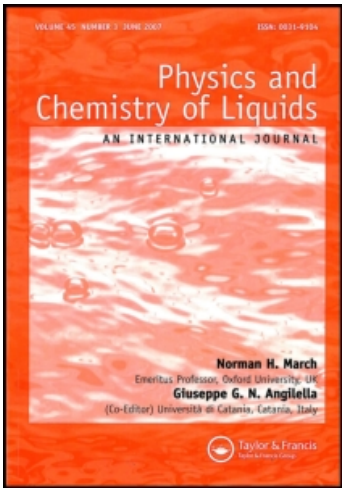

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J. M. Resa[a]; C. Gonzalez[a]; R. G. Concha[a]; M. Iglesias[b]
[a] Dpto. de Ingenieria Química, Universidad del Pais Vasco, Vitoria, España [b] Departament d'Enginyeria Química, Escola Tècnica Superior d'Enginyeria Química, Universitat Rovira i Virgili, Campus Sescelades, 43007 Tarragona, España

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ULTRASONIC VELOCITY MEASUREMENTS FOR BUTYL ACETATE + HYDROCARBON MIXTURES

J.M. RESA[a,*], C. GONZALEZ[a], R.G. CONCHA[a] and M. IGLESIAS[b,†]

[a]*Dpto. de Ingenieria Química, Universidad del Pais Vasco, Apto. 450, Vitoria, España;*
[b]*Departament d'Enginyeria Química, Escola Tècnica Superior d'Enginyeria Química, Universitat Rovira i Virgili, Avinguda Països Catalans 26, Campus Sescelades, 43007 Tarragona, España*

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This article presents ultrasonic velocities and isentropic compressibilities of mixtures enclosing butyl acetate and aromatic hydrocarbons (toluene, ethylbenzene, *p*-xylene, mesitylene, isopropylbenzene, butylbenzene, isobutylbenzene, or *t*-butylbenzene) that have been measured at several temperatures and atmospheric conditions. The values of these properties were calculated over the whole range of composition, different acoustic magnitudes being computed due to their importance in the study of specific molecular interactions and theoretical calculations. The application of different models to predict the mixing trend in terms of isentropic compressibility shows adequate agreement between experimental and computed sets of data both in magnitude or sign.

Keywords: Ultrasonic velocity; Isentropic compressibility; Derived properties; Estimation; Binary mixtures; Butyl acetate; Aromatic hydrocarbons; Temperature

1. INTRODUCTION

As a continuation of the previous works [1–6], this article is devoted to the study of thermodynamic properties of mixtures with chemicals containing the ester group into aromatic environment. With this aim, our research team carried out a collection of studies focused on acetate mixtures to analyze the influence of the position of alkyl groups in the aromatic ring and the temperature dependence of the thermophysical properties. Butyl acetate is used widely in the perfume industry, applied as solvent in the production of different synthetic products (synthetic resins, agricultural chemicals, adhesives, paint, etc) and as flavoring agent for foods and pharmaceuticals. Our purpose is to discuss the dependence of the isentropic compressibility on mixing and other acoustic parameters on the composition and molecular structure, in order to provide a better understanding concerning the factors that contribute to the special behavior in enclosing slight polar molecules into aromatic solvents, where the factors short chain and different molecular nature may be taken into account. In this work

*Corresponding author. Fax: +34945013014. E-mail: iqpredij@vc.ehu.es
†Fax: +34 977 559621

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we present data of the mixtures enclosing butyl acetate + (toluene, ethylbenzene, *p*-xylene, mesitylene, isopropylbenzene, butylbenzene, isobutylbenzene, or *t*-butylbenzene) that have been measured at the range 293.15–313.15 K and atmospheric condition. Due to the importance of theoretical models on industrial design, different procedures (Danusso and Nomoto equations) [7,8] and theories (Free Length Theory (FLT), and Collision Factor Theory (CFT)) [9–11] for the isentropic compressibilities were applied, the obtained results being analyzed, and commented upon. We have attempted to explain the physico-chemical behavior of the mixtures indicated above, in order to explore the strength and nature of the interactions between the components by deriving various thermodynamic parameters from the ultrasonic velocity and density data [6]. Various parameters such as intermolecular free length (L_f), van der Waals' constant (b), molecular radius (r), geometrical volume (B), molar surface area (Y), available volume (V_a), volume at absolute zero (V_0), molar sound velocity (R), collision factor (S), specific acoustic impedance (Z), relative association (R_A), and molecular association (M_A) were computed, some of them direct application for predictions. The analysis of excess acoustic magnitudes pointed out the availability of weaker interactions among the heaviest, unalike molecules at increasing temperatures. Attending to the deviation of computed data, we arrive at the conclusion that the application of the FLT model produces theoretically close results.

2. EXPERIMENTAL SECTION

All the chemicals were supplied by Fluka, except butyl acetate, which was supplied by Panreac, and with mole fraction purities better than 0.990, as checked by gas chromatography. The liquids were degassed in an ultrasonic bath for 4 h at least. Solution composition were determined gravimetrically using a Salter ER-182A balance with a precision of $\pm 1 \times 10^{-4}$ g, special care being taken during solution preparation to avoid evaporation losses. The ultrasonic velocities were measured with a precision of $\pm 1\ \mathrm{ms}^{-1}$ using an Anton Paar DSA-48 digital device. Calibration of the apparatus was performed periodically, in accordance with technical specifications, using Millipore quality water (resistivity, 18.2 MΩ cm) and ambient air. Maximum deviation in the calculation of changes of isentropic compressibility for these mixtures have been estimated with a precision of $1\ \mathrm{T\,Pa}^{-1}$. The values of the pure components [12,13], as well as open literature data, are given in Table I. Further details about technical procedures or manipulation could be found in earlier works.

3. DATA PROCEDURE

3.1. Correlation of Derived Magnitude

The experimental data of ultrasonic velocity, isentropic compressibility (by means of the Newton–Laplace equation), as well as the variation of isentropic compressibility calculated by means of the Eq. (1), are presented in Table II

$$\delta Q = Q_{\mathrm{mix}} - \sum_{i=1}^{N} x_i Q_i. \tag{1}$$

TABLE I Comparison of experimental and literature data for pure liquids at 298.15 K

Compound	M ($g\,mol^{-1}$)	u ($m\,s^{-1}$) (*exp*)	u ($m\,s^{-1}$) (*lit*)[a]
Butyl acetate	116.16	1191.3	1190.0[b]
Toluene	92.14	1304.2	1305.0
Ethylbenzene	106.167	1318.8	1319.0
p-Xylene	106.167	1309.4	1309.7
Mesitylene	120.194	1336.0	1336.8
Isopropylbenzene	120.194	1307.5	1307.7
Butylbenzene	134.221	1333.8	1334.1
Isobutylbenzene	134.221	1296.7	1296.9
t-Butylbenzene	134.221	1315.2	1315.6

[a][4]; [b][13].

