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Temperature Dependence of Densities and Excess Molar Volumes of the Ternary Mixture (1-Butanol + Chloroform + Benzene) and its Binary Constituents (1-Butanol + Chloroform and 1-Butanol + Benzene)

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Abstract Densities ρ of the 1-butanol + chloroform + benzene ternary mixture and the 1-butanol + chloroform and 1-butanol + benzene binaries have been measured at six temperatures (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K and atmospheric pressure, using an oscillating U-tube densimeter. From these densities, excess molar volumes (V^{E}) were calculated and fitted to the Redlich–Kister equation for all binary mixtures and to the Nagata and Tamura equation for the ternary system. The Radojković et al. equation has been used to predict excess molar volumes of the ternary mixtures. Also, V^{E} data of the binary systems were correlated by the van der Waals (vdW1) and Twu–Coon–Bluck–Tilton (TCBT) mixing rules coupled with the Peng–Robinson–Stryjek–Vera (PRSV) equation of state. The prediction and correlation of V^{E} data for the ternary system were performed by the same models.

Keywords Benzene · Binary mixtures · 1-Butanol · Chloroform · Cubic EOS mixing rules · Densities · Excess molar volumes · Ternary mixture

1 Introduction

The study of thermodynamic properties of binary and ternary mixtures contributes to an understanding of the behavior of different liquids and functional groups. This information is very useful in the design of industrial processes and in the development of theories for the liquid state and predictive methods.

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This article is a continuation of our studies [1–6] of the excess molar volumes, V^E, for binaries and multicomponent mixtures containing different types of organic solvents widely used in various industries [3,4].

Experimental V^E data provide better insight into molecular interactions and can be used for testing of various correlation and prediction thermodynamic models, including cubic equations of state (CEOS).

Thus, in the current article, the experimental V^E results were used to analyze factors influencing molecular interactions and packing phenomena between unlike and like molecules.

In this article experimental measurements of the density of the 1-butanol (1) + chloroform (2) + benzene (3) ternary mixture and the 1-butanol (1) + chloroform (2) and 1-butanol (1) + benzene (3) binary constituents are presented, at temperatures of (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K and atmospheric pressure. The density data have been used to calculate excess molar volumes of the mixtures.

For the binary mixtures the ρ and V^E literature data cover the following temperatures: 303.15 K [7] for the 1-butanol (1) + chloroform (2) mixture and 293.15 K [8], 298.15 K [9], 303.15 K [10], and 308.15 K [9,11] for the 1-butanol (1) + benzene (3) mixture. Although literature V^E data were reported at several temperatures for the 1-butanol (1) + benzene (3) system, no values of V^E have been found for the entire temperature range studied here, especially for the 1-butanol (1) + chloroform (2) mixture. Also, to the best of our knowledge, literature data are not available for the investigated ternary system.

V^E's of the binary mixtures were fitted using the Redlich–Kister expansion [12], and the ternary data with the Nagata and Tamura [13] equation, while the Radojković et al. [14] equation was used for the prediction of the ternary data. The correlation of the binary data was performed by the PRSV CEOS using the selected mixing rules: (i) the composition-dependent van der Waals one-fluid (vdW1) mixing rules [15] and (ii) the mixing rules that incorporate the excess free energy model G^E developed by Twu and co-workers (TCBT) [16]. The prediction of V^E of the ternary system was performed by the same vdW1 and TCBT models. For correlation of V^E of the ternary data, only TCBT mixing rules were used.

2 Experimental

2.1 Materials

1-Butanol (Merck) was supplied with a purity >99.5 mass% (p.a.), chloroform (stabilized with amylene) by Riedel-de Haën with a purity of 99.8 mass%, while benzene by Aldrich with a purity of 99.9 mass% (HPLC). Table 1 lists the measured densities

Table 1 Densities ρ of the pure components at 298.15 K and atmospheric pressure

Component	$\rho(\mathrm{g \cdot cm^{-3}})$	
	Experimental	Literature
1-Butanol	0.805762	0.80575 [17]
Chloroform	1.479148	1.47970 [17], 1.47919 [18]
Benzene	0.873582	0.87360 [17]

of the pure components at 298.15, and they agree within ±4 × 10^{-5} g · cm^{-3} with most of the corresponding literature values [17,18].

2.2 Measurements

The density of the mixtures and the corresponding pure substances was measured with an Anton Paar Model DMA 5000 digital vibrating U-tube densimeter, provided with automatic viscosity correction, having a stated accuracy of ±5 × 10^{-6} g · cm^{-3}. The temperature in the cell was regulated to ±0.001 K with a built-in solid-state thermostat. The temperature in the cell was measured by means of two integrated Pt 100 platinum thermometers, and the stability was better then ±0.002 K. The reliability of the apparatus was verified daily with dry air and distilled freshly degassed water. To minimize the errors in composition, all mixtures were prepared by mass using the cell and the procedure described previously [19,20] and a Mettler AG 204 balance with a precision of 1 × 10^{-4} g. The uncertainty of the mole fraction calculation was less than ±1 × 10^{-4}. All molar quantities were based on the IUPAC relative atomic mass table. The experimental uncertainty in density is about ±1 × 10^{-5} g · cm^{-3}, while the average uncertainty in the excess molar volume is estimated to be less than 3 × 10^{-3} cm^3 · mol^{-1}.

3 Results and Discussion

3.1 Excess Molar Volumes

The excess molar volumes V^{E} were calculated from the equation,

$$V^{\mathrm{E}} = \sum_{i=1}^{n} x_i M_i \left[(1/\rho) - (1/\rho_i)\right] \tag{1}$$

where n is the number of components; x_i is the mole fraction of component i in the mixture while M_i is its molar mass; ρ and ρ_i are the measured densities of the mixture and pure component i, respectively.

Tables 2 and 3 list the measured densities ρ and the corresponding values of V^{E} for the 1-butanol (1) + chloroform (2) and 1-butanol (1) + benzene (3) binary systems as well as for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system. The experimental results for the chloroform (2) + benzene (3) binary system have been presented in our previous paper [4].

Data for the binary mixtures were fitted to a Redlich–Kister [12] (RK) polynomial of the type,

$$V_{ij}^{\mathrm{E}} = x_i x_j \sum_{p=0}^{k} A_p \left(2x_i - 1\right)^p \tag{2}$$

Table 2 Experimental densities ρ and excess molar volumes V^E for the 1-butanol + chloroform and 1-butanol + benzene binary systems, at $T = (288.15–313.15)$ K and atmospheric pressure

x_1	ρ $(\mathrm{g \cdot cm^{-3}})$	V^E $(\mathrm{cm^3 \cdot mol^{-1}})$	x_1	ρ $(\mathrm{g \cdot cm^{-3}})$	V^E $(\mathrm{cm^3 \cdot mol^{-1}})$	x_1	ρ $(\mathrm{g \cdot cm^{-3}})$	V^E $(\mathrm{cm^3 \cdot mol^{-1}})$
1-Butanol (1) + chloroform (2)								
$T = 288.15$ K								
0.0000	1.498077	0.0000	0.3474	1.238343	0.0432	0.7008	1.001030	−0.1334
0.0493	1.458967	0.0428	0.4003	1.201440	0.0163	0.7485	0.970420	−0.1414
0.0994	1.420117	0.0696	0.4610	1.159744	−0.0166	0.7987	0.938452	−0.1352
0.1499	1.381858	0.0777	0.4993	1.133810	−0.0406	0.8495	0.906492	−0.1256
0.2003	1.344302	0.0806	0.5517	1.098600	−0.0661	0.8953	0.877854	−0.0982
0.2476	1.309654	0.0759	0.5989	1.067377	−0.0904	0.9475	0.845530	−0.0551
0.2790	1.286969	0.0684	0.6510	1.033234	−0.1118	1.0000	0.813373	0.0000
$T = 293.15$ K								
0.0000	1.488638	0.0000	0.3474	1.231070	0.0593	0.7008	0.995760	−0.1209
0.0493	1.449824	0.0477	0.4003	1.194482	0.0330	0.7485	0.965404	−0.1308
0.0994	1.411277	0.0788	0.4610	1.153143	0.0001	0.7987	0.933697	−0.1268
0.1499	1.373340	0.0894	0.4993	1.127428	−0.0239	0.8495	0.901999	−0.1203
0.2003	1.336110	0.0940	0.5517	1.092600	−0.0496	0.8953	0.873588	−0.0953
0.2476	1.301761	0.0906	0.5989	1.061553	−0.0749	0.9475	0.841510	−0.0547
0.2790	1.279278	0.0834	0.6510	1.027696	−0.0976	1.0000	0.809573	0.0000
$T = 298.15$ K								
0.0000	1.479148	0.0000	0.3474	1.223746	0.0771	0.7008	0.990450	−0.1063
0.0493	1.440633	0.0528	0.4003	1.187479	0.0511	0.7485	0.960349	−0.1181
0.0994	1.402389	0.0883	0.4610	1.146500	0.0182	0.7987	0.928907	−0.1166
0.1499	1.364771	0.1019	0.4993	1.121002	−0.0057	0.8495	0.897472	−0.1130
0.2003	1.327863	0.1086	0.5517	1.086400	−0.0318	0.8953	0.869292	−0.0908
0.2476	1.293819	0.1064	0.5989	1.055688	−0.0577	0.9475	0.837462	−0.0526
0.2790	1.271534	0.0998	0.6510	1.022116	−0.0815	1.0000	0.805762	0.0000
$T = 303.15$ K								
0.0000	1.469612	0.0000	0.3474	1.216374	0.0957	0.7008	0.985097	−0.0906
0.0493	1.431398	0.0578	0.4003	1.180425	0.0704	0.7485	0.955255	−0.1047
0.0994	1.393449	0.0984	0.4610	1.139809	0.0373	0.7987	0.924082	−0.1059
0.1499	1.356152	0.1150	0.4993	1.114527	0.0138	0.8495	0.892910	−0.1052
0.2003	1.319568	0.1238	0.5517	1.080300	−0.0130	0.8953	0.864961	−0.0856
0.2476	1.285822	0.1233	0.5989	1.049776	−0.0393	0.9475	0.833386	−0.0506
0.2790	1.263746	0.1168	0.6510	1.016495	−0.0645	1.0000	0.801923	0.0000
$T = 308.15$ K								
0.0000	1.460025	0.0000	0.3474	1.208943	0.1157	0.7008	0.979698	−0.0739
0.0493	1.422115	0.0628	0.4003	1.173313	0.0910	0.7485	0.950115	−0.0901
0.0994	1.384450	0.1094	0.4610	1.133064	0.0577	0.7987	0.919208	−0.0937
0.1499	1.347474	0.1291	0.4993	1.107999	0.0345	0.8495	0.888303	−0.0961
0.2003	1.311210	0.1404	0.5517	1.074000	0.0074	0.8953	0.860590	−0.0797
0.2476	1.277767	0.1413	0.5989	1.043814	−0.0196	0.9475	0.829272	−0.0479
0.2790	1.255896	0.1352	0.6510	1.010818	−0.0456	1.0000	0.798053	0.0000
$T = 313.15$ K								
0.0000	1.450413	0.0000	0.3474	1.201478	0.1361	0.7008	0.974260	−0.0568
0.0493	1.412816	0.0674	0.4003	1.166161	0.1125	0.7485	0.944940	−0.0755
0.0994	1.375410	0.1214	0.4610	1.126294	0.0777	0.7987	0.914297	−0.0813
0.1499	1.338756	0.1441	0.4993	1.101418	0.0570	0.8495	0.883670	−0.0881
0.2003	1.302801	0.1586	0.5517	1.067800	0.0273	0.8953	0.856188	−0.0743
0.2476	1.269664	0.1608	0.5989	1.037803	0.0015	0.9475	0.825138	−0.0471
0.2790	1.248018	0.1536	0.6510	1.005107	−0.0267	1.0000	0.794147	0.0000
1-Butanol (1) + benzene (3)								
$T = 288.15$ K								
0.0000	0.884246	0.0000	0.2997	0.860741	0.1863	0.7010	0.833239	0.0938

