested in a comprehensive study of Cl−O interactions. Here we present results for the binary systems formed between the above-cited ether and each of the four isomeric chlorobutanes.

We recently published kinematic and absolute viscosities for these mixtures.[10] In order to extend this study, we present here speeds of sound and refractive indices together with densities over the temperature range (283.15 to 313.15) K. From these values we obtained excess volumes, V^E, excess isentropic compressibilities, κ_S^E, and refractive index deviations, Δn_D. The values of these derived properties behave regularly for the four systems over the entire composition range in the temperature range studied. As far as we know, these properties of the four systems have not been previously reported in the literature.

Experimental Section

The compounds used were 1-chlorobutane, 2-chlorobutane, 2-methyl-2-chloropropane, and diisopropyl ether (mass fraction greater than 0.99) obtained from Aldrich and 2-methyl-1-chloropropane (mass fraction greater than 0.99) provided by Fluka. The purities of the chemical were checked by comparing the values of their different properties with those from the literature. In all cases, the purity was sufficient to fulfill our purposes, and no additional purification was necessary.

Refractive indices at the 589.3 nm sodium D wavelength were measured using a high-precision automatic refractometer (Abbemat-HP, Dr. Wolfgang Kernchen GMBH, Germany) whose temperature was internally controlled to within ± 0.01 K. The apparatus was calibrated with deionized, double-distilled water. The uncertainty in the measurements was $\pm 1 \times 10^{-6}$.

Densities, ρ, and speeds of sound, u, of the pure compounds and their mixtures were determined with an Anton Paar DSA-5000 vibrating-tube densimeter and sound analyzer automatically thermostatted to within ± 0.001 K. The uncertainty in the density measurements after proper adjustment with deionized, doubly distilled water and dry air was $\pm 1 \times 10^{-3}$ kg·m^{-3}, and the corresponding uncertainty in the speed of sound measurements was ± 0.01 m·s^{-1}.

The mixtures were prepared by mass using a Sartorius semimicro balance CP225-D with an uncertainty of $\pm 10^{-5}$ g. The maximum estimated error in the mole fraction was $\pm 1 \times 10^{-4}$.

Values of the properties for the pure compounds at the working temperatures along with literature values at 298.15 K are collected in Table 1.[11,12]

Results and Discussion

Excess volumes, V^E, were calculated from the density of the mixture, ρ, the densities, ρ_i, and molar masses, M_i, of the pure compounds, and the corresponding mole fractions, x_i, by means of the equation

$$V^E = \sum_i x_i \left(\frac{M_i}{\rho} - \frac{M_i}{\rho_i} \right) \quad (1)$$

Isentropic compressibilities, κ_S, were calculated from the experimental densities and speeds of sound using the Newton−Laplace relation, $\kappa_S = (\rho \cdot u^2)^{-1}$. From these values, excess isentropic compressibilities, κ_S^E, were estimated as

$$\kappa_S^E = \kappa_S - \kappa_S^{id} \quad (2)$$

where κ_S^{id} was obtained according to Benson and Kiyohara:[13]

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Table 1. Properties of the Pure Compounds and Comparison of Refractive Indices and Densities with Literature Values at $T = 298.15$ K