In this equation, δQ is the variation of a magnitude Q (κ_S, isentropic compressibilities), Q_i is the pure solvent magnitude, x_i is the mole fraction, and N is the number of components in the mixtures. The derived magnitudes of the binary mixtures were fitted using the Redlich–Kister expression [14]

$$\delta Q = x_i x_j \cdot \left(\sum_{p=0}^{S} B_p (x_i - x_j)^p \right). \tag{2}$$

The B_p parameters were expanded as quadratic dependent functions of temperature as is expressed in Eq. (3), as we used previously [5–6]

$$B_p = \sum_{q=0}^{2} B_{pq} \cdot T^q, \tag{3}$$

where B_{pq} are the fitting parameters obtained by least-squares method (Marquardt algorithm, [15]) with all the data being weighted equally and T is the temperature in Kelvin degrees. The fitting parameters are given in Table III, with the corresponding root mean square deviations (σ). This magnitude was computed using Eq. (4), where z is the value of the property, and n_{DAT} is the number of experimental data

$$\sigma = \left(\frac{\sum_{i=1}^{n_{\mathrm{DAT}}} \left(z_{\mathrm{exp}} - z_{\mathrm{pred}} \right)^2}{n_{\mathrm{DAT}}} \right)^{1/2}. \tag{4}$$

For example, in the Fig. 1(a), the changes of isentropic compressibilities have been plotted along the mole fraction for the binaries butyl acetate + (toluene, ethylbenzene, *p*-xylene, mesitylene, isopropylbenzene, butylbenzene, isobutylbenzene, or *t*-butylbenzene) at 298.15 K, and for the systems butyl acetate + ethylbenzene, isopropylbenzene and *t*-butylbenzene the influence of temperature is shown in Fig. 1(b). In these figures two main effects may be observed: first, the decreasing tendency of derived magnitude of rising temperatures and, second, a similar trend when molecular weight is increased.

TABLE II Ultrasonic velocity, isentropic compressibility and change of isentropic compressibility of the binary mixtures (butyl acetate + aromatic hydrocarbon) as function of temperature

x_1	u ($m\,s^{-1}$)	κ_s ($T\,Pa^{-1}$)	$\delta\kappa_s$ ($T\,Pa^{-1}$)	x_1	u ($m\,s^{-1}$)	κ_s ($T\,Pa^{-1}$)	$\delta\kappa_s$ ($T\,Pa^{-1}$)
Toluene							
293.15 K							
1.0000	1211.9	772.6	0.0	0.4468	1269.3	709.4	1.3
0.9449	1216.9	766.6	0.5	0.4011	1274.6	704.0	1.2
0.8971	1221.5	761.2	0.6	0.3447	1281.5	697.2	0.9
0.8404	1227.0	754.9	0.9	0.2985	1287.3	691.6	0.7
0.7972	1231.3	750.1	1.1	0.2502	1293.3	685.8	0.6
0.7516	1235.9	744.9	1.2	0.2001	1299.6	679.8	0.4
0.7000	1241.3	739.0	1.3	0.1500	1306.1	673.9	0.3
0.6517	1246.4	733.4	1.4	0.0998	1312.6	667.9	0.2
0.5999	1252.0	727.4	1.4	0.0499	1319.3	662.0	0.1
0.5524	1257.2	721.9	1.4	0.0000	1326.0	656.1	0.0
0.4994	1263.2	715.6	1.4				
298.15 K							
1.0000	1191.3	804.1	0.0	0.4468	1248.1	737.7	1.2
0.9449	1196.2	798.0	0.6	0.4011	1253.4	732.0	1.1
0.8971	1200.6	792.5	1.0	0.3447	1260.1	724.9	1.0
0.8404	1206.1	785.6	1.1	0.2985	1265.9	719.0	0.7
0.7972	1210.4	780.6	1.3	0.2502	1271.8	712.9	0.6
0.7516	1215.0	775.0	1.3	0.2001	1278.1	706.7	0.4
0.7000	1220.3	768.8	1.5	0.1500	1284.5	700.3	0.3
0.6517	1225.4	762.9	1.4	0.0998	1291.0	694.1	0.2
0.5999	1231.0	756.5	1.4	0.0499	1297.6	687.9	0.1
0.5524	1236.1	750.8	1.5	0.0000	1304.2	681.7	0.0
0.4994	1242.1	744.2	1.3				
303.15 K							
1.0000	1170.6	837.4	0.0	0.4468	1227.0	767.5	1.3
0.9449	1175.5	830.9	0.6	0.4011	1232.4	761.3	1.1
0.8971	1179.9	825.2	1.0	0.3447	1239.0	753.9	1.0
0.8404	1185.3	818.1	1.2	0.2985	1244.7	747.7	0.7
0.7972	1189.6	812.7	1.4	0.2502	1250.6	741.3	0.5
0.7516	1194.1	806.9	1.4	0.2001	1256.9	734.6	0.2
0.7000	1199.4	800.3	1.5	0.1500	1263.2	728.0	0.2
0.6517	1204.5	794.0	1.5	0.0998	1269.6	721.5	0.1
0.5999	1210.0	787.4	1.5	0.0499	1276.1	715.0	0.0
0.5524	1215.1	781.3	1.5	0.0000	1282.7	708.5	0.0
0.4994	1221.2	774.1	1.2				
308.15 K							
1.0000	1150.2	872.6	0.0	0.4468	1205.9	799.0	1.4
0.9449	1155.0	865.7	0.6	0.4011	1211.2	792.6	1.2
0.8971	1159.2	859.8	1.1	0.3447	1217.8	784.7	1.0
0.8404	1164.6	852.4	1.4	0.2985	1223.4	778.2	0.7
0.7972	1168.8	846.6	1.5	0.2502	1229.3	771.4	0.5
0.7516	1173.4	840.4	1.5	0.2001	1235.5	764.4	0.3
0.7000	1178.6	833.5	1.6	0.1500	1241.7	757.6	0.3
0.6517	1183.7	826.9	1.5	0.0998	1248.1	750.6	0.1
0.5999	1189.1	819.9	1.6	0.0499	1254.6	743.7	0.0
0.5524	1194.1	813.5	1.6	0.0000	1261.0	737.0	0.0
0.4994	1200.1	806.1	1.4				
313.15 K							
1.0000	1130.0	909.4	0.0	0.4468	1184.5	832.7	1.9
0.9449	1134.9	902.0	0.4	0.4011	1189.7	826.1	1.8
0.8971	1138.7	896.2	1.5	0.3447	1196.2	817.8	1.5
0.8404	1144.0	888.5	1.8	0.2985	1201.8	810.9	1.2
0.7972	1148.0	882.6	2.0	0.2502	1207.6	803.8	1.0