Table 2 continued

x_1	ρ $(\mathrm{g \cdot cm^{-3}})$	V^{E} $(\mathrm{cm^3 \cdot mol^{-1}})$	x_1	ρ $(\mathrm{g \cdot cm^{-3}})$	V^{E} $(\mathrm{cm^3 \cdot mol^{-1}})$	x_1	ρ $(\mathrm{g \cdot cm^{-3}})$	V^{E} $(\mathrm{cm^3 \cdot mol^{-1}})$
0.0193	0.882483	0.0353	0.3532	0.856936	0.1846	0.7502	0.829979	0.0749
0.0534	0.879595	0.0758	0.4019	0.853504	0.1809	0.7945	0.827051	0.0579
0.1013	0.875720	0.1157	0.4525	0.850000	0.1716	0.8511	0.823296	0.0389
0.1509	0.871829	0.1462	0.4998	0.846738	0.1625	0.8961	0.820299	0.0260
0.2016	0.867984	0.1654	0.5532	0.843129	0.1455	0.9510	0.816663	0.0091
0.2018	0.867955	0.1669	0.6004	0.839985	0.1265	1.0000	0.813373	0.0000
0.2500	0.864382	0.1780	0.6493	0.836693	0.1115			
$T = 293.15\,\mathrm{K}$								
0.0000	0.878918	0.0000	0.2997	0.855806	0.1984	0.7010	0.828949	0.1016
0.0193	0.877168	0.0377	0.3532	0.852081	0.1972	0.7502	0.825772	0.0813
0.0534	0.874309	0.0815	0.4019	0.848721	0.1939	0.7945	0.822920	0.0629
0.1013	0.870495	0.1237	0.4525	0.845300	0.1840	0.8511	0.819258	0.0424
0.1509	0.866677	0.1555	0.4998	0.842111	0.1748	0.8961	0.816336	0.0282
0.2016	0.862908	0.1756	0.5532	0.838594	0.1565	0.9510	0.812791	0.0096
0.2018	0.862874	0.1777	0.6004	0.835529	0.1365	1.0000	0.809573	0.0000
0.2500	0.859372	0.1896	0.6493	0.832317	0.1205			
$T = 298.15\,\mathrm{K}$								
0.0000	0.873582	0.0000	0.2997	0.850849	0.2120	0.7010	0.824631	0.1114
0.0193	0.871844	0.0402	0.3532	0.847201	0.2116	0.7502	0.821537	0.0898
0.0534	0.869007	0.0881	0.4019	0.843914	0.2086	0.7945	0.818759	0.0701
0.1013	0.865255	0.1326	0.4525	0.840574	0.1984	0.8511	0.815196	0.0475
0.1509	0.861506	0.1660	0.4998	0.837460	0.1889	0.8961	0.812348	0.0320
0.2016	0.857807	0.1876	0.5532	0.834030	0.1697	0.9510	0.808897	0.0113
0.2018	0.857776	0.1894	0.6004	0.831042	0.1488	1.0000	0.805762	0.0000
0.2500	0.854344	0.2023	0.6493	0.827910	0.1320			
$T = 303.15\,\mathrm{K}$								
0.0000	0.868233	0.0000	0.2997	0.845866	0.2268	0.7010	0.820282	0.1223
0.0193	0.866507	0.0428	0.3532	0.842294	0.2272	0.7502	0.817269	0.0993
0.0534	0.863694	0.0945	0.4019	0.839080	0.2245	0.7945	0.814569	0.0779
0.1013	0.859995	0.1422	0.4525	0.835817	0.2142	0.8511	0.811102	0.0533
0.1509	0.856309	0.1778	0.4998	0.832778	0.2042	0.8961	0.808331	0.0361
0.2016	0.852685	0.2004	0.5532	0.829436	0.1841	0.9510	0.804977	0.0129
0.2018	0.852651	0.2026	0.6004	0.826525	0.1622	1.0000	0.801923	0.0000
0.2500	0.849285	0.2167	0.6493	0.823473	0.1443			
$T = 308.15\,\mathrm{K}$								
0.0000	0.862871	0.0000	0.2997	0.840854	0.2430	0.7010	0.815895	0.1346
0.0193	0.861158	0.0452	0.3532	0.837357	0.2442	0.7502	0.812965	0.1100
0.0534	0.858360	0.1019	0.4019	0.834214	0.2418	0.7945	0.810343	0.0867
0.1013	0.854713	0.1528	0.4525	0.831029	0.2313	0.8511	0.806975	0.0596
0.1509	0.851089	0.1907	0.4998	0.828059	0.2214	0.8961	0.804274	0.0415
0.2016	0.847536	0.2145	0.5532	0.824804	0.2002	0.9510	0.801025	0.0147
0.2018	0.847499	0.2170	0.6004	0.821974	0.1769	1.0000	0.798053	0.0000
0.2500	0.844201	0.2322	0.6493	0.819001	0.1580			
$T = 313.15\,\mathrm{K}$								
0.0000	0.857498	0.0000	0.2997	0.835830	0.2587	0.7010	0.811483	0.1466
0.0193	0.855809	0.0465	0.3532	0.832400	0.2615	0.7502	0.808640	0.1199
0.0534	0.853019	0.1088	0.4019	0.829324	0.2597	0.7945	0.806094	0.0946
0.1013	0.849433	0.1619	0.4525	0.826217	0.2488	0.8511	0.802822	0.0653
0.1509	0.845861	0.2030	0.4998	0.823320	0.2385	0.8961	0.800189	0.0463
0.2016	0.842375	0.2283	0.5532	0.820157	0.2155	0.9510	0.797051	0.0151
0.2018	0.842342	0.2305	0.6004	0.817402	0.1912	1.0000	0.794147	0.0000
0.2500	0.839110	0.2468	0.6493	0.814449	0.1778			

Table 3 Experimental densities ρ and excess molar volumes V^E for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system at $T = (288.15–313.15)$ K and atmospheric pressure