	n_D		ρ/kg·m^{-3}				
T/K	exptl	lit	exptl	lit	u/m·s^{-1}	C_p/J·mol^{-1}·K^{-1}	10^3·α_{exptl}/K^{-1}
			1-Chlorobutane				
283.15	1.407504		897.339		1180.14	155.96	1.221
288.15	1.404813		891.855		1159.51	157.06	1.235
293.15	1.402123		886.335		1138.84	158.10	1.249
298.15	1.399500	1.39996[a]	880.705	880.95[a]	1118.18	159.16	1.264
303.15	1.396716		875.204		1097.64	160.17	1.280
308.15	1.393949		869.585		1077.18	161.44	1.296
313.15	1.391309		863.882		1056.91	162.65	1.313
			2-Chlorobutane				
283.15	1.402257		884.340		1127.71	156.16	1.259
288.15	1.399533		878.756		1107.25	157.29	1.276
293.15	1.396800		873.130		1086.74	158.40	1.292
298.15	1.394036	1.3942[a]	867.474	867.1[b]	1066.24	159.49	1.309
303.15	1.391249		861.779		1045.88	160.58	1.326
308.15	1.388444		856.044		1025.33	161.65	1.345
313.15	1.385618		850.266		1005.32	162.70	1.365
			1-Chloro-2-methylpropane				
283.15	1.403542		888.845		1141.74	156.78	1.266
288.15	1.400797		883.211		1120.72	158.03	1.281
293.15	1.398017		877.539		1099.63	159.31	1.297
298.15	1.395285	1.3951[a]	871.533	871.7[a]	1078.68	160.63	1.312
303.15	1.392451		866.096		1057.76	161.98	1.329
308.15	1.389626		860.319		1036.97	163.36	1.347
313.15	1.386827		853.902		1016.27	164.78	1.367
			2-Chloro-2-methylpropane				
283.15	1.391153		855.249		1046.93	155.76	1.399
288.15	1.388209		849.243		1025.50	157.75	1.420
293.15	1.385217		843.191		1004.08	159.78	1.441
298.15	1.382254	1.3828[a]	837.096	836.1[a]	983.25	161.86	1.461
303.15	1.379211		830.958		961.51	163.98	1.483
308.15	1.376189		824.772		940.46	166.16	1.506
313.15	1.373115		818.536		919.41	168.37	1.531
			Diisopropyl Ether				
283.15	1.373582		733.833		1065.52	210.64	1.396
288.15	1.370844		728.692		1043.14	212.43	1.417
293.15	1.368118		723.509		1020.62	214.25	1.438
298.15	1.365249	1.3655[a]	718.289	718.54[a]	998.27	216.12	1.459
303.15	1.362417		713.032		976.02	218.03	1.481
308.15	1.359563		707.727		953.94	219.97	1.505
313.15	1.356672		702.378		932.01	221.95	1.531

[a] Data from ref 11. [b] Data from ref 12.

$$\kappa_S^{id} = \sum_i \phi_i \left[\kappa_{S,i} + \frac{T V_i \alpha_i^2}{C_{p,i}} \right] - T \left(\sum_i x_i V_i \right) \frac{\left(\sum_i \phi_i \alpha_i \right)^2}{\sum_i x_i C_{p,i}} \tag{3}$$

where ϕ_i is the volume fraction of component i in the mixture referred to the unmixed state; x_i is the corresponding mole fraction; T is the absolute temperature; and $\kappa_{S,i}$, V_i, α_i, and $C_{p,i}$ are the isentropic compressibility, molar volume, thermal expansion coefficient, and molar constant-pressure heat capacity of pure component i, respectively. Molar heat capacities for isomeric chlorobutanes were calculated using different heat capacity group-contribution methods,[14−17] and those corresponding to diisopropyl ether were taken from the literature.[18] Thermal expansion coefficients were derived from our own density measurements by means of the following equation:

$$\alpha_i = \frac{1}{\rho_i} \left(\frac{\partial \rho_i}{\partial T} \right)_p \tag{4}$$

Values of all of these properties for the pure substances over the temperature range studied are listed in Table 1.

Refractive index deviations, Δn_D, were calculated following the suggestions of Fialkov and Fenerli[19] and Fialkov[20] by means of the equation

$$\Delta n_D = n_D - \sum_i \phi_i n_{D,i} \tag{5}$$

where n_D is the refractive index of the mixture and $n_{D,i}$ is the refractive index of component i.

Values of the measured thermophysical properties (densities, speeds of sound, and refractive indices) together with the corresponding excess or deviation properties can be found in the Supporting Information.