(*continued*)

TABLE II Continued

x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})	x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})
0.7516	1152.6	876.1	2.0	0.2001	1213.8	796.4	0.6
0.7000	1157.7	868.8	2.0	0.1500	1220.0	789.1	0.5
0.6517	1162.7	861.9	2.0	0.0998	1226.3	781.8	0.3
0.5999	1168.0	854.7	2.1	0.0499	1232.6	774.6	0.2
0.5524	1173.1	847.8	2.0	0.0000	1239.2	767.3	0.0
0.4994	1178.8	840.2	2.0				
Ethylbenzene							
293.15 K							
1.0000	1211.9	772.7	0.0	0.4448	1280.1	698.4	−2.0
0.9505	1217.5	766.2	−0.1	0.3989	1286.1	692.4	−2.0
0.9009	1223.2	759.6	−0.2	0.3526	1292.1	686.5	−1.9
0.8511	1229.1	752.9	−0.4	0.2929	1300.0	678.9	−1.8
0.8016	1234.9	746.3	−0.6	0.2540	1305.2	673.9	−1.6
0.7555	1240.5	740.1	−0.7	0.2024	1312.2	667.3	−1.5
0.7003	1247.3	732.7	−1.0	0.1488	1319.5	660.6	−1.3
0.6456	1254.2	725.3	−1.3	0.1008	1326.0	654.7	−1.0
0.6041	1259.5	719.6	−1.6	0.0544	1332.5	648.9	−0.7
0.5505	1266.4	712.4	−1.8	0.0000	1339.8	642.5	0.0
0.5021	1272.7	705.9	−2.0				
298.15 K							
1.0000	1191.3	804.3	0.0	0.4448	1259.2	725.6	−2.1
0.9505	1196.8	797.4	0.0	0.3989	1265.2	719.2	−2.2
0.9009	1202.5	790.3	−0.3	0.3526	1271.1	713.1	−2.0
0.8511	1208.4	783.3	−0.5	0.2929	1279.0	705.0	−1.9
0.8016	1214.3	776.1	−0.8	0.2540	1284.3	699.7	−1.8
0.7555	1219.8	769.7	−0.8	0.2024	1291.2	692.7	−1.6
0.7003	1226.5	761.8	−1.1	0.1488	1298.5	685.6	−1.4
0.6456	1233.5	753.9	−1.5	0.1008	1305.1	679.2	−1.1
0.6041	1238.8	747.9	−1.8	0.0544	1311.5	673.3	−0.7
0.5505	1245.6	740.3	−2.0	0.0000	1318.8	666.5	0.0
0.5021	1251.9	733.4	−2.2				
303.15 K							
1.0000	1170.6	837.8	0.0	0.4448	1238.5	754.2	−2.4
0.9505	1176.1	830.5	0.0	0.3989	1244.4	747.5	−2.4
0.9009	1181.9	822.9	−0.3	0.3526	1250.3	740.9	−2.2
0.8511	1187.7	815.5	−0.5	0.2929	1258.2	732.3	−2.1
0.8016	1193.6	807.9	−0.9	0.2540	1263.5	726.7	−2.0
0.7555	1199.1	801.0	−1.0	0.2024	1270.4	719.4	−1.8
0.7003	1205.8	792.7	−1.2	0.1488	1277.7	711.7	−1.6
0.6456	1212.7	784.4	−1.6	0.1008	1284.3	705.1	−1.3
0.6041	1218.1	777.8	−2.0	0.0544	1290.7	698.7	−0.9
0.5505	1224.9	769.8	−2.2	0.0000	1297.9	691.6	0.0
0.5021	1231.1	762.6	−2.4				
308.15 K							
1.0000	1150.2	873.1	0.0	0.4448	1217.8	784.3	−2.6
0.9505	1155.6	865.4	0.0	0.3989	1223.8	777.2	−2.6
0.9009	1161.3	857.4	−0.3	0.3526	1229.8	770.1	−2.5
0.8511	1167.2	849.4	−0.6	0.2929	1237.7	761.0	−2.4
0.8016	1173.1	841.3	−1.0	0.2540	1242.8	755.1	−2.2
0.7555	1178.6	834.0	−1.1	0.2024	1249.8	747.2	−2.0
0.7003	1185.4	825.0	−1.6	0.1488	1257.1	739.2	−1.7
0.6456	1192.2	816.2	−1.9	0.1008	1263.6	732.1	−1.4
0.6041	1197.6	809.3	−2.3	0.0544	1270.0	725.3	−0.9
0.5505	1204.3	800.9	−2.4	0.0000	1277.2	717.8	0.0
0.5021	1210.6	793.1	−2.7				

(*continued*)