x_1	x_2	ρ $(g \cdot cm^{-3})$	V^E $(cm^3 \cdot mol^{-1})$	x_1	x_2	ρ $(g \cdot cm^{-3})$	V^E $(cm^3 \cdot mol^{-1})$
$T = 288.15$ K							
0.0906	0.0999	0.931435	0.1738	0.5389	0.1010	0.899497	0.1145
0.0787	0.2010	0.989208	0.2135	0.4856	0.1974	0.956866	0.1359
0.0698	0.2996	1.046683	0.2336	0.4200	0.2995	1.019836	0.1492
0.0591	0.4023	1.108113	0.2377	0.3606	0.4006	1.083361	0.1538
0.0547	0.4980	1.166249	0.2289	0.3000	0.4971	1.145811	0.1552
0.0405	0.5972	1.228764	0.2122	0.2388	0.5967	1.211706	0.1546
0.0294	0.6816	1.282824	0.2016	0.1801	0.6987	1.280679	0.1487
0.0203	0.7851	1.351079	0.1311	0.1207	0.7997	1.351169	0.1209
0.1793	0.0999	0.924387	0.2138	0.0615	0.8957	1.420354	0.0837
0.1712	0.1977	0.979833	0.2437	0.7128	0.1020	0.888415	0.0144
0.1417	0.3001	1.040893	0.2593	0.6404	0.2010	0.948600	0.0082
0.1197	0.3995	1.101288	0.2499	0.5584	0.2992	1.010178	0.0314
0.1001	0.5004	1.163756	0.2353	0.4790	0.4004	1.074927	0.0493
0.0793	0.5994	1.226676	0.2127	0.3993	0.4995	1.139982	0.0727
0.0588	0.7018	1.293355	0.1745	0.3206	0.5992	1.206986	0.0913
0.0433	0.7983	1.357306	0.1367	0.2393	0.6997	1.276532	0.1087
0.0186	0.9020	1.428941	0.0739	0.1605	0.7998	1.347822	0.0992
0.3607	0.0993	0.910702	0.2050	0.0809	0.8963	1.418925	0.0791
0.3199	0.2003	0.970092	0.2271	0.8111	0.0999	0.881131	−0.0822
0.2776	0.3061	1.033855	0.2362	0.7185	0.1999	0.942900	−0.0636
0.2384	0.3991	1.091477	0.2324	0.6289	0.2991	1.005673	−0.0556
0.1979	0.5010	1.155872	0.2256	0.5411	0.3998	1.070364	−0.0161
0.1587	0.5980	1.218808	0.2062	0.4498	0.5004	1.137082	0.0122
0.1217	0.6993	1.286139	0.1653	0.3579	0.6015	1.205629	0.0594
0.0803	0.7980	1.353781	0.1284	0.2669	0.6985	1.273712	0.0798
0.0410	0.8957	1.422419	0.0811	0.1791	0.7991	1.345658	0.0964
$T = 293.15$ K							
0.0906	0.0999	0.925887	0.1778	0.5389	0.1010	0.894582	0.1296
0.0787	0.2010	0.983315	0.2141	0.4856	0.1974	0.951609	0.1455
0.0698	0.2996	1.040436	0.2320	0.4200	0.2995	1.014123	0.1585
0.0591	0.4023	1.101474	0.2346	0.3606	0.4006	1.077169	0.1639
0.0547	0.4980	1.159228	0.2256	0.3000	0.4971	1.139140	0.1650
0.0405	0.5972	1.221313	0.2085	0.2388	0.5967	1.204553	0.1616
0.0294	0.6816	1.275166	0.1867	0.1801	0.6987	1.272941	0.1579
0.0203	0.7851	1.342752	0.1284	0.1207	0.7997	1.342891	0.1273
0.1793	0.0999	0.918970	0.1778	0.0615	0.8957	1.411506	0.0887
0.1712	0.1977	0.974084	0.2482	0.7128	0.1020	0.883840	0.0218
0.1417	0.3001	1.034746	0.2614	0.6404	0.2010	0.943582	0.0179
0.1197	0.3995	1.094734	0.2510	0.5584	0.2992	1.004682	0.0429
0.1001	0.5004	1.156780	0.2354	0.4790	0.4004	1.068925	0.0619
0.0793	0.5994	1.219254	0.2127	0.3993	0.4995	1.133454	0.0861
0.0588	0.7018	1.285446	0.1748	0.3206	0.5992	1.199949	0.1019
0.0433	0.7983	1.348934	0.1370	0.2393	0.6997	1.268877	0.1213
0.0186	0.9020	1.420062	0.0720	0.1605	0.7998	1.339580	0.1095
0.3607	0.0993	0.905562	0.2148	0.0809	0.8963	1.410088	0.0863
0.3199	0.2003	0.964564	0.2349	0.8111	0.0999	0.876597	−0.0636
0.2776	0.3061	1.027894	0.2427	0.7185	0.1999	0.938013	−0.0543
0.2384	0.3991	1.085106	0.2383	0.6289	0.2991	1.000288	−0.0435
0.1979	0.5010	1.149034	0.2311	0.5411	0.3998	1.064458	−0.0020
0.1587	0.5980	1.211497	0.2117	0.4498	0.5004	1.130614	0.0282
0.1217	0.6993	1.278317	0.1706	0.3579	0.6015	1.198647	0.0710

Table 3 continued

x_1	x_2	ρ $(\text{g} \cdot \text{cm}^{-3})$	V^{E} $(\text{cm}^3 \cdot \text{mol}^{-1})$	x_1	x_2	ρ $(\text{g} \cdot \text{cm}^{-3})$	V^{E} $(\text{cm}^3 \cdot \text{mol}^{-1})$
0.0803	0.7980	1.345434	0.1330	0.2669	0.6985	1.266105	0.0936
0.0410	0.8957	1.413555	0.0837	0.1791	0.7991	1.337448	0.1079
$T = 298.15\,\text{K}$							
0.0906	0.0999	0.920323	0.1823	0.5389	0.1010	0.889639	0.1465
0.0787	0.2010	0.977401	0.2154	0.4856	0.1974	0.946317	0.1571
0.0698	0.2996	1.034161	0.2314	0.4200	0.2995	1.008370	0.1698
0.0591	0.4023	1.094806	0.2321	0.3606	0.4006	1.070941	0.1752
0.0547	0.4980	1.152171	0.2230	0.3000	0.4971	1.132428	0.1761
0.0405	0.5972	1.213828	0.2050	0.2388	0.5967	1.197330	0.1716
0.0294	0.6816	1.267429	0.1744	0.1801	0.6987	1.265158	0.1680
0.0203	0.7851	1.334382	0.1259	0.1207	0.7997	1.334546	0.1356
0.1793	0.0999	0.913529	0.2285	0.0615	0.8957	1.402612	0.0939
0.1712	0.1977	0.968308	0.2539	0.7128	0.1020	0.879232	0.0314
0.1417	0.3001	1.028567	0.2647	0.6404	0.2010	0.938529	0.0295
0.1197	0.3995	1.088148	0.2530	0.5584	0.2992	0.999147	0.0563
0.1001	0.5004	1.149765	0.2366	0.4790	0.4004	1.062876	0.0767
0.0793	0.5994	1.211791	0.2135	0.3993	0.4995	1.126878	0.1013
0.0588	0.7018	1.277502	0.1751	0.3206	0.5992	1.192843	0.1154
0.0433	0.7983	1.340520	0.1374	0.2393	0.6997	1.261173	0.1350
0.0186	0.9020	1.411118	0.0713	0.1605	0.7998	1.331279	0.1212
0.3607	0.0993	0.900395	0.2262	0.0809	0.8963	1.401202	0.0939
0.3199	0.2003	0.959004	0.2444	0.8111	0.0999	0.872028	−0.0423
0.2776	0.3061	1.021894	0.2510	0.7185	0.1999	0.933090	−0.0430
0.2384	0.3991	1.078697	0.2456	0.6289	0.2991	0.994861	−0.0292
0.1979	0.5010	1.142154	0.2379	0.5411	0.3998	1.058510	0.0139
0.1587	0.5980	1.204145	0.2180	0.4498	0.5004	1.124115	0.0448
0.1217	0.6993	1.270448	0.1769	0.3579	0.6015	1.191589	0.0861
0.0803	0.7980	1.337037	0.1385	0.2669	0.6985	1.258449	0.1086
0.0410	0.8957	1.404643	0.0865	0.1791	0.7991	1.329180	0.1207
$T = 303.15\,\text{K}$							
0.0906	0.0999	0.914732	0.1879	0.5389	0.1010	0.884667	0.1641
0.0787	0.2010	0.971460	0.2174	0.4856	0.1974	0.940990	0.1697
0.0698	0.2996	1.027856	0.2314	0.4200	0.2995	1.002577	0.1823
0.0591	0.4023	1.088107	0.2299	0.3606	0.4006	1.064666	0.1880
0.0547	0.4980	1.145079	0.2209	0.3000	0.4971	1.125667	0.1886
0.0405	0.5972	1.206307	0.2018	0.2388	0.5967	1.190050	0.1834
0.0294	0.6816	1.259585	0.1668	0.1801	0.6987	1.257328	0.1789
0.0203	0.7851	1.325972	0.1235	0.1207	0.7997	1.326143	0.1450
0.1793	0.0999	0.908057	0.2379	0.0615	0.8957	1.393672	0.0993
0.1712	0.1977	0.962500	0.2606	0.7128	0.1020	0.874591	0.0418
0.1417	0.3001	1.022349	0.2694	0.6404	0.2010	0.933435	0.0424
0.1197	0.3995	1.081525	0.2559	0.5584	0.2992	0.993567	0.0712
0.1001	0.5004	1.142715	0.2382	0.4790	0.4004	1.056782	0.0927
0.0793	0.5994	1.204292	0.2145	0.3993	0.4995	1.120257	0.1176
0.0588	0.7018	1.269511	0.1762	0.3206	0.5992	1.185676	0.1309
0.0433	0.7983	1.332062	0.1382	0.2393	0.6997	1.253417	0.1498
0.0186	0.9020	1.402114	0.0715	0.1605	0.7998	1.322923	0.1339
0.3607	0.0993	0.895193	0.2392	0.0809	0.8963	1.392267	0.1020
0.3199	0.2003	0.953408	0.2552	0.8111	0.0999	0.867437	−0.0214
0.2776	0.3061	1.015857	0.2604	0.7185	0.1999	0.928130	−0.0308
0.2384	0.3991	1.072249	0.2539	0.6289	0.2991	0.989396	−0.0141
0.1979	0.5010	1.135231	0.2458	0.5411	0.3998	1.052519	0.0309
0.1587	0.5980	1.196748	0.2253	0.4498	0.5004	1.117570	0.0624