The values of V^E, κ_S^E, and Δn_D (denoted as Q in eq 6) were correlated with the Redlich−Kister polynomial equation:

$$Q = y_1 y_2 \sum_{j=0}^{r} A_j (y_1 - y_2)^j \tag{6}$$

where A_j are adjustable parameters and y_i is the mole fraction x_i of component i when $Q = V^E$ or κ_S^E and the volume fraction

Table 2. Values of the Parameters A_j (j = 0 to 3) and Standard Deviations, $\sigma(Q)$, of the Redlich−Kister Equation

Q	T/K	A_0	A_1	A_2	A_3	$\sigma(Q)$
		1-Chlorobutane (1) + Diisopropyl Ether (2)				
$10^6 \cdot V^E/m^3 \cdot mol^{-1}$	283.15	−1.5479	−0.0566	−0.3511	0.5266	0.0029
	288.15	−1.5730	−0.0781	−0.3806	0.6141	0.0057
	293.15	−1.6044	−0.0727	−0.3830	0.6128	0.0059
	298.15	−1.6317	−0.0519	−0.4010	0.5814	0.0071
	303.15	−1.6680	−0.0405	−0.3948	0.5512	0.0072
	308.15	−1.7062	−0.0434	−0.4002	0.5671	0.0075
	313.15	−1.7432	−0.0636	−0.4046	0.6039	0.0076
κ_S^E/TPa^{-1}	283.15	−178.75	−15.72	−12.60	9.55	0.15
	288.15	−191.43	−17.83	−13.90	11.11	0.24
	293.15	−206.23	−19.27	−16.10	13.72	0.23
	298.15	−222.19	−21.59	−15.18	13.60	0.21
	303.15	−240.53	−20.23	−17.29	11.49	0.20
	308.15	−259.85	−23.26	−18.62	12.71	0.19
	313.15	−281.14	−24.08	−21.02	15.18	0.33
Δn_D	283.15	0.004621	0.000019	−0.001130	0.000595	0.000017
	288.15	0.004703	−0.000041	−0.001117	0.000583	0.000016
	293.15	0.004782	−0.000027	−0.001122	0.000512	0.000014
	298.15	0.004849	−0.000115	−0.000967	0.000735	0.000016
	303.15	0.004891	0.000013	−0.000840	0.000574	0.000018
	308.15	0.004951	0.000038	−0.000761	0.000682	0.000018
	313.15	0.005018	−0.000017	−0.000717	0.000719	0.000016
		2-Chlorobutane (1) + Diisopropyl Ether (2)				
$10^6 \cdot V^E/m^3 \cdot mol^{-1}$	283.15	−1.0804	−0.0147	−0.1135	0.2490	0.0024
	288.15	−1.0960	−0.0062	−0.1182	0.2083	0.0020
	293.15	−1.1143	−0.0248	−0.1249	0.2491	0.0027
	298.15	−1.1303	−0.0287	−0.1129	0.2437	0.0022
	303.15	−1.1482	−0.0314	−0.1204	0.2557	0.0032
	308.15	−1.1660	−0.0312	−0.1172	0.2415	0.0027
	313.15	−1.1859	−0.0400	−0.1247	0.2610	0.0031
κ_S^E/TPa^{-1}	283.15	−111.92	−14.53	−6.19	5.11	0.04
	288.15	−119.58	−15.68	−6.63	6.57	0.04
	293.15	−129.38	−16.34	−6.79	7.29	0.07
	298.15	−138.99	−20.38	−7.66	13.46	0.05
	303.15	−149.45	−19.58	−7.70	9.92	0.07
	308.15	−161.25	−21.52	−6.35	9.60	0.07