TABLE II Continued

x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})	x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})
313.15 K							
1.0000	1130.0	910.0	0.0	0.4448	1197.5	815.6	−2.8
0.9505	1135.5	901.7	−0.1	0.3989	1203.4	808.2	−2.7
0.9009	1141.2	893.2	−0.4	0.3526	1209.4	800.6	−2.7
0.8511	1146.9	884.9	−0.6	0.2929	1217.3	791.0	−2.5
0.8016	1152.8	876.3	−1.0	0.2540	1222.4	784.7	−2.3
0.7555	1158.3	868.4	−1.3	0.2024	1229.5	776.3	−2.2
0.7003	1165.1	858.9	−1.6	0.1488	1236.7	767.8	−1.9
0.6456	1171.9	849.6	−1.9	0.1008	1243.2	760.4	−1.4
0.6041	1177.2	842.4	−2.3	0.0544	1249.7	753.1	−1.0
0.5505	1184.0	833.3	−2.6	0.0000	1256.9	745.1	0.0
0.5021	1190.2	825.1	−2.8				
p-Xylene							
293.15 K							
1.0000	1211.9	772.7	0.0	0.4519	1274.7	706.5	−2.5
0.9489	1217.5	766.4	−0.4	0.4040	1280.4	701.0	−2.5
0.8979	1222.9	760.4	−0.4	0.3519	1286.8	694.9	−2.6
0.8519	1228.0	754.7	−0.8	0.3077	1292.2	689.9	−2.4
0.7990	1234.0	748.2	−1.1	0.2480	1299.6	683.0	−2.3
0.7490	1239.8	741.9	−1.6	0.2012	1305.3	678.0	−1.9
0.6993	1245.4	736.0	−1.7	0.1494	1311.9	672.1	−1.8
0.6518	1251.0	730.2	−2.1	0.1014	1317.6	667.1	−1.2
0.5991	1257.0	724.0	−2.1	0.0494	1324.3	661.4	−0.9
0.5505	1262.9	718.1	−2.4	0.0000	1330.2	656.5	0.0
0.4999	1268.8	712.2	−2.4				
298.15 K							
1.0000	1191.3	804.3	0.0	0.4519	1253.9	734.0	−2.7
0.9489	1196.7	797.7	−0.3	0.4040	1259.6	728.2	−2.6
0.8979	1202.2	791.3	−0.4	0.3519	1266.0	721.7	−2.7
0.8519	1207.4	785.1	−0.9	0.3077	1271.3	716.5	−2.4
0.7990	1213.2	778.5	−1.0	0.2480	1278.8	709.1	−2.4
0.7490	1219.0	771.8	−1.6	0.2012	1284.4	703.8	−2.0
0.6993	1224.6	765.5	−1.7	0.1494	1291.0	697.6	−1.8
0.6518	1230.3	759.1	−2.2	0.1014	1296.9	692.2	−1.3
0.5991	1236.3	752.7	−2.2	0.0494	1303.5	686.2	−0.9
0.5505	1242.1	746.4	−2.5	0.0000	1309.4	681.0	0.0
0.4999	1248.1	740.1	−2.5				
303.15 K							
1.0000	1170.6	837.8	0.0	0.4519	1233.1	763.1	−2.8
0.9489	1176.0	830.9	−0.1	0.4040	1238.8	757.0	−2.7
0.8979	1181.4	824.1	−0.3	0.3519	1245.2	750.1	−2.7
0.8519	1186.7	817.4	−0.9	0.3077	1250.5	744.5	−2.5
0.7990	1192.5	810.3	−1.1	0.2480	1258.0	736.7	−2.5
0.7490	1198.3	803.3	−1.6	0.2012	1263.7	730.9	−2.1
0.6993	1203.8	796.7	−1.7	0.1494	1270.3	724.3	−1.9
0.6518	1209.4	790.0	−2.1	0.1014	1276.1	718.6	−1.3
0.5991	1215.5	783.0	−2.2	0.0494	1282.8	712.1	−1.0
0.5505	1221.3	776.3	−2.5	0.0000	1288.7	706.7	0.0
0.4999	1227.2	769.6	−2.6				
308.15 K							
1.0000	1150.2	873.1	0.0	0.4519	1212.5	793.7	−2.9
0.9489	1155.5	865.9	−0.1	0.4040	1218.1	787.2	−2.8
0.8979	1160.8	858.7	−0.1	0.3519	1224.5	779.9	−2.8
0.8519	1166.2	851.4	−1.0	0.3077	1229.8	773.9	−2.6
0.7990	1171.8	844.0	−1.0	0.2480	1237.4	765.5	−2.6
0.7490	1177.6	836.5	−1.6	0.2012	1243.0	759.4	−2.2

(*continued*)

TABLE II Continued

x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})	x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})
0.6993	1183.2	829.4	−1.7	0.1494	1249.7	752.3	−2.1
0.6518	1188.8	822.3	−2.2	0.1014	1255.5	746.3	−1.4
0.5991	1194.9	814.8	−2.3	0.0494	1262.1	739.4	−1.0
0.5505	1200.7	807.7	−2.7	0.0000	1268.1	733.6	0.0
0.4999	1206.7	800.6	−2.7				
313.15 K							
1.0000	1130.0	910.0	0.0	0.4519	1191.75	826.2	−2.9
0.9489	1135.3	902.3	−0.1	0.4040	1197.405	819.2	−2.8
0.8979	1140.7	894.5	−0.4	0.3519	1203.804	811.4	−3.0
0.8519	1145.7	887.5	−0.6	0.3077	1209.075	805.1	−2.7
0.7990	1151.4	879.4	−0.9	0.2480	1216.503	796.3	−2.7
0.7490	1157.1	871.6	−1.4	0.2012	1222.235	789.7	−2.4
0.6993	1162.7	863.9	−1.8	0.1494	1228.796	782.3	−2.2
0.6518	1168.2	856.5	−2.1	0.1014	1234.728	775.7	−1.7
0.5991	1174.3	848.4	−2.4	0.0494	1241.108	768.7	−1.0
0.5505	1180.0	841.1	−2.6	0.0000	1247.051	762.4	0.0
0.4999	1185.9	833.5	−2.7				
Mesitylene							
293.15 K							
1.0000	1211.9	772.7	0.0	0.4499	1288.7	691.0	−2.2
0.9494	1218.5	765.3	−0.1	0.3998	1296.2	683.7	−2.4
0.8998	1225.1	758.0	−0.2	0.3481	1303.8	676.3	−2.3
0.8531	1231.4	751.1	−0.4	0.2995	1311.0	669.4	−2.2
0.8007	1238.7	743.1	−0.8	0.2516	1318.2	662.5	−2.1
0.7495	1245.7	735.5	−1.0	0.2009	1325.9	655.3	−2.0
0.7020	1252.4	728.4	−1.3	0.1506	1333.5	648.4	−1.7
0.6518	1259.4	720.9	−1.5	0.1002	1341.1	641.5	−1.2
0.5990	1267.0	713.0	−1.7	0.0516	1348.7	634.9	−0.8
0.5517	1273.9	705.9	−2.1	0.0000	1356.3	628.3	0.0
0.5012	1281.2	698.5	−2.1				
298.15 K							
1.0000	1191.3	804.3	0.0	0.4499	1268.2	717.2	−2.5
0.9494	1197.9	796.4	−0.1	0.3998	1275.7	709.4	−2.6
0.8998	1204.5	788.6	−0.2	0.3481	1283.3	701.6	−2.5
0.8531	1210.9	781.1	−0.6	0.2995	1290.5	694.3	−2.3
0.8007	1218.0	772.8	−0.8	0.2516	1297.8	686.9	−2.4
0.7495	1225.1	764.7	−1.1	0.2009	1305.5	679.3	−2.2
0.7020	1231.8	757.0	−1.5	0.1506	1313.2	671.8	−1.9
0.6518	1239.0	748.9	−1.8	0.1002	1320.8	664.6	−1.4
0.5990	1246.4	740.7	−1.9	0.0516	1328.4	657.5	−1.1
0.5517	1253.4	733.0	−2.3	0.0000	1336.0	650.6	0.0
0.5012	1260.7	725.2	−2.4				
303.15 K							
1.0000	1170.6	837.8	0.0	0.4499	1247.8	744.8	−2.8
0.9494	1177.3	829.4	−0.1	0.3998	1255.2	736.6	−2.8
0.8998	1183.9	821.0	−0.3	0.3481	1262.9	728.1	−2.8
0.8531	1190.3	813.0	−0.7	0.2995	1270.2	720.3	−2.6
0.8007	1197.5	804.1	−1.0	0.2516	1277.6	712.4	−2.7
0.7495	1204.6	795.4	−1.3	0.2009	1285.4	704.2	−2.5
0.7020	1211.3	787.2	−1.7	0.1506	1293.0	696.4	−2.1
0.6518	1218.5	778.5	−2.1	0.1002	1300.6	688.8	−1.5
0.5990	1226.0	769.7	−2.3	0.0516	1308.4	681.1	−1.2
0.5517	1233.0	761.6	−2.7	0.0000	1315.9	673.8	0.0
0.5012	1240.3	753.3	−2.7				