Table 3 continued

x_1	x_2	ρ $(\text{g}\cdot\text{cm}^{-3})$	V^E $(\text{cm}^3\cdot\text{mol}^{-1})$	x_1	x_2	ρ $(\text{g}\cdot\text{cm}^{-3})$	V^E $(\text{cm}^3\cdot\text{mol}^{-1})$
0.1217	0.6993	1.262540	0.1835	0.3579	0.6015	1.184465	0.1035
0.0803	0.7980	1.328606	0.1436	0.2669	0.6985	1.250742	0.1246
0.0410	0.8957	1.395692	0.0892	0.1791	0.7991	1.320855	0.1347
$T = 308.15\,\text{K}$							
0.0906	0.0999	0.909117	0.1942	0.5389	0.1010	0.879675	0.1814
0.0787	0.2010	0.965493	0.2199	0.4856	0.1974	0.935620	0.1838
0.0698	0.2996	1.021520	0.2320	0.4200	0.2995	0.996737	0.1964
0.0591	0.4023	1.081372	0.2285	0.3606	0.4006	1.058343	0.2022
0.0547	0.4980	1.137945	0.2197	0.3000	0.4971	1.118863	0.2019
0.0405	0.5972	1.198745	0.1991	0.2388	0.5967	1.182714	0.1966
0.0294	0.6816	1.251642	0.1631	0.1801	0.6987	1.249442	0.1910
0.0203	0.7851	1.317514	0.1215	0.1207	0.7997	1.317691	0.1550
0.1793	0.0999	0.902557	0.2484	0.0615	0.8957	1.384679	0.1051
0.1712	0.1977	0.956662	0.2683	0.7128	0.1020	0.869909	0.0534
0.1417	0.3001	1.016091	0.2755	0.6404	0.2010	0.928301	0.0563
0.1197	0.3995	1.074857	0.2603	0.5584	0.2992	0.987945	0.0871
0.1001	0.5004	1.135626	0.2404	0.4790	0.4004	1.050635	0.1104
0.0793	0.5994	1.196753	0.2160	0.3993	0.4995	1.113580	0.1355
0.0588	0.7018	1.261470	0.1781	0.3206	0.5992	1.178458	0.1474
0.0433	0.7983	1.323565	0.1388	0.2393	0.6997	1.245604	0.1659
0.0186	0.9020	1.393049	0.0726	0.1605	0.7998	1.314511	0.1476
0.3607	0.0993	0.889956	0.2536	0.0809	0.8963	1.383274	0.1109
0.3199	0.2003	0.947777	0.2670	0.8111	0.0999	0.862844	−0.0032
0.2776	0.3061	1.009777	0.2713	0.7185	0.1999	0.923125	−0.0174
0.2384	0.3991	1.065755	0.2636	0.6289	0.2991	0.983881	0.0025
0.1979	0.5010	1.128264	0.2545	0.5411	0.3998	1.046476	0.0493
0.1587	0.5980	1.189307	0.2333	0.4498	0.5004	1.110971	0.0814
0.1217	0.6993	1.254576	0.1913	0.3579	0.6015	1.177285	0.1222
0.0803	0.7980	1.320130	0.1490	0.2669	0.6985	1.242979	0.1417
0.0410	0.8957	1.386690	0.0921	0.1791	0.7991	1.312472	0.1497
$T = 313.15\,\text{K}$							
0.0906	0.0999	0.903502	0.1992	0.5389	0.1010	0.874675	0.1969
0.0787	0.2010	0.959515	0.2220	0.4856	0.1974	0.930242	0.1962
0.0698	0.2996	1.015161	0.2332	0.4200	0.2995	0.990878	0.2099
0.0591	0.4023	1.074634	0.2259	0.3606	0.4006	1.052000	0.2159
0.0547	0.4980	1.130771	0.2200	0.3000	0.4971	1.112032	0.2153
0.0405	0.5972	1.191159	0.1966	0.2388	0.5967	1.175356	0.2096
0.0294	0.6816	1.243655	0.1609	0.1801	0.6987	1.241530	0.2032
0.0203	0.7851	1.309028	0.1198	0.1207	0.7997	1.309220	0.1646
0.1793	0.0999	0.897040	0.2590	0.0615	0.8957	1.375665	0.1108
0.1712	0.1977	0.950816	0.2750	0.7128	0.1020	0.865196	0.0652
0.1417	0.3001	1.009798	0.2831	0.6404	0.2010	0.923143	0.0696
0.1197	0.3995	1.068159	0.2655	0.5584	0.2992	0.982294	0.1028
0.1001	0.5004	1.128523	0.2421	0.4790	0.4004	1.044466	0.1274
0.0793	0.5994	1.189204	0.2166	0.3993	0.4995	1.106856	0.1549
0.0588	0.7018	1.253412	0.1797	0.3206	0.5992	1.171241	0.1618
0.0433	0.7983	1.315067	0.1380	0.2393	0.6997	1.237743	0.1834
0.0186	0.9020	1.383942	0.0747	0.1605	0.7998	1.306053	0.1627
0.3607	0.0993	0.884700	0.2679	0.0809	0.8963	1.374240	0.1208
0.3199	0.2003	0.942119	0.2794	0.8111	0.0999	0.858299	0.0064
0.2776	0.3061	1.003675	0.2821	0.7185	0.1999	0.918097	−0.0049
0.2384	0.3991	1.059428	0.2575	0.6289	0.2991	0.978341	0.0184
0.1979	0.5010	1.121270	0.2636	0.5411	0.3998	1.040403	0.0676

Table 3 continued

x_1	x_2	ρ $(\mathrm{g \cdot cm^{-3}})$	V^E $(\mathrm{cm^3 \cdot mol^{-1}})$	x_1	x_2	ρ $(\mathrm{g \cdot cm^{-3}})$	V^E $(\mathrm{cm^3 \cdot mol^{-1}})$
0.1587	0.5980	1.181862	0.2398	0.4498	0.5004	1.104344	0.1003
0.1217	0.6993	1.246591	0.1989	0.3579	0.6015	1.170087	0.1402
0.0803	0.7980	1.311632	0.1543	0.2669	0.6985	1.235174	0.1599
0.0410	0.8957	1.377672	0.0946	0.1791	0.7991	1.304056	0.1652

Table 4 Parameters A_p of Eq. 2 and the corresponding σ for the binary mixtures

T (K)	A_0	A_1	A_2	A_3	$\sigma\,(\mathrm{cm^3 \cdot mol^{-1}})$
1-Butanol (1) + chloroform (2)					
288.15	−0.1560	−1.1307	−0.0291	−0.0178	0.0024
293.15	−0.0893	−1.1449	−0.0304	−0.0563	0.0023
298.15	−0.0162	−1.1487	−0.0234	−0.0999	0.0023
303.15	0.0616	−1.1487	−0.0036	−0.1630	0.0023
308.15	0.1429	−1.1688	0.0071	−0.1847	0.0022
313.15	0.2277	−1.1652	0.0147	−0.2317	0.0037
1-Butanol (1) + benzene (3)					
288.15	0.6370	−0.5121	0.1825	−0.1858	0.0027
293.15	0.6827	−0.5362	0.1967	−0.2141	0.0031
298.15	0.7429	−0.5456	0.1876	−0.2473	0.0035
303.15	0.8026	−0.5673	0.2010	−0.2891	0.0038
308.15	0.8636	−0.5964	0.2457	−0.2946	0.0041
313.15	0.9346	−0.5902	0.2435	−0.3799	0.0044

where A_p denotes the adjustable parameters and $k + 1$ is their number determined by means of the F-test [21].

Adjustable parameters of the fits at each temperature separately and the corresponding root-mean-square deviations (rmsd), σ, defined by the equation,

$$\sigma = \left(\sum_{i=1}^{m} \left(V^{E}_{\mathrm{exp},i} - V^{E}_{\mathrm{cal},i} \right)^2 / m \right)^{1/2} \tag{3}$$

are given in Table 4. In Eq. 3, m is the number of experimental data points.

The ternary V^E's were predicted using the Radojković et al. [14] equation;

$$V^E_{123} = V^E_{12} + V^E_{13} + V^E_{23} \tag{4}$$

where V^E_{12}, V^E_{13}, and V^E_{23} represent the binary excess molar volumes calculated by Eq. 2, while x_1, x_2, and x_3 are the mole fractions of the ternary system.

The ternary V^E were correlated by the Nagata and Tamura [13] model;

$$\begin{aligned} V^E_{123} = V^E_{12} + V^E_{13} + V^E_{23} + x_1x_2x_3RT(B_0 - B_1x_1 - B_2x_2 - B_3x_1^2 \\ - B_4x_2^2 - B_5x_1x_2 - B_6x_1^3 - B_7x_2^3 - B_8x_1^2x_2) \end{aligned} \tag{5}$$

where $B_0, B_1, \ldots, B_8$ are the adjustable parameters of the ternary contribution obtained from the ternary experimental V^E data. These fitted parameters of Eq. 5 along with the corresponding σ for Eqs. 4 and 5, calculated according to Eq. 3, are given in Table 5.

In Fig. 1a, b the experimental V^E data for the 1-butanol (1) + chloroform (2) and 1-butanol (1) + benzene (3) binary systems were plotted for the following investigated temperatures: (288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K. As can be seen from Fig. 1a, the 1-butanol (1) + chloroform (2) system exhibits an S-shape of the $V^E - x_1$ curves (maximum with positive and minimum with negative values of V^E), with V^E values increasing with temperature from 288.15 K to 313.15 K. As can be seen from Fig. 1b, the 1-butanol (1) + benzene (3) system shows positive V^E values over the whole concentration range, also with V^E values increasing with increasing temperature. Comparisons of our experimental results of V^E for the 1-butanol (1) + benzene (3) system at (293.15, 298.15, 303.15, and 308.15) K with the data reported previously [8–10] show that our V^E data are in very good agreement (for the maximum V^E values, at $x_1 = 0.35$, the difference is less than 4% for all studied temperatures). Larger disagreements exist only for the case of data reported by Bhardway et al. [11] at 308.15 K (nearly 15%). Since the 1-butanol (1) + chloroform (2) system exhibits an S-shape of the $V^E - x_1$ curves, comparisons between the experimental and literature data [7] at 303.15 K were performed in the area of maximum (at $x_1 = 0.2$) and minimum V^E values (at $x_1 = 0.8$). The maximum experimental V^E value is higher comparing to the literature (about 10%), while V^E values for the minimum are in very good agreement (the difference is about 3%).

For the investigated mixtures, V^E data can be explained qualitatively on the basis of the following resulting opposite contributions that are predominant in a certain mole-fraction region: (i) the positive values in the 1-butanol lower region may be due to the disruptive or stretching effects on the self-associated molecular structure of 1-butanol, (ii) the negative values are thought to be due to the specific interactions between unlike molecules, and (iii) the accommodation of benzene or chloroform in the intermolecular space of the 1-butanol network structure leads to more dense packing and results in the volume reduction that occurs in the region rich in 1-butanol. The magnitude and sign of V^E have been interpreted as the result of a balance between these effects.