	313.15	−173.51	−24.26	−8.47	10.87	0.06
Δn_D	283.15	0.002639	0.000029	−0.001184	0.000345	0.000005
	288.15	0.002669	−0.000005	−0.001060	0.000467	0.000005
	293.15	0.002687	−0.000048	−0.001021	0.000552	0.000005
	298.15	0.002707	−0.000077	−0.000971	0.000607	0.000004
	303.15	0.002727	−0.000034	−0.000874	0.000603	0.000003
	308.15	0.002752	0.000000	−0.000813	0.000488	0.000004
	313.15	0.002765	−0.000011	−0.000731	0.000500	0.000006
		2-Methyl-1-chloropropane (1) + Diisopropyl Ether (2)				
$10^6 \cdot V^E/m^3 \cdot mol^{-1}$	283.15	−1.1873	0.1967	0.1503	−0.5825	0.0028
	288.15	−1.2037	0.2132	0.1520	−0.6015	0.0027
	293.15	−1.2170	0.2045	0.1417	−0.5661	0.0029
	298.15	−1.2370	0.2010	0.1661	−0.5515	0.0030
	303.15	−1.2561	0.2240	0.1721	−0.6321	0.0032
	308.15	−1.2732	0.2238	0.1775	−0.6371	0.0030
	313.15	−1.2906	0.2180	0.1774	−0.6260	0.0031
κ_S^E/TPa^{-1}	283.15	−125.38	−10.83	6.82	−19.98	0.07
	288.15	−133.57	−10.75	5.11	−21.94	0.05
	293.15	−143.99	−11.06	6.20	−24.28	0.06
	298.15	−153.95	−12.18	4.86	−25.14	0.07
	303.15	−165.40	−12.98	5.22	−27.32	0.06
	308.15	−177.10	−16.05	5.50	−24.79	0.08
	313.15	−191.69	−16.17	6.27	−27.47	0.09
Δn_D	283.15	0.003261	−0.000316	−0.000235	−0.000029	0.000009
	288.15	0.003294	−0.000334	−0.000260	−0.000044	0.000008
	293.15	0.003320	−0.000384	−0.000264	0.000057	0.000008
	298.15	0.003350	−0.000415	−0.000271	0.000061	0.000009
	303.15	0.003382	−0.000431	−0.000308	0.000035	0.000008
	308.15	0.003409	−0.000468	−0.000320	0.000061	0.000009
	313.15	0.003440	−0.000505	−0.000345	0.000087	0.000009
		2-Methyl-2-chloropropane (1) + Diisopropyl Ether (2)				
$10^6 \cdot V^E/m^3 \cdot mol^{-1}$	283.15	−0.2141	0.0175	0.1434	−0.1415	0.0005
	288.15	−0.2215	0.0191	0.1420	−0.1437	0.0005
	293.15	−0.2288	0.0068	0.1514	−0.1172	0.0006
	298.15	−0.2371	0.0007	0.1486	−0.1166	0.0006
	303.15	−0.2427	−0.0026	0.1548	−0.1152	0.0006
	308.15	−0.2507	−0.0029	0.1457	−0.1278	0.0007
	313.15	−0.2578	−0.0030	0.1607	−0.1416	0.0006
κ_S^E/TPa^{-1}	283.15	−26.68	−5.70	−0.20	0.34	0.02
	288.15	−27.79	−6.49	−0.24	0.79	0.02
	293.15	−29.19	−7.04	0.04	0.45	0.03
	298.15	−30.62	−7.91	0.06	0.03	0.02
	303.15	−31.44	−9.34	0.02	0.37	0.04
	308.15	−32.79	−10.37	−0.58	0.99	0.05
	313.15	−34.04	−12.43	−0.57	3.13	0.05