(*continued*)

TABLE II Continued

x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})	x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})
308.15 K							
1.0000	1150.2	873.1	0.0	0.4499	1227.5	773.8	−3.1
0.9494	1156.9	864.0	−0.2	0.3998	1235.0	764.9	−3.2
0.8998	1163.4	855.1	−0.4	0.3481	1242.8	755.9	−3.1
0.8531	1169.9	846.5	−0.9	0.2995	1250.1	747.5	−3.0
0.8007	1177.0	837.1	−1.1	0.2516	1257.4	739.2	−3.0
0.7495	1184.2	827.6	−1.6	0.2009	1265.3	730.4	−2.8
0.7020	1190.9	819.0	−2.0	0.1506	1272.9	722.2	−2.3
0.6518	1198.2	809.7	−2.5	0.1002	1280.5	714.1	−1.6
0.5990	1205.8	800.2	−2.8	0.0516	1288.3	705.8	−1.3
0.5517	1212.7	791.6	−3.0	0.0000	1295.9	698.1	0.0
0.5012	1220.1	782.7	−3.1				
313.15 K							
1.0000	1129.7	910.5	0.0	0.4499	1207.4	804.1	−3.4
0.9494	1136.4	900.8	−0.2	0.3998	1214.9	794.7	−3.4
0.8998	1143.1	891.1	−0.6	0.3481	1222.7	785.0	−3.4
0.8531	1149.5	881.8	−1.1	0.2995	1230.1	776.0	−3.3
0.8007	1156.7	871.7	−1.4	0.2516	1237.5	767.1	−3.2
0.7495	1164.0	861.6	−2.0	0.2009	1245.5	757.7	−3.1
0.7020	1170.8	852.2	−2.4	0.1506	1253.1	748.9	−2.5
0.6518	1178.0	842.4	−2.9	0.1002	1260.8	740.2	−1.7
0.5990	1185.6	832.3	−3.1	0.0516	1268.7	731.4	−1.4
0.5517	1192.5	823.2	−3.3	0.0000	1276.3	723.2	0.0
0.5012	1199.9	813.6	−3.5				
Isopropylbenzene							
293.15 K							
1.0000	1211.9	772.7	0.0	0.4514	1276.4	705.2	−4.4
0.9500	1217.9	766.0	−0.9	0.4021	1282.0	699.8	−4.2
0.8992	1223.8	759.5	−1.7	0.3578	1287.2	694.8	−4.0
0.8497	1229.7	753.1	−2.3	0.3036	1293.4	689.0	−3.7
0.8007	1235.5	746.9	−2.9	0.2496	1299.7	683.2	−3.2
0.7493	1241.5	740.4	−3.4	0.2043	1304.9	678.4	−2.9
0.6996	1247.3	734.4	−3.7	0.1510	1311.1	672.8	−2.3
0.6500	1253.2	728.4	−4.1	0.0998	1316.9	667.6	−1.7
0.6017	1258.8	722.6	−4.3	0.0521	1322.4	662.7	−1.0
0.5550	1264.3	717.1	−4.5	0.0000	1328.2	657.7	0.0
0.4994	1270.8	710.7	−4.4				
298.15 K							
1.0000	1191.3	804.3	0.0	0.4514	1255.7	732.5	−4.7
0.9500	1197.3	797.0	−1.1	0.4021	1261.3	726.8	−4.5
0.8992	1203.2	790.2	−1.8	0.3578	1266.4	721.5	−4.3
0.8497	1209.0	783.4	−2.5	0.3036	1272.7	715.3	−3.9
0.8007	1214.8	776.8	−3.1	0.2496	1278.9	709.2	−3.4
0.7493	1220.9	769.9	−3.7	0.2043	1284.2	704.0	−3.0
0.6996	1226.6	763.6	−4.0	0.1510	1290.3	698.1	−2.4
0.6500	1232.5	757.1	−4.4	0.0998	1296.2	692.5	−1.8
0.6017	1238.2	750.9	−4.7	0.0521	1301.6	687.5	−1.0
0.5550	1243.7	745.1	−4.8	0.0000	1307.5	682.1	0.0
0.4994	1250.1	738.3	−4.8				
303.15 K							
1.0000	1170.6	837.8	0.0	0.4514	1235.0	761.3	−5.0
0.9500	1176.6	830.2	−1.0	0.4021	1240.8	754.9	−5.0
0.8992	1182.5	822.8	−1.8	0.3578	1245.9	749.4	−4.7
0.8497	1188.3	815.6	−2.6	0.3036	1252.1	742.8	−4.3
0.8007	1194.1	808.5	−3.3	0.2496	1258.3	736.3	−3.8
0.7493	1200.1	801.3	−3.8	0.2043	1263.6	730.8	−3.3

(*continued*)