V^E's of the 1-butanol (1) + chloroform (2) mixture plotted in Fig. 1a exhibit the S-shape form of the $V^E - x_1$ curves. The positive values in the 1-butanol lower region are a consequence of a rupture of the hydrogen bonding of a self-associated aggregate of 1-butanol and a steric effect between the alkyl chain of the alcohol and the Cl atom of the chloroform. The maximum values of V^E appear at smaller x_1 where the dissociation of 1-butanol agglomerates is more extensive. On the other hand, the presence of a larger amount of 1-butanol has an effect of changing the positive sign of V^E to negative, suggesting that a more compact structure is obtained. Namely, chloroform molecules are fitted into a three-dimensional associated 1-butanol network showing that their breaking is not complete. Also, the negative V^E values arise from changes of free volumes at the real condition and specific interactions between the 1-butanol chain fragment and molecules of chloroform. The disruptive effect of self-associated aggregates of 1-butanol increases with increasing temperature, while the

Table 5 Parameters B_i of Eq. 5 and the corresponding σ of the prediction, Eq. 4, and correlation, Eq. 5, for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system

T (K)	288.15	293.15	298.15	303.15	308.15	313.15
Prediction						
σ (cm^3 · mol^{-1})	0.0289	0.0291	0.0293	0.0297	0.0306	0.0303
Correlation						
B_0	0.1538×10^{-3}	0.1928×10^{-3}	0.3019×10^{-3}	0.4563×10^{-3}	0.4875×10^{-3}	0.7643×10^{-3}
B_1	-0.1400×10^{-2}	-0.1469×10^{-2}	-0.1197×10^{-2}	-0.4973×10^{-3}	-0.6068×10^{-3}	0.8462×10^{-3}
B_2	-0.4987×10^{-2}	-0.4595×10^{-2}	-0.4061×10^{-2}	-0.3511×10^{-2}	-0.3116×10^{-2}	-0.2063×10^{-2}
B_3	0.3263×10^{-3}	0.1158×10^{-2}	0.1871×10^{-2}	0.1417×10^{-2}	0.1954×10^{-2}	-0.7815×10^{-3}
B_4	0.8547×10^{-2}	0.7256×10^{-2}	0.6306×10^{-2}	0.5629×10^{-2}	0.4220×10^{-2}	0.2233×10^{-2}
B_5	0.1130×10^{-1}	0.1088×10^{-1}	0.9545×10^{-2}	0.7364×10^{-2}	0.7620×10^{-2}	0.6361×10^{-2}
B_6	0.4206×10^{-2}	0.2605×10^{-2}	0.8080×10^{-3}	-0.1179×10^{-3}	-0.9328×10^{-3}	0.7429×10^{-3}
B_7	-0.5114×10^{-2}	-0.3927×10^{-2}	-0.3302×10^{-2}	-0.2780×10^{-2}	-0.1638×10^{-2}	-0.2917×10^{-3}
B_8	-0.1649×10^{-1}	-0.1489×10^{-1}	-0.1259×10^{-1}	-0.8915×10^{-2}	-0.8869×10^{-2}	-0.7672×10^{-2}
σ (cm^3 · mol^{-1})	0.0059	0.0044	0.0035	0.0035	0.0040	0.0049

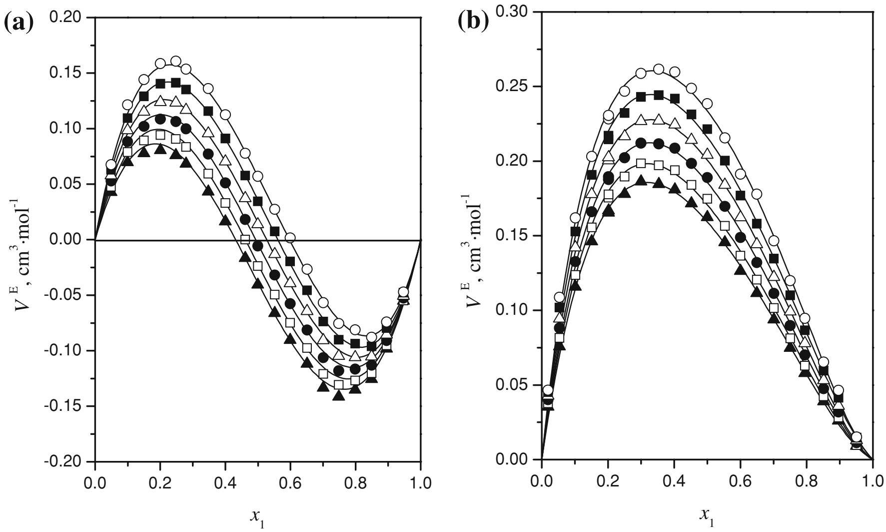

Fig. 1 Experimental values of V^E data for (**a**) 1-butanol (1) + chloroform (2) and (**b**) 1-butanol (1) + benzene (2). Symbols refer to experimental points at: ▲ 288.15 K; □ 293.15 K; ● 298.15 K; △ 303.15 K; ■ 308.15 K; and ○ 313.15 K, while the lines represent the results calculated by Eq. 2

number of cross-associated H bonds decreases in the alcohol-rich region causing less negative V^E.

Table 2 and Fig. 1b show that experimental V^E data of the 1-butanol (1) + benzene (3) mixture are positive over the whole composition range at all investigated temperatures. These positive values of V^E can be qualitatively explained by disruptive or stretching effects on the self-associated molecular structure of 1-butanol. The possible formation of weak H$\cdots\pi$ bonding between the OH group of 1-butanol and π electrons of the benzene ring has not resulted in negative V^E values. As suggested by Assarson and Eirich [22], components of similar molecular sizes such as 1-butanol and benzene (vdW volumes of 52.4 cm$^3\cdot$ mol^{-1} and 48.4 cm$^3\cdot$ mol^{-1}, respectively) mix with positive values of V^E. From Table 2 and Fig. 1b, it can be seen that in all cases V^E of this system increases with increasing temperature. It is clear that a rupture of the hydrogen bonding of self-associated molecules of 1-butanol increases with increasing temperature leading to higher positive V^E results. The factors that cause changes of V^E for the chloroform (2) + benzene (3) binary mixture have been described previously [3,4].

Ternary V^E data can be plotted for lines of constant $z(= x_1/x_3)$. Figure 2 shows experimental values of V^E at 303.15 K and fitted lines of z obtained by means of Eq. 5. From this figure it is observed that a larger amount of benzene up to z_3 gives expansive values of V^E which change in a contractive way when adding a large amount of 1-butanol (z_5 and z_6) at a lower mole fraction of chloroform. This effect could be attributed to the interaction of 1-butanol and benzene with chloroform. Isolines at constant values of the ternary V^E at 288.15 K and 315.15 K obtained by Eq. 5 were plotted in Fig. 3a and b, respectively. Positive V^E values were obtained over most of

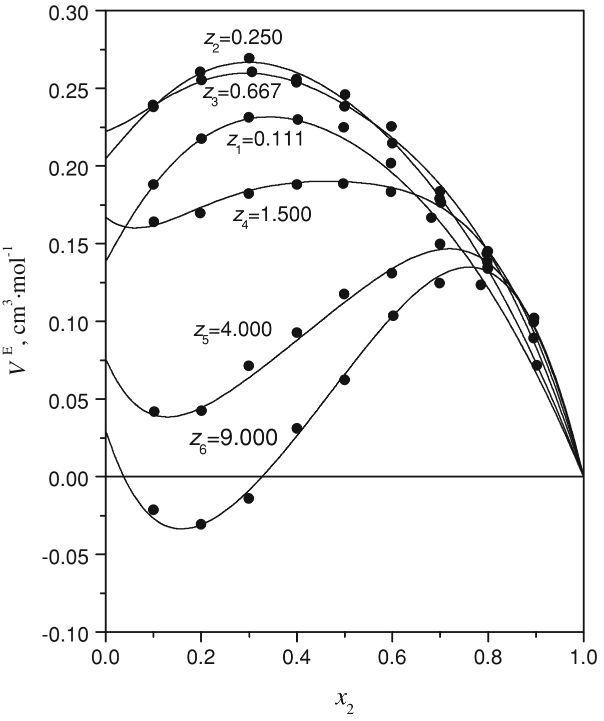

Fig. 2 Excess molar volumes (V^E) for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system, at 303.15 K and atmospheric pressure, along the curves of constant ratio $z = x_1/x_3$ as a function of the chloroform composition. Symbols represent the experimental points. Solid curves were calculated by Eq. 5

the composition range, except in the region which is close to 1-butanol in the binary mixture with chloroform where the sign is negative. Namely, the latter contractive trend of V^E shown in Fig. 1a is due to greater packing in this system. This situation could be also confirmed in Fig. 2 as already pointed out for $z_6 = 9.000$ and in the low region of chloroform at 303.15 K. Maximum values of V^E appear close to the chloroform (2) + benzene (3) binary mixture suggesting that the unpacking effect, which is the result of complex formation of chloroform (2) + benzene (3) and the disruptive effect on the self-associated molecules of 1-butanol, are more dominant. The increase in temperature, as can be seen from Fig. 3a and b, only confirms this viewpoint.

It is also observed that maximum values of V^E increase with increasing temperature. As expected, this expansive trend with increasing temperature means that the negative region of V^E is diminished. As shown in Fig. 3c and d, the ternary contribution ΔV^E_{123} is positive and relatively significant with a maximum V^E located around the center of the triangular diagram at 288.15 K, and shifted toward the chloroform (2) + benzene (3) binary system at 313.15 K. ΔV^E_{123} is about 38% at 288.15 K and about 26% at 313.15 K of the total magnitude of V^E_{123}, respectively.