Table 2. Continued

Q	T/K	A_0	A_1	A_2	A_3	$\sigma(Q)$
Δn_D	283.15	0.000193	−0.000005	−0.000032	0.000063	0.000001
	288.15	0.000200	0.000000	−0.000024	0.000059	0.000001
	293.15	0.000207	0.000004	−0.000022	0.000055	0.000001
	298.15	0.000214	0.000015	−0.000018	0.000033	0.000001
	303.15	0.000221	0.000011	−0.000020	0.000046	0.000001
	308.15	0.000229	0.000013	−0.000020	0.000053	0.000001
	313.15	0.000237	0.000016	−0.000013	0.000065	0.000001

ϕ_i of component i when $Q = \Delta n_D$. The values of the parameters A_j together with the standard deviation σ for each property Q are given in Table 2, and V^E, κ_S^E, and Δn_D are graphically represented in Figures 1 to 3, respectively.

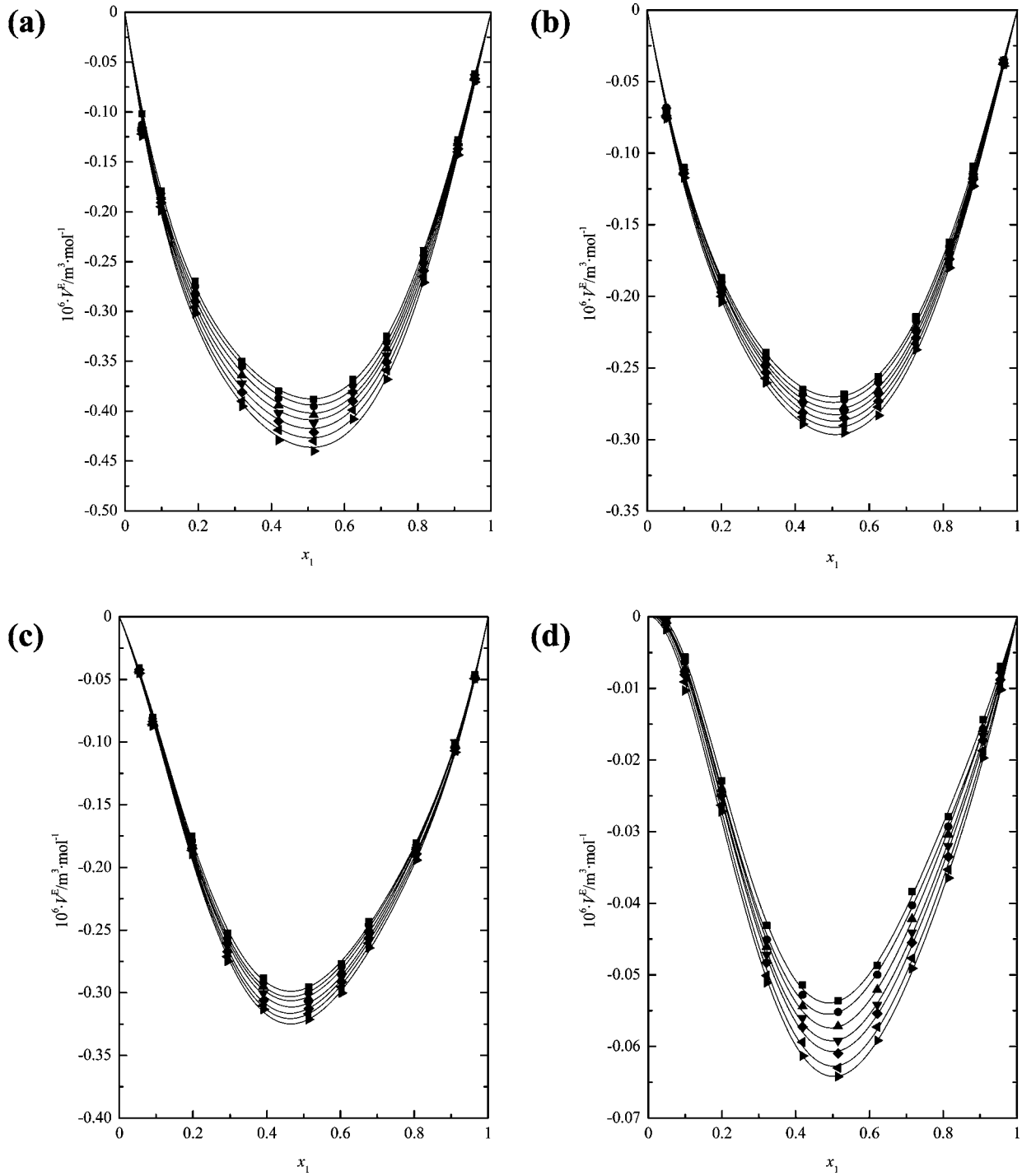

Figure 1. Excess volumes, V^E, of isomeric chlorobutane (1) + diisopropyl ether (2) as functions of the chlorobutane mole fraction, x_1: (a) 1-chlorobutane; (b) 2-chlorobutane; (c) 2-methyl-1-chloropropane; (d) 2-methyl-2-chloropropane. Experimental data: ■, 283.15 K; ●, 288.15 K; ▲, 293.15 K; ▼, 298.15 K; ◆, 303.15 K; left-pointing triangles, 308.15 K; right-pointing triangles, 313.15 K. Solid curves are fits to the Redlich−Kister equation.