TABLE II Continued

x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})	x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})
0.6996	1205.9	794.4	−4.3	0.1510	1269.7	724.6	−2.7
0.6500	1211.8	787.5	−4.7	0.0998	1275.6	718.7	−1.9
0.6017	1217.5	781.0	−4.9	0.0521	1281.1	713.2	−1.2
0.5550	1223.0	774.6	−5.2	0.0000	1286.9	707.6	0.0
0.4994	1229.4	767.4	−5.2				
308.15 K							
1.0000	1150.2	873.1	0.0	0.4514	1214.5	791.4	−5.5
0.9500	1156.1	865.1	−1.1	0.4021	1220.3	784.8	−5.3
0.8992	1162.0	857.1	−2.0	0.3578	1225.4	778.8	−5.1
0.8497	1167.8	849.4	−2.8	0.3036	1231.6	771.8	−4.6
0.8007	1173.6	841.9	−3.5	0.2496	1237.9	764.8	−4.1
0.7493	1179.7	834.0	−4.3	0.2043	1243.1	759.1	−3.5
0.6996	1185.5	826.8	−4.6	0.1510	1249.2	752.4	−2.8
0.6500	1191.4	819.3	−5.2	0.0998	1255.2	746.0	−2.1
0.6017	1197.0	812.4	−5.4	0.0521	1260.7	740.3	−1.2
0.5550	1202.5	805.7	−5.6	0.0000	1266.5	734.2	0.0
0.4994	1209.0	798.0	−5.6				
313.15 K							
1.0000	1130.0	910.0	0.0	0.4514	1194.4	822.9	−5.8
0.9500	1135.9	901.4	−1.2	0.4021	1200.1	815.8	−5.5
0.8992	1141.8	892.9	−2.1	0.3578	1205.2	809.6	−5.2
0.8497	1147.6	884.8	−2.9	0.3036	1211.5	802.0	−4.7
0.8007	1153.4	876.8	−3.7	0.2496	1217.7	794.5	−4.2
0.7493	1159.4	868.4	−4.4	0.2043	1223.0	788.4	−3.6
0.6996	1165.2	860.6	−4.9	0.1510	1229.2	781.3	−2.9
0.6500	1171.1	852.7	−5.4	0.0998	1235.2	774.4	−2.1
0.6017	1176.8	845.2	−5.7	0.0521	1240.6	768.2	−1.2
0.5550	1182.3	838.2	−5.8	0.0000	1246.6	761.7	0.0
0.4994	1188.8	829.9	−5.8				
Butylbenzene							
293.15 K							
1.0000	1211.9	772.7	0.0	0.4500	1292.3	689.5	−7.4
0.9493	1219.5	764.2	−1.6	0.3997	1299.4	682.8	−7.1
0.8999	1227.3	755.7	−3.2	0.3501	1306.3	676.3	−6.7
0.8489	1234.7	747.7	−4.2	0.3023	1312.8	670.3	−6.1
0.8010	1241.6	740.4	−4.9	0.2515	1320.0	663.9	−5.6
0.7517	1249.0	732.6	−5.9	0.1989	1326.8	657.8	−4.4
0.6998	1256.7	724.6	−6.7	0.1545	1332.9	652.5	−3.6
0.6499	1263.9	717.4	−7.0	0.1016	1339.8	646.4	−2.4
0.6004	1271.0	710.3	−7.3	0.0490	1347.2	640.0	−1.5
0.5496	1278.2	703.1	−7.5	0.0000	1353.4	634.8	0.0
0.4993	1285.4	696.1	−7.5				
298.15 K							
1.0000	1191.3	804.3	0.0	0.4500	1272.2	715.1	−8.0
0.9493	1198.8	795.3	−1.5	0.3997	1279.4	707.9	−7.8
0.8999	1206.7	786.0	−3.5	0.3501	1286.3	701.1	−7.3
0.8489	1214.0	777.6	−4.3	0.3023	1292.8	694.7	−6.6
0.8010	1221.0	769.7	−5.2	0.2515	1300.0	687.7	−6.0
0.7517	1228.5	761.4	−6.3	0.1989	1306.8	681.3	−4.7
0.6998	1236.3	752.8	−7.2	0.1545	1313.1	675.4	−4.0
0.6499	1243.5	745.0	−7.6	0.1016	1320.0	669.1	−2.6
0.6004	1250.7	737.4	−7.9	0.0490	1327.5	662.3	−1.6
0.5496	1258.0	729.7	−8.1	0.0000	1333.8	656.7	0.0
0.4993	1265.2	722.2	−8.2				

(*continued*)

TABLE II Continued

x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})	x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})
303.15 K							
1.0000	1170.6	837.8	0.0	0.4500	1252.1	742.0	−8.7
0.9493	1178.2	828.1	−1.6	0.3997	1259.5	734.1	−8.6
0.8999	1186.1	818.2	−3.7	0.3501	1266.5	726.8	−8.1
0.8489	1193.6	809.1	−4.8	0.3023	1273.0	720.1	−7.2
0.8010	1200.6	800.6	−5.6	0.2515	1280.2	712.7	−6.6
0.7517	1208.1	791.6	−6.9	0.1989	1287.2	705.7	−5.2
0.6998	1216.0	782.3	−7.9	0.1545	1293.4	699.5	−4.4
0.6499	1223.3	774.0	−8.3	0.1016	1300.4	692.6	−2.9
0.6004	1230.5	765.8	−8.7	0.0490	1307.9	685.4	−1.8
0.5496	1237.9	757.6	−8.9	0.0000	1314.3	679.4	0.0
0.4993	1245.2	749.5	−8.9				
308.15 K							
1.0000	1150.2	873.1	0.0	0.4500	1232.3	770.2	−9.5
0.9493	1157.7	862.8	−1.6	0.3997	1239.7	761.7	−9.4
0.8999	1165.7	852.1	−4.0	0.3501	1246.8	753.8	−8.9
0.8489	1173.3	842.1	−5.3	0.3023	1253.3	746.6	−7.9
0.8010	1180.3	833.1	−6.2	0.2515	1260.6	738.7	−7.2
0.7517	1187.9	823.4	−7.5	0.1989	1267.6	731.3	−5.7
0.6998	1195.8	813.6	−8.5	0.1545	1273.9	724.6	−4.8
0.6499	1203.2	804.5	−9.1	0.1016	1281.0	717.3	−3.1
0.6004	1210.5	795.6	−9.5	0.0490	1288.5	709.6	−1.9
0.5496	1217.9	786.8	−9.7	0.0000	1295.0	703.1	0.0
0.4993	1225.3	778.2	−9.8				
313.15 K							
1.0000	1130.0	910.0	0.0	0.4500	1212.6	799.5	−10.4
0.9493	1137.7	898.8	−2.0	0.3997	1220.0	790.6	−10.1
0.8999	1145.5	887.6	−4.2	0.3501	1227.2	782.0	−9.7
0.8489	1153.3	876.6	−5.9	0.3023	1233.9	774.3	−8.8
0.8010	1160.3	867.0	−6.8	0.2515	1241.1	765.9	−7.8
0.7517	1167.9	856.7	−8.1	0.1989	1248.2	757.9	−6.3
0.6998	1175.8	846.2	−9.2	0.1545	1254.5	750.9	−5.3
0.6499	1183.2	836.5	−9.8	0.1016	1261.7	743.0	−3.5
0.6004	1190.6	827.0	−10.3	0.0490	1269.2	734.9	−2.0
0.5496	1198.0	817.6	−10.5	0.0000	1275.7	728.0	0.0
0.4993	1205.5	808.2	−10.7				
Isobutylbenzene							
293.15 K							
1.0000	1211.9	772.7	0.0	0.4537	1271.5	715.5	−4.7
0.9482	1217.9	766.7	−1.0	0.3994	1277.2	710.3	−4.6
0.8995	1223.2	761.5	−1.6	0.3619	1280.9	707.0	−4.3
0.8469	1229.2	755.4	−2.5	0.3027	1287.0	701.7	−3.9
0.7981	1234.6	750.2	−3.0	0.2486	1292.3	697.0	−3.5
0.7510	1239.8	745.1	−3.6	0.2010	1297.1	692.8	−3.0
0.6954	1245.8	739.4	−4.1	0.1619	1300.9	689.6	−2.5
0.6485	1250.9	734.6	−4.3	0.1042	1306.4	684.9	−1.7
0.5973	1256.4	729.3	−4.6	0.0560	1311.0	681.0	−0.9
0.5506	1261.3	724.9	−4.6	0.0000	1316.5	676.5	0.0
0.5056	1266.1	720.5	−4.7				
298.15 K							
1.0000	1191.3	804.3	0.0	0.4537	1251.2	742.7	−4.9
0.9482	1197.1	798.0	−0.9	0.3994	1256.9	737.2	−4.8
0.8995	1202.5	792.3	−1.6	0.3619	1260.7	733.6	−4.5
0.8469	1208.6	785.8	−2.6	0.3027	1266.9	727.7	−4.3
0.7981	1214.0	780.1	−3.2	0.2486	1272.3	722.7	−3.6
0.7510	1219.3	774.7	−3.8	0.2010	1277.1	718.2	−3.2