The three-dimensional surfaces of V^E_{123} generated from the Nagata and Tamura Eq. 5 at 288.15 K and 313.15 K were plotted in Fig. 4a and b, respectively. The ternary V^E_{123}

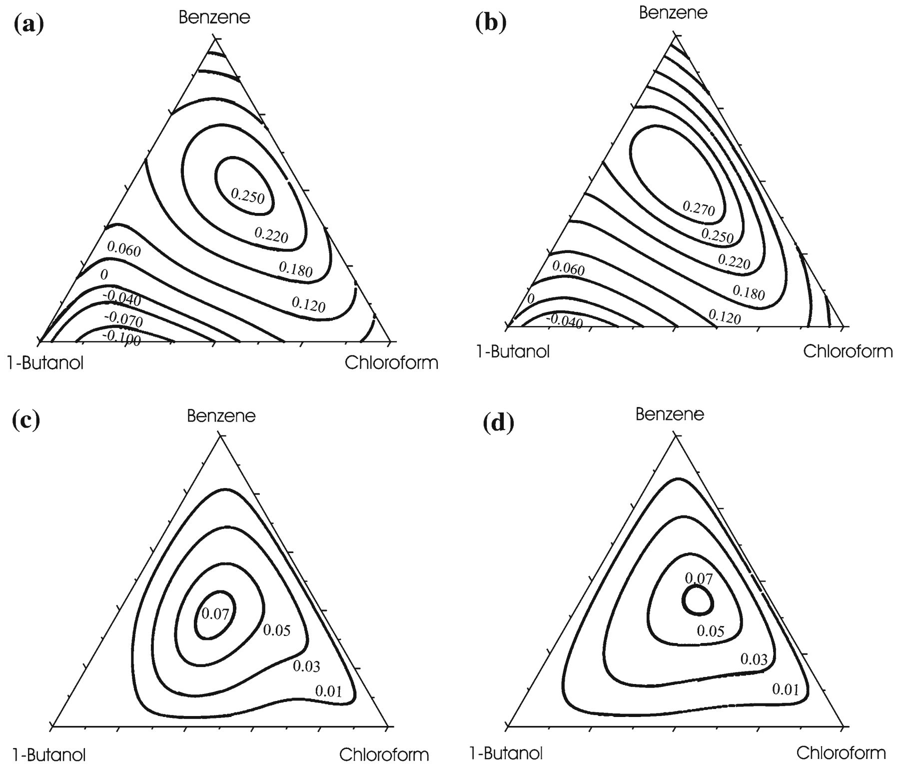

Fig. 3 Curves of constant $V^{\mathrm{E}}_{123}(\mathrm{cm}^3 \cdot \mathrm{mol}^{-1})$ for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system, at (**a**) 288.15 K and (**b**) 313.15 K. Lines represent results calculated by Eq. 5. Curves of ternary contribution $\Delta V^{\mathrm{E}}(\mathrm{cm}^3 \cdot \mathrm{mol}^{-1})$, $\Delta V^{\mathrm{E}} = V^{\mathrm{E}}_{123} - V^{\mathrm{E}}_{12} - V^{\mathrm{E}}_{13} - V^{\mathrm{E}}_{23}$, for the same system at (**c**) 288.15 K, and (**d**) 313.15 K. Lines represent results calculated by the ternary contribution of Eq. 5

show large positive and small negative values, and they show insignificant changes with increasing temperature.

3.2 Cubic EOS Mixing Rules

Stryjek and Vera [23] proposed a two-parameter cubic equation of state (PRSV CEOS) as a modification of the Peng–Robinson equation in the following form:

$$P = \frac{RT}{V - b} - \frac{a}{V\,(V + b) + b\,(V - b)} \tag{6}$$

where P, T, and V are the pressure, temperature, and molar volume, respectively, and R is the universal gas constant.

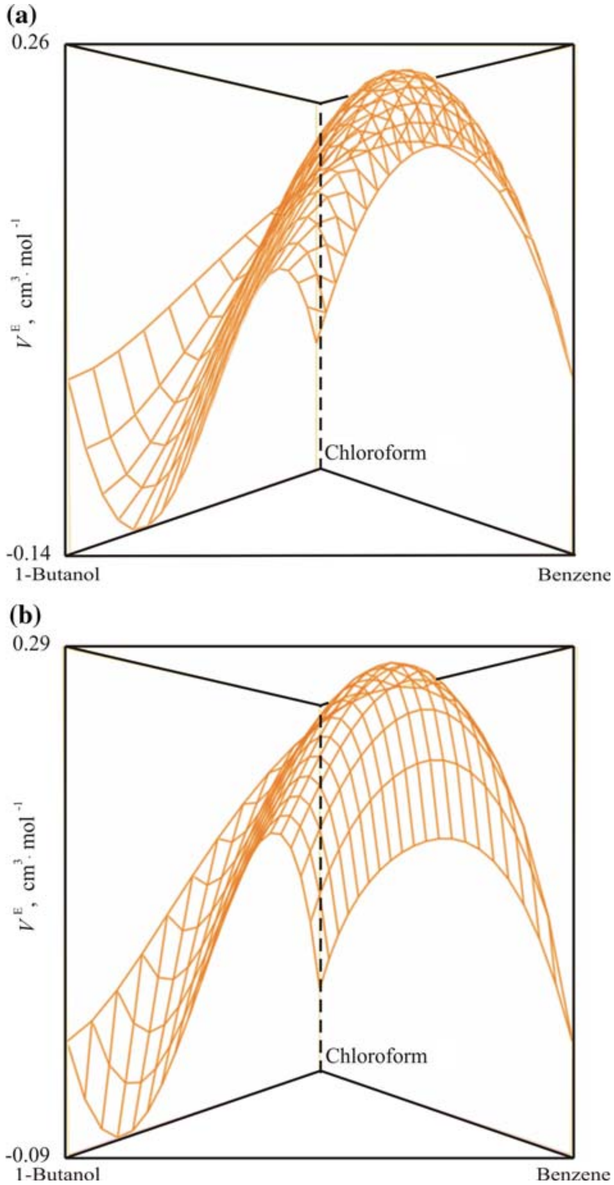

Fig. 4 Three-dimensional surfaces for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system at (**a**) 288.15 K and (**b**) 313.15 K, generated by Eq. 5

The temperature-dependent energy a_i and covolume b_i are pure component parameters obtained from

$$a_i(T) = 0.457235\frac{(RT_{\mathrm{c}i})^2}{P_{\mathrm{c}i}}\left[1 + m_i\left(1 - T_{\mathrm{r}i}^{1/2}\right)\right]^2 \qquad (7)$$

$$b_i = 0.077796 \frac{RT_{ci}}{P_{ci}} \tag{8}$$

where T_{ci} and P_{ci} are the critical temperature and critical pressure of component i, respectively.

In Eq. 7, m is a parameter given by

$$m_i = k_{0i} + k_{1i} \left(1 + T_{ri}^{1/2}\right)(0.7 - T_{ri}) \text{ and} \tag{9}$$

$$k_{0i} = 0.378893 + 1.4897153\omega_i - 0.1713848\omega_i^2 + 0.0196554\omega_i^3 \tag{10}$$

where T_{ri} stands for the reduced temperature (T/T_{ci}), ω_i is the acentric factor, and k_{1i} denotes the pure substance adjustable parameter [23].

Two different mixing rules for determining the PRSV CEOS mixing parameters a and b were investigated here: vdW1 and TCBT. The vdW1 mixing rule [15] is expressed as

$$a = \sum_i \sum_j x_i x_j \left(a_i a_j\right)^{1/2} \left[1 - k_{ij} + l_{ij}\left(x_i - x_j\right)\right] \tag{11}$$

and

$$b = \sum_i \sum_j x_i x_j \left(b_i b_j\right)^{1/2} \left(1 - m_{ij}\right) \tag{12}$$

where k_{ij}, l_{ij}, and m_{ij} are the adjustable binary interaction parameters, estimated for both binary mixtures. Since the TCBT mixing rule [16] has been applied successfully in our previous articles [1–4], it was used here. This mixing rule, developed for no reference pressure conditions and based on the van der Waals reference fluid (vdW), can be represented as

$$\begin{aligned} \frac{G^E}{RT} - \frac{G^E_{\text{vdW}}}{RT} + (Z - Z_{\text{vdW}}) = \ln\left[\left(\frac{V^*_{\text{vdW}} - 1}{V^* - 1}\right)\left(\frac{b_{\text{vdW}}}{b}\right)\right] \\ - \frac{1}{w - u}\left[\frac{a^*}{b^*}\ln\left(\frac{V^* + w}{V^* + u}\right)\right. \\ \left. - \frac{a^*_{\text{vdW}}}{b^*_{\text{vdW}}}\ln\left(\frac{V^*_{\text{vdW}} + w}{V^*_{\text{vdW}} + u}\right)\right] \end{aligned} \tag{13}$$

where G^E_{vdW} is calculated for the PRSV CEOS. Parameters a_{vdW} and b_{vdW} were calculated by Eqs. 11 and 12. All reduced parameters a^*, b^*, a^*_{vdW}, and b^*_{vdW} are determined as follows:

$$a^* = Pa/R^2T^2 \quad b^* = Pb/RT \tag{14}$$

The reduced volume $V^* = V/b = Z/b^*$ is defined at P and T of the mixture. Equation 6 given in the form for the factor compressibility Z was used to calculate Z and Z_{vdW}. Bearing in mind that V^* does not have an explicit solution, an iterative technique was required for the calculation.

The NRTL equation [24] was applied as the G^{E} model in Eq. 13 according to the expression,

$$\frac{G^{\mathrm{E}}}{RT} = \sum_i x_i \frac{\sum_j x_j G_{ji} \tau_{ji}}{\sum_k x_k G_{ki}} \tag{15}$$

where for binary mixtures,

$$\begin{aligned} G_{12} &= \exp\left(-\alpha_{12}\tau_{12}\right) \quad G_{21} = \exp\left(-\alpha_{12}\tau_{21}\right) \\ \tau_{12} &= \frac{\Delta g_{12}}{RT} = \left(g_{12} - g_{22}\right)/RT \quad \tau_{21} = \frac{\Delta g_{21}}{RT} = \left(g_{21} - g_{11}\right)/RT \end{aligned} \tag{16}$$

and for a ternary mixture,

$$\tau'_{ij} = \tau_{ij} + \frac{\sum_{k=1}^{n} x_k \Delta g_{ijk}}{RT} \tag{17}$$

Δg_{12} and Δg_{21} are the binary energy parameters and Δg_{ijk} represents the ternary contribution.

The temperature-dependent parameters for the CEOS and CEOS/G^{E} models used in the investigated temperature range were obtained as

$$Y = Y_1 + Y_2 T \tag{18}$$

where $Y = k_{ij}, l_{ij}, m_{ij}, \Delta g_{12}$, and Δg_{21}. Corresponding models applied here were made by using adequate equations, and they are listed in Table 6. Parameters or coefficients of these models were obtained by minimizing the following objective function:

$$\mathrm{OF} = \frac{1}{m} \sum_{i=1}^{m} \left(\frac{V_{\exp}^{\mathrm{E}} - V_{\mathrm{cal}}^{\mathrm{E}}}{V_{\exp}^{\mathrm{E}}} \right)_i^2 \to \min \tag{19}$$

using the Marquardt optimization technique [25].