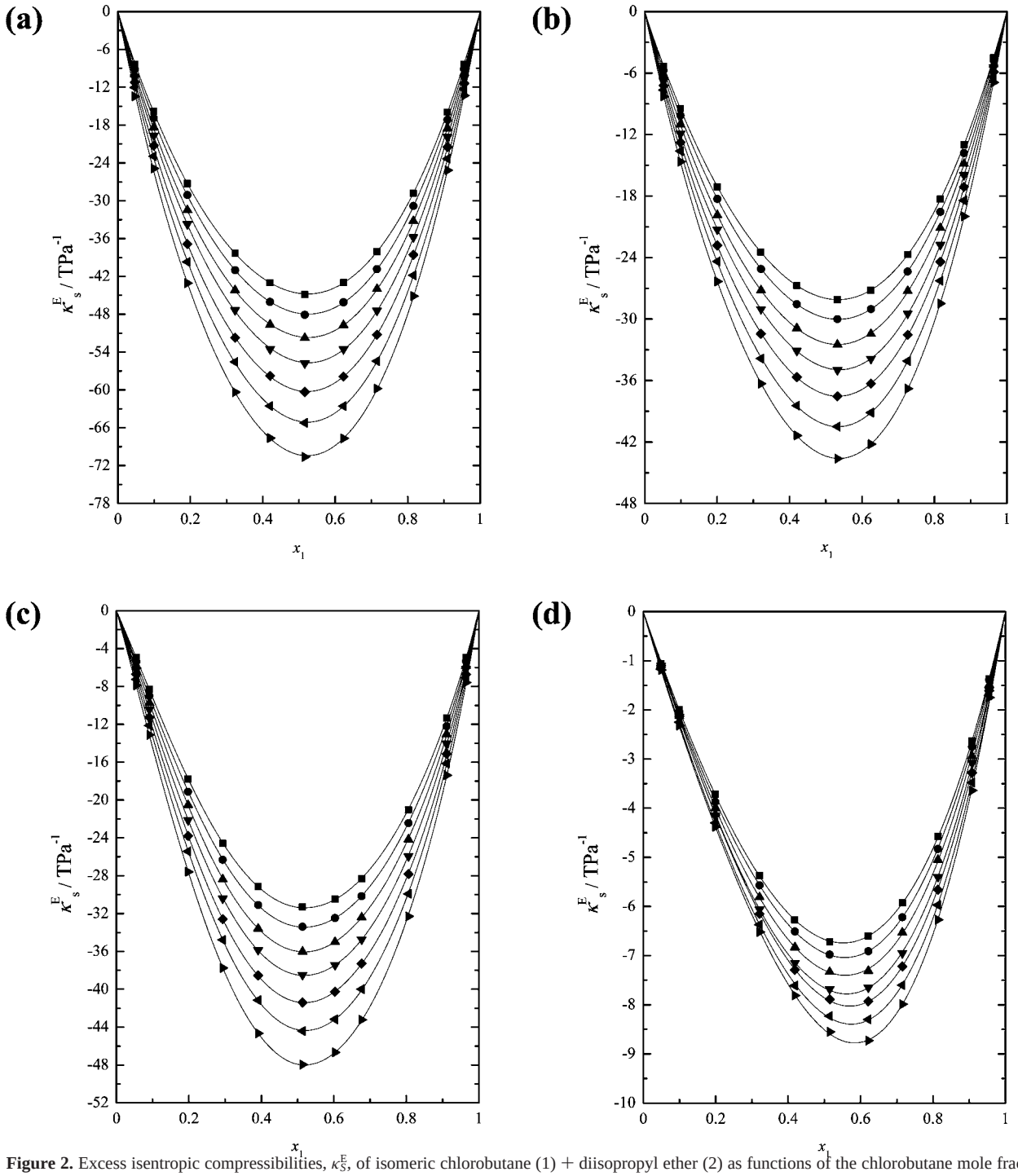

Figure 2. Excess isentropic compressibilities, κ_S^E, of isomeric chlorobutane (1) + diisopropyl ether (2) as functions of the chlorobutane mole fraction, x_1: (a) 1-chlorobutane; (b) 2-chlorobutane; (c) 2-methyl-1-chloropropane; (d) 2-methyl-2-chloropropane. Experimental data: ■, 283.15 K; ●, 288.15 K; ▲, 293.15 K; ▼, 298.15 K; ◆, 303.15 K; left-pointing triangles, 308.15 K; right-pointing triangles, 313.15 K. Solid curves are fits to the Redlich−Kister equation.

The excess volumes are negative at the seven temperatures studied over the whole composition range. Their values become more negative as the temperature increases. The minimum is always placed at an x_1 value close to 0.5. It is remarkable that the values for the mixture 2-methyl-2-chloropropane + diisopropyl ether are close to zero (in absolute terms, always smaller than 0.1 cm^3·mol^{-1}) while those for the rest of the systems studied are between 5 and 7 times greater.

The excess isentropic compressibilities follow the same trend, and two facts should be emphasized. The first is that the minimum values for the mixture 2-methyl-2-chloropropane + diisopropyl ether are shifted toward $x_1 = 0.6$. The second fact is the noticeable difference between the observed values, as the minima for the above-cited system are 10 times lower than those for the mixture containing 1-chlorobutane at a given temperature. Mixtures involving the other two chlorinated isomers have intermediate values.

The refractive index deviations are positive for the four mixtures, independent of temperature and composition. The values increase as the temperature increases, with the maxima located at values of ϕ_1 close to 0.5. Once again, the mixture 2-methyl-2-chloropropane + diisopropyl ether presents values very different than the rest, being in this case 10 times lower than those for the other three chlorinated systems. Qualitatively,