(*continued*)

TABLE II Continued

x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})	x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})
0.6954	1225.4	768.4	−4.3	0.1619	1280.8	714.9	−2.5
0.6485	1230.4	763.3	−4.5	0.1042	1286.6	709.5	−1.8
0.5973	1236.1	757.6	−5.0	0.0560	1291.1	705.5	−0.8
0.5506	1241.0	752.8	−4.9	0.0000	1296.7	700.6	0.0
0.5056	1245.8	748.0	−5.0				
303.15 K							
1.0000	1170.6	837.8	0.0	0.4537	1231.0	771.3	−5.3
0.9482	1176.6	830.8	−1.1	0.3994	1236.7	765.4	−5.1
0.8995	1181.9	824.9	−1.6	0.3619	1240.7	761.4	−5.0
0.8469	1188.1	817.8	−2.8	0.3027	1246.8	755.1	−4.6
0.7981	1193.5	811.7	−3.4	0.2486	1252.2	749.7	−3.9
0.7510	1198.7	805.9	−4.0	0.2010	1257.1	744.9	−3.4
0.6954	1205.1	798.9	−4.8	0.1619	1260.9	741.2	−2.7
0.6485	1210.0	793.5	−4.9	0.1042	1266.7	735.6	−1.9
0.5973	1215.7	787.4	−5.3	0.0560	1271.3	731.2	−0.8
0.5506	1220.7	782.1	−5.3	0.0000	1277.0	725.8	0.0
0.5056	1225.5	777.1	−5.3				
308.15 K							
1.0000	1150.2	873.1	0.0	0.4537	1211.0	801.2	−5.8
0.9482	1156.1	865.7	−1.1	0.3994	1216.8	794.8	−5.6
0.8995	1161.6	859.0	−1.9	0.3619	1220.7	790.5	−5.4
0.8469	1167.7	851.5	−3.1	0.3027	1227.0	783.7	−5.0
0.7981	1173.1	845.0	−3.6	0.2486	1232.4	778.0	−4.2
0.7510	1178.5	838.6	−4.4	0.2010	1237.4	772.7	−3.7
0.6954	1184.8	831.1	−5.1	0.1619	1241.2	768.7	−2.9
0.6485	1189.9	825.2	−5.4	0.1042	1247.1	762.6	−2.1
0.5973	1195.5	818.6	−5.7	0.0560	1251.8	757.9	−1.0
0.5506	1200.6	812.8	−5.9	0.0000	1257.5	752.1	0.0
0.5056	1205.4	807.5	−5.8				
313.15 K							
1.0000	1130.0	910.0	0.0	0.4537	1191.3	832.4	−6.2
0.9482	1135.7	902.5	−0.7	0.3994	1197.1	825.5	−6.0
0.8995	1141.2	895.2	−1.7	0.3619	1201.1	820.8	−5.7
0.8469	1147.4	887.0	−3.0	0.3027	1207.5	813.5	−5.3
0.7981	1152.8	880.0	−3.6	0.2486	1213.0	807.2	−4.6
0.7510	1158.3	873.0	−4.5	0.2010	1218.0	801.5	−4.0
0.6954	1164.7	864.8	−5.3	0.1619	1221.9	797.2	−3.2
0.6485	1169.8	858.4	−5.6	0.1042	1227.8	790.7	−2.1
0.5973	1175.7	851.2	−6.1	0.0560	1232.7	785.3	−1.2
0.5506	1180.8	844.9	−6.3	0.0000	1238.4	779.3	0.0
0.5056	1185.6	839.2	−6.2				
t-Butylbenzene							
293.15 K							
1.0000	1211.9	772.7	0.0	0.4489	1283.7	695.4	−8.0
0.9500	1218.6	764.9	−1.5	0.4061	1289.0	690.2	−7.8
0.9005	1225.4	757.1	−3.1	0.3516	1295.5	683.9	−7.2
0.8509	1232.1	749.7	−4.3	0.3008	1301.6	678.1	−6.7
0.8013	1238.8	742.2	−5.5	0.2511	1307.5	672.5	−6.0
0.7489	1245.6	734.8	−6.3	0.1995	1313.5	667.0	−5.0
0.7006	1251.9	728.1	−6.9	0.1522	1318.9	662.0	−4.0
0.6496	1258.6	721.0	−7.7	0.1000	1325.0	656.5	−3.0
0.6070	1263.9	715.4	−7.9	0.0517	1329.9	652.1	−1.2
0.5499	1271.1	708.0	−8.1	0.0000	1335.9	646.9	0.0
0.4994	1277.5	701.6	−8.2				