The obtained results of V^{E} calculation were assessed by the percentage average absolute deviation PD(V^{E})

$$\mathrm{PD}(V^{\mathrm{E}}) = \frac{100}{m} \sum_{i=1}^{m} \left| \frac{V_{\exp}^{\mathrm{E}} - V_{\mathrm{cal}}^{\mathrm{E}}}{\left(V_{\exp}^{\mathrm{E}}\right)_{\max}} \right|_i \tag{20}$$

where $\left(V_{\exp}^{\mathrm{E}}\right)_{\max}$ denotes the maximum absolute value of experimental V^{E} points.

Table 6 Coefficients and results of correlation of the V^E data, given by PD(V^E) and σ, obtained by the temperature-independent PRSV CEOS models for the investigated binary systems at the temperatures (288.15–313.15) K and atmospheric pressure

T (K)	$k_{ij,1}$	$l_{ij,1}$	$m_{ij,1}$	$\Delta g_{12,1}$ (J · mol^{-1})	$\Delta g_{21,1}$ (J · mol^{-1})	PD(V^E) (%)	σ (cm^3 · mol^{-1})
1-Butanol (1) + chloroform (2)							
288.15							
vdW1-2[a]	0.1181		0.0046			5.02	0.0077
vdW1-3[b]	0.1612	0.0168	0.0111			1.80	0.0031
TCBT-2[c]				-0.227514×10^{4}	0.358796×10^{4}	11.95	0.0191
TCBT-3[d]	−0.1021			-0.208666×10^{4}	-0.166802×10^{4}	1.45	0.0026
293.15							
vdW1-2	0.1163		0.0046			5.51	0.0079
vdW1-3	0.1583	0.0161	0.0112			2.18	0.0036
TCBT-2				-0.228780×10^{4}	0.359391×10^{4}	12.86	0.0190
TCBT-3	−0.1030			-0.207367×10^{4}	-0.164897×10^{4}	1.51	0.0024
298.15							
vdW1-2	0.1140		0.0045			5.94	0.0078
vdW1-3	0.1536	0.0150	0.0109			2.73	0.0040
TCBT-2				-0.228963×10^{4}	0.357902×10^{4}	13.88	0.0187
TCBT-3	−0.1048			-0.207702×10^{4}	-0.164153×10^{4}	1.69	0.0023
303.15							
vdW1-2	0.1117		0.0044			5.53	0.0078
vdW1-3	0.1490	0.0139	0.0106			2.94	0.0044
TCBT-2				-0.228586×10^{4}	0.355394×10^{4}	12.88	0.0184
TCBT-3	−0.1042			-0.203210×10^{4}	-0.159719×10^{4}	1.54	0.0025
308.15							
vdW1-2	0.1094		0.0042			4.67	0.0078
vdW1-3	0.1435	0.0126	0.0101			2.89	0.0049
TCBT-2				-0.227858×10^{4}	0.352440×10^{4}	10.90	0.0180
TCBT-3	−0.1066			-0.205027×10^{4}	-0.158964×10^{4}	1.50	0.0028
313.15							
vdW1-2	0.1064		0.0039			4.63	0.0091
vdW1-3	0.1418	0.0129	0.0103			3.23	0.0064
TCBT-2				-0.226975×10^{4}	0.349191×10^{4}	9.92	0.0185
TCBT-3	−0.1068			-0.201376×10^{4}	-0.156483×10^{4}	1.98	0.0045
288.15–313.15							
vdW1-2	0.1056		0.0033			10.32	0.0162
vdW1-3	0.0788	−0.0118	−0.0010			8.39	0.0129
TCBT-2				-0.225785×10^{4}	0.350293×10^{4}	15.22	0.0249
TCBT-3	−0.0352			0.433231×10^{4}	-0.366352×10^{4}	6.32	0.0106
1-Butanol (1) + benzene (3)							
288.15							
vdW1-2	0.0725		0.0012			2.15	0.0054
vdW1-3	−0.0101	−0.0261	−0.0099			1.53	0.0035
TCBT-2				-0.874348×10^{3}	0.170486×10^{4}	1.31	0.0037
TCBT-3	−0.0010			-0.959123×10^{3}	0.176730×10^{4}	1.31	0.0036
293.15							
vdW1-2	0.0734		0.0015			2.21	0.0060
vdW1-3	−0.1147	−0.0598	−0.0238			1.02	0.0030
TCBT-2				-0.927679×10^{3}	0.175449×10^{4}	1.42	0.0042
TCBT-3	−0.0017			-0.106730×10^{4}	0.185799×10^{4}	1.42	0.0041
298.15							
vdW1-2	0.0738		0.0017			2.32	0.0068

Table 6 continued

T (K)	$k_{ij,1}$	$l_{ij,1}$	$m_{ij,1}$	$\Delta g_{12,1}$ (J · mol^{-1})	$\Delta g_{21,1}$ (J · mol^{-1})	PD(V^E) (%)	σ (cm^3 · mol^{-1})
vdW1-3	−0.1097	−0.0572	−0.0239			1.08	0.0035
TCBT-2				-0.954670×10^3	0.176918×10^4	1.47	0.0050
TCBT-3	−0.0011			-0.104883×10^4	0.184507×10^4	1.45	0.0048
303.15							
vdW1-2	0.0743		0.0020			2.43	0.0076
vdW1-3	−0.1042	−0.0546	−0.0239			1.15	0.0040
TCBT-2				-0.101517×10^4	0.183326×10^4	1.50	0.0053
TCBT-3	−0.0048			-0.137346×10^4	0.210231×10^4	1.50	0.0052
308.15							
vdW1-2	0.0747		0.0022			2.55	0.0085
vdW1-3	−0.0978	−0.0518	−0.0238			1.26	0.0046
TCBT-2				-0.103397×10^4	0.184074×10^4	1.59	0.0062
TCBT-3	−0.0058			-0.150969×10^4	0.223456×10^4	1.58	0.0058
313.15							
vdW1-2	0.0747		0.0024			2.66	0.0092
vdW1-3	−0.1001	−0.0515	−0.0249			1.41	0.0052
TCBT-2				-0.105207×10^4	0.184635×10^4	1.77	0.0072
TCBT-3	−0.0061			-0.156877×10^4	0.229562×10^4	1.73	0.0063
288.15–313.15							
vdW1-2	−0.0677		0.0009			4.55	0.0117
vdW1-3	0.0423	−0.0096	−0.0029			1.77	0.0056
TCBT-2				-0.882690×10^3	0.165950×10^4	10.31	0.0270
TCBT-3	−0.0287			0.226899×10^4	-0.230477×10^4	2.76	0.0083

[a] Eqs. 6–12, 18; $l_{ij} = 0$

[b] Eqs. 6–12, 18

[c] Eqs. 6–16, 18; $k_{ij} = l_{ij} = m_{ij} = 0$; $\alpha_{ij} = 0.3$

[d] Eqs. 6–16, 18; $l_{ij} = m_{ij} = 0$; $\alpha_{ij} = 0.3$

The fitting parameters of the temperature-independent vdW1 and TCBT models, as well as PD(V^E) and σ are shown in Table 6. As can be seen from Table 6, the best agreement with experimental data was achieved by the three-parameter vdW1-3 and TCBT-3 models. The PD(V^E) for the 1-butanol (1) + chloroform (2) system for both models increase with increasing temperature. It means that the 1-butanol (1) + chloroform (2) system with the S-shape of the $V^E - x_1$ curve is not easy to fit. The temperature-independent vdW1-2 and TCBT-2 models gave relatively large deviations for each separate isotherm, while all models do not work well for the whole temperature range.

A different situation was found for the 1-butanol (1) + benzene (3) binary system where the results obtained with all models are better, particularly those achieved by the vdW1-3 model which is simpler than TCBT-3. The dissimilar fitting of aforementioned systems can be observed in Fig. 5a and b. Figure 5a shows a different quality of the sigmoidal $V^E - x_1$ fit for the 1-butanol (1) + chloroform (2) system, resulting from the temperature-independent TCBT-2 and TCBT-3 models at 288.15 K and 313.15 K. Namely, the TCBT-2 model fails in the case of maximum and minimum V^E data fitting. Contrarily, as shown in Fig. 5b, the temperature-independent two-parameter vdW1-2 and

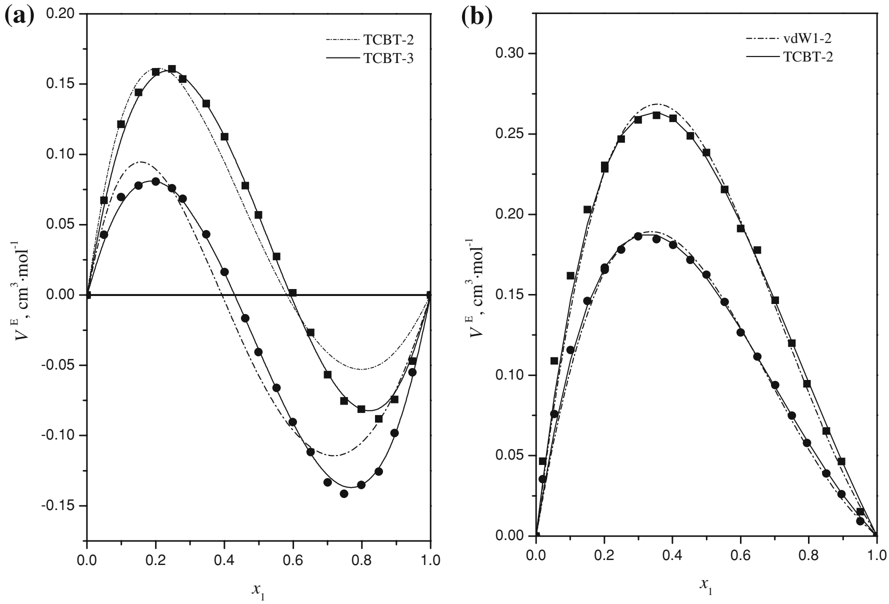

Fig. 5 Correlation of V^E data for the binary systems: (**a**) 1-butanol (1) + chloroform (2) and (**b**) 1-butanol (1) + benzene (3). Symbols refer to experimental points at: ●, 288.15 K; ■, 298.15 K, while the lines represent the results calculated by PRSV CEOS models

TCBT-2 models gave a similar quality of results, which could be considered as satisfactory. The results obtained over the whole temperature range by temperature-dependent CEOS and CEOS/G^E models together with their coefficients are listed in Table 7. For the 1-butanol (1) + chloroform (2) system, low PD(V^E) and σ were obtained only for the TCBT-3 model, and are better than those obtained by the temperature-independent TCBT-3 model (Table 6). For the 1-butanol (1) + benzene (3) mixture, better results for PD(V^E) and σ calculations were achieved by temperature-dependent TCBT-2 and TCBT-3 models, compared to the vdW1-2 and vdW1-3 models.