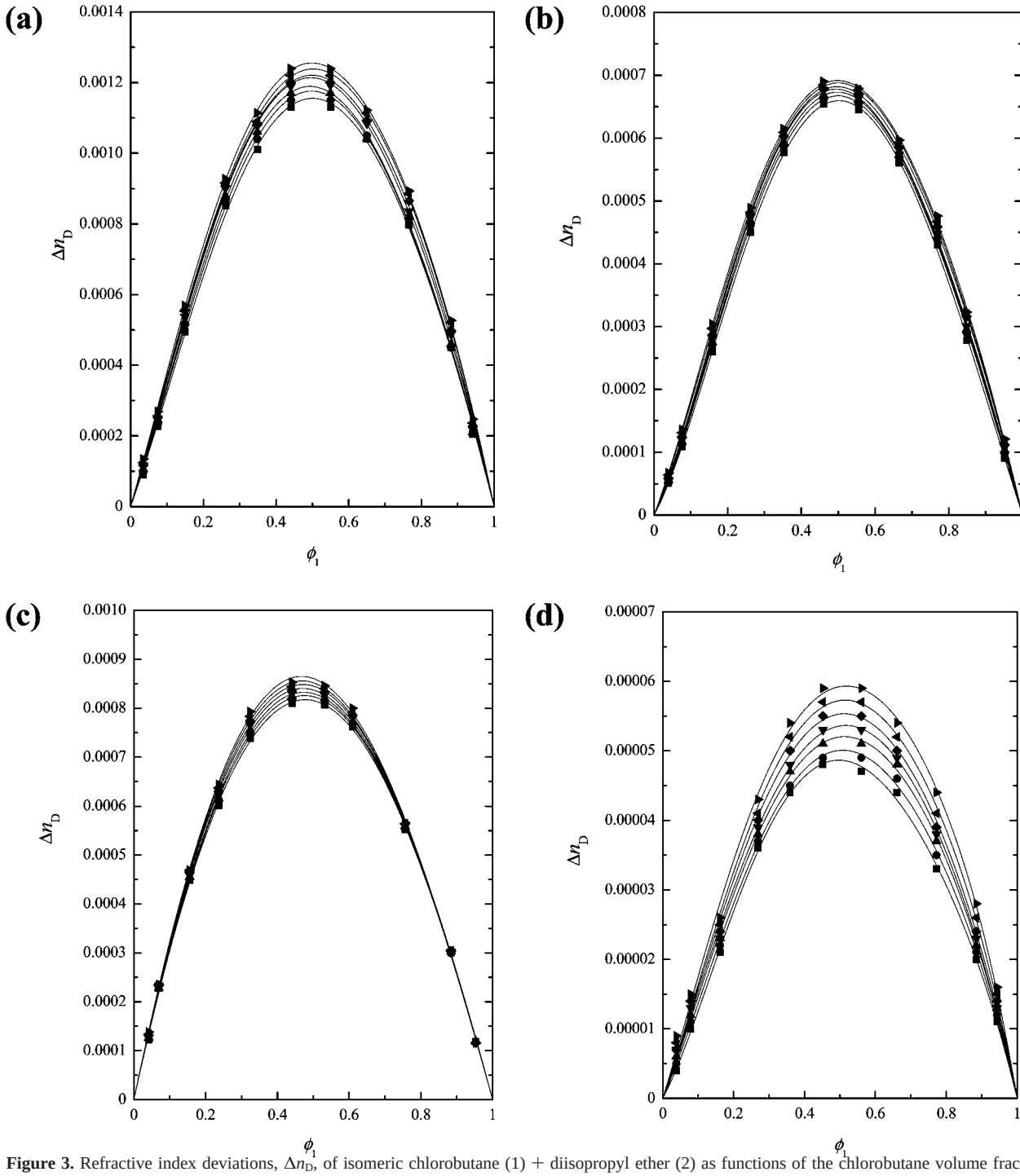

Figure 3. Refractive index deviations, Δn_D, of isomeric chlorobutane (1) + diisopropyl ether (2) as functions of the chlorobutane volume fraction, ϕ_1: (a) 1-chlorobutane; (b) 2-chlorobutane; (c) 2-methyl-1-chloropropane; (d) 2-methyl-2-chloropropane. Experimental data: ■, 283.15 K; ●, 288.15 K; ▲, 293.15 K; ▼, 298.15 K; ◆, 303.15 K; left-pointing triangles, 308.15 K; right-pointing triangles, 313.15 K. Solid curves are fits to the Redlich−Kister equation.

a symmetrical correspondence between these curves and those for the excess volume can be observed, confirming the suggestions previously stated.[21] Moreover, it can be noted that relative values for 2-methyl-2-chloropropane + diisopropyl ether and the rest of the chlorinated compounds are about the same for these two properties.

The results can be interpreted by taking into account the molecular characteristics of the pure compounds, which are usually divided into structural and energetic effects. The negative values of V^E and κ_S^E and positive values of Δn_D could suggest an appreciable contribution by Cl−O interactions established during mixing process. In addition, the Cl−O interaction is more easily established in terms of size effects and steric hindrance when the chlorine atom in the haloalkane is linked to a terminal carbon atom of the alkyl chain, and the latter is completely linear so that such contribution should be stronger.

In order to corroborate this hypothesis, it is necessary to consider the absolute viscosity deviations for the same systems.[10] The actual values for this property are always negative and very close to zero for the four systems (in absolute terms, < 0.01 for 1- and 2-chlorobutane, < 0.02 for 2-methyl-1-chloropropane, and < 0.05 for 2-methyl-2-chloropropane). Moreover, they become less negative as the temperature rises, and according to Fort and Moore,[22] negative values of this property indicate

that dispersion forces are predominant. Thus, we can rule out the Cl−O interaction as responsible for the observed behavior, since the viscosity deviations should be positive.

Therefore, the present data should be explained only by means of structural terms such as the different molecular geometries of haloalkanes and the structural compatibility between every chloroalkane and the ether. Such effects, rather than Cl−O interactions between unlike molecules, play the decisive role over the determined properties.

Supporting Information Available:

Thermophysical and derived properties for the binary mixtures isomeric chlorobutane (1) + diisopropyl ether (2). This material is available free of charge via the Internet at http://pubs.acs.org.

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