Prediction of V^E for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system at each temperature and over the whole range of temperature, were carried out using the CEOS and CEOS/G^E models, with binary interaction parameters of these models generated from binary data. The corresponding PD(V^E) and σ are given in Table 8. It is evident that predictions carried out by the simple vdW1-2 model could be treated as acceptable and similar to those obtained by Radojkovic et al., Eq. 4. The results for other models are poor, except those achieved by the temperature-independent vdW1-3 model for the whole temperature range. Correlation of ternary V^E data of this system, using only TCBT models was based on the ternary contribution incorporated in Eq. 17. As can be seen from Table 9, better agreement with experimental V^E data for each temperature and the whole temperature range was obtained with the TCBT-3 model. However, for the whole temperature range, the TCBT-2 model with temperature-dependent parameters works satisfactorily.

Table 7 Coefficients and results of correlation of the V^{E} data, given by PD(V^{E}) and σ, obtained by the temperature-dependent PRSV CEOS models for the investigated binary systems over the temperature range (288.15–313.15) K and atmospheric pressure

	$k_{ij,1}$ $k_{ij,2}(\mathrm{K}^{-1})$	$l_{ij,1}$ $l_{ij,2}(\mathrm{K}^{-1})$	$m_{ij,1}$ $m_{ij,2}(\mathrm{K}^{-1})$	$\Delta g_{12,1}(\mathrm{J \cdot mol^{-1}})$ $\Delta g_{12,2}(\mathrm{J \cdot mol^{-1} \cdot K^{-1}})$	$\Delta g_{21,1}(\mathrm{J \cdot mol^{-1}})$ $\Delta g_{21,2}(\mathrm{J \cdot mol^{-1} \cdot K^{-1}})$	PD(V^{E}) (%)	σ ($\mathrm{cm^3 \cdot mol^{-1}}$)
1-Butanol (1) + chloroform (2)							
vdW1-2[a]	0.2429		0.0109			5.23	0.0081
	-0.433×10^{-3}		-0.218×10^{-4}				
vdW1-3[b]	−0.6247	−0.4709	0.0113			5.22	0.0082
	0.119×10^{-2}	0.107×10^{-2}	-0.199×10^{-3}				
TCBT-2[c]				-0.244877×10^{4}	0.490222×10^{4}	12.24	0.0185
				0.487381×10^{0}	-0.433531×10^{1}		
TCBT-3[d]	−0.1048			-0.479366×10^{4}	-0.279641×10^{4}	2.90	0.0055
				0.910166×10^{1}	0.388945×10^{1}		
1-Butanol (1) + benzene (3)							
vdW1-2	0.0473		−0.0120			2.39	0.0072
	0.884×10^{-4}		0.462×10^{-4}				
vdW1-3	4.5371	1.3592	0.6512			4.01	0.0102
	-0.152×10^{-1}	-0.464×10^{-2}	-0.222×10^{-2}				
TCBT-2				0.535297×10^{3}	0.101258×10^{4}	1.91	0.0058
				-0.518576×10^{1}	0.281591×10^{1}		
TCBT-3	0.0178			0.187177×10^{4}	0.134081×10^{4}	1.90	0.0062
				-0.638858×10^{1}	0.584935×10^{0}		

[a] Eqs. 6–12, 18; $l_{ij} = 0$

[b] Eqs. 6–12, 18

[c] Eqs. 6–16, 18; $k_{ij} = l_{ij} = m_{ij} = 0$; $\alpha_{ij} = 0.3$

[d] Eqs. 6–16, 18; $l_{ij} = m_{ij} = 0$; $\alpha_{ij} = 0.3$

Table 8 Results of prediction of V^{E}, given by PD(V^{E}) and σ, for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system

T (K)	vdW1-2[a] PD(V^{E}) (%)	σ ($\mathrm{cm}^3 \cdot \mathrm{mol}^{-1}$)	vdW1-3[b] PD(V^{E}) (%)	σ ($\mathrm{cm}^3 \cdot \mathrm{mol}^{-1}$)	TCBT-2[c] PD(V^{E}) (%)	σ ($\mathrm{cm}^3 \cdot \mathrm{mol}^{-1}$)	TCBT-3[d] PD(V^{E}) (%)	σ ($\mathrm{cm}^3 \cdot \mathrm{mol}^{-1}$)
288.15	5.51	0.0175	7.72	0.0233	hv[g]	hv	15.83	0.0552
293.15	5.32	0.0168	20.98	0.0645	hv	hv	27.62	0.0870
298.15	5.06	0.0162	20.67	0.0638	hv	hv	18.77	0.0642
303.15	4.87	0.0160	20.25	0.0632	hv	hv	12.47	0.0425
308.15	4.75	0.0162	19.49	0.0618	hv	hv	18.80	0.0722
313.15	4.84	0.0175	19.83	0.0639	hv	hv	19.17	0.0712
288.15–313.15[e]	5.07	0.0186	2.62	0.0094	14.37	0.0506	11.75	0.0381
288.15–313.15[f]	5.03	0.0167	31.72	0.1027	hv	hv	hv	hv

[a] Eqs. 6–12, 18; $l_{ij} = 0$

[b] Eqs. 6–12, 18

[c] Eqs. 6–16, 18; $k_{ij} = l_{ij} = m_{ij} = 0$; $\alpha_{ij} = 0.3$

[d] Eqs. 6–16, 18; $l_{ij} = m_{ij} = 0$; $\alpha_{ij} = 0.3$

[e] Prediction of V^{E} using temperature-independent parameters

[f] Prediction of V^{E} using temperature-dependent parameters

[g] hv—high value

Table 9 Correlation of V^E for the 1-butanol (1) + chloroform (2) + benzene (3) ternary system

T (K)	$\Delta g_{123}(\mathrm{J \cdot mol^{-1}})$ $\Delta g_{132}(\mathrm{J \cdot mol^{-1}})$	$\Delta g_{213}(\mathrm{J \cdot mol^{-1}})$ $\Delta g_{231}(\mathrm{J \cdot mol^{-1}})$	$\Delta g_{312}(\mathrm{J \cdot mol^{-1}})$ $\Delta g_{321}(\mathrm{J \cdot mol^{-1}})$	PD(V^E) (%)	σ ($\mathrm{cm^3 \cdot mol^{-1}}$)
288.15					
TCBT-2[a]	0.242155×10^4	-0.354164×10^4	-0.100651×10^4	2.66	0.0111
	-0.432052×10^3	0.419419×10^4	0.134159×10^6		
TCBT-3[b]	0.758883×10^4	-0.940626×10^3	-0.578481×10^4	1.67	0.0064
	0.903925×10^4	-0.422690×10^2	-0.894742×10^4		
293.15					
TCBT-2	0.243634×10^4	-0.350073×10^4	-0.102652×10^4	2.34	0.0094
	-0.406890×10^3	0.410023×10^4	0.117706×10^6		
TCBT-3	-0.341819×10^4	0.130816×10^3	-0.235320×10^3	1.60	0.0060
	0.756450×10^4	-0.313663×10^4	0.649785×10^4		
298.15					
TCBT-2	0.243936×10^4	-0.340318×10^4	-0.900287×10^3	2.00	0.0077
	-0.478844×10^3	0.395155×10^4	0.986065×10^5		
TCBT-3	0.726134×10^4	-0.451356×10^3	-0.575173×10^4	1.38	0.0044
	0.809144×10^4	-0.530041×10^3	-0.837497×10^4		
303.15					
TCBT-2	0.237066×10^4	-0.305383×10^4	-0.815095×10^3	1.76	0.0066
	-0.492765×10^3	0.363026×10^4	-0.286823×10^4		
TCBT-3	-0.397164×10^4	-0.388234×10^3	0.960691×10^3	1.16	0.0041
	0.827809×10^4	-0.341436×10^4	0.724872×10^4		
308.15					
TCBT-2	0.237568×10^4	-0.306729×10^4	-0.652608×10^3	1.64	0.0061
	-0.610811×10^3	0.360214×10^4	-0.148557×10^5		
TCBT-3	-0.429031×10^4	-0.257027×10^3	-0.250666×10^3	1.24	0.0042
	0.961359×10^4	-0.378274×10^4	0.836248×10^4		
313.15					
TCBT-2	0.246110×10^4	-0.328388×10^4	-0.470757×10^3	1.72	0.0066
	-0.660702×10^3	0.346506×10^4	0.275323×10^6		
TCBT-3	-0.447078×10^4	-0.104401×10^4	0.148843×10^4	1.38	0.0049
	0.988870×10^4	-0.380606×10^4	0.874493×10^4		
288.15–313.15[c]					
TCBT-2	0.331960×10^4	-0.259234×10^4	-0.828002×10^3	8.14	0.0265
	0.367322×10^4	0.840441×10^3	-0.591097×10^4		
TCBT-3	0.115991×10^4	-0.388894×10^2	-0.692183×10^3	2.38	0.0083
	-0.299962×10^4	0.301905×10^4	0.894278×10^3		
288.15–313.15[d]					
TCBT-2	0.266526×10^4	-0.517119×10^4	0.465144×10^4	2.87	0.0107
	-0.290106×10^4	0.464600×10^4	0.128070×10^6		
TCBT-3	0.209318×10^4	0.196298×10^4	-0.427686×10^4	4.00	0.0142
	-0.110182×10^4	0.379155×10^4	-0.548159×10^5		

[a] Eqs. 6–18; $k_{ij} = l_{ij} = m_{ij} = 0$; $\alpha_{ij} = 0.3$

[b] Eqs. 6–18; $l_{ij} = m_{ij} = 0$; $\alpha_{ij} = 0.3$

[c] Correlation of V^E using temperature-independent binary parameters

[d] Correlation of V^E using temperature-dependent binary parameters

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