(*continued*)

TABLE II Continued

x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})	x_1	u (m s^{-1})	κ_s (T Pa^{-1})	$\delta\kappa_s$ (T Pa^{-1})
298.15 K							
1.0000	1191.3	804.3	0.0	0.4489	1262.9	722.1	−8.4
0.9500	1197.8	796.2	−1.4	0.4061	1268.3	716.6	−8.2
0.9005	1204.5	788.1	−2.9	0.3516	1274.7	709.9	−7.6
0.8509	1211.2	780.0	−4.3	0.3008	1281.0	703.6	−7.1
0.8013	1218.0	772.0	−5.7	0.2511	1286.7	697.8	−6.3
0.7489	1224.9	764.0	−6.7	0.1995	1292.8	691.9	−5.3
0.7006	1231.0	757.0	−7.2	0.1522	1298.1	686.8	−4.1
0.6496	1237.8	749.3	−8.1	0.1000	1304.3	680.7	−3.2
0.6070	1243.1	743.5	−8.2	0.0517	1309.3	676.1	−1.3
0.5499	1250.3	735.6	−8.5	0.0000	1315.2	670.5	0.0
0.4994	1256.8	728.7	−8.7				
303.15 K							
1.0000	1170.6	837.8	0.0	0.4489	1242.3	750.2	−9.0
0.9500	1177.1	829.3	−1.3	0.4061	1247.7	744.2	−8.8
0.9005	1183.8	820.6	−3.0	0.3516	1254.1	737.2	−8.1
0.8509	1190.5	812.0	−4.5	0.3008	1260.5	730.3	−7.7
0.8013	1197.3	803.4	−6.0	0.2511	1266.2	724.3	−6.6
0.7489	1204.2	794.8	−7.1	0.1995	1272.3	717.9	−5.7
0.7006	1210.3	787.4	−7.6	0.1522	1277.5	712.5	−4.3
0.6496	1217.2	779.1	−8.7	0.1000	1283.8	706.0	−3.3
0.6070	1222.4	773.0	−8.7	0.0517	1288.8	701.0	−1.4
0.5499	1229.7	764.6	−9.0	0.0000	1294.8	695.1	0.0
0.4994	1236.1	757.1	−9.2				
308.15 K							
1.0000	1150.2	873.1	0.0	0.4489	1221.9	779.5	−9.6
0.9500	1156.5	864.2	−1.3	0.4061	1227.3	773.1	−9.5
0.9005	1163.2	854.9	−3.0	0.3516	1233.7	765.7	−8.6
0.8509	1170.0	845.6	−4.8	0.3008	1240.0	758.5	−8.1
0.8013	1176.8	836.4	−6.4	0.2511	1245.8	751.9	−7.1
0.7489	1183.7	827.2	−7.6	0.1995	1252.0	745.0	−6.1
0.7006	1189.9	819.2	−8.2	0.1522	1257.2	739.3	−4.6
0.6496	1196.7	810.5	−9.2	0.1000	1263.6	732.4	−3.6
0.6070	1202.0	803.9	−9.4	0.0517	1268.5	727.2	−1.4
0.5499	1209.2	794.9	−9.6	0.0000	1274.6	720.7	0.0
0.4994	1215.7	787.0	−9.8				
313.15 K							
1.0000	1130.0	910.0	0.0	0.4489	1201.3	810.7	−10.1
0.9500	1136.0	901.0	−0.9	0.4061	1206.6	804.2	−9.7
0.9005	1142.6	891.2	−2.7	0.3516	1213.1	796.0	−9.1
0.8509	1149.3	881.4	−4.5	0.3008	1219.3	788.4	−8.4
0.8013	1156.0	871.7	−6.1	0.2511	1225.1	781.5	−7.4
0.7489	1162.9	862.0	−7.3	0.1995	1231.4	774.1	−6.4
0.7006	1169.2	853.2	−8.3	0.1522	1236.8	767.7	−5.1
0.6496	1175.9	844.1	−9.2	0.1000	1242.9	760.7	−3.7
0.6070	1181.5	836.6	−9.8	0.0517	1247.9	755.0	−1.5
0.5499	1188.6	827.1	−10.0	0.0000	1254.0	748.2	0.0
0.4994	1195.0	818.9	−10.1				

3.2. Acoustic Parameters

We have attempted to explain the physico-chemical behavior of the mixtures indicated above, in order to explore the strength and nature of the interactions between the components by deriving various thermodynamic parameters from the ultrasonic velocity and density data. The parameters derived from the experimental measured data were

TABLE III Fitting parameters of Eqs. (2) and (3), and root mean square deviation, σ (TPa^{-1}) by means of Eq. (4)

Butyl acetate + toluene				*Butyl acetate + isopropylbenzene*			
$B_{00} = 1155.7$	$B_{01} = -7.6904$	$B_{02} = 0.0129$		$B_{00} = 197.2$	$B_{01} = -1.1485$	$B_{02} = 0.0014$	
$B_{10} = -67.5$	$B_{11} = 0.3973$	$B_{12} = -0.0005$		$B_{10} = -529.9$	$B_{11} = 3.5003$	$B_{12} = -0.0058$	
$B_{20} = 739.3$	$B_{21} = -5.1049$	$B_{22} = 0.0088$	$\sigma = 0.20$	$B_{20} = -27.5$	$B_{21} = 0.0832$	$B_{22} = 0.0001$	$\sigma = 0.11$
$B_{30} = -1457.6$	$B_{31} = 9.4775$	$B_{32} = -0.0154$		$B_{30} = 371.1$	$B_{31} = -2.4749$	$B_{32} = 0.0041$	
$B_{40} = -2248.5$	$B_{41} = 15.0770$	$B_{42} = -0.0252$		$B_{40} = 38.7$	$B_{41} = -0.2659$	$B_{42} = 0.0004$	
Butyl acetate + ethylbenzene				*Butyl acetate + butylbenzene*			
$B_{00} = 88.4$	$B_{01} = -0.4794$	$B_{02} = 0.0005$		$B_{00} = -223.6$	$B_{01} = 1.8628$	$B_{02} = -0.0041$	
$B_{10} = 593.3$	$B_{11} = -3.8896$	$B_{12} = 0.0064$		$B_{10} = 655.9$	$B_{11} = -4.3622$	$B_{12} = 0.0072$	
$B_{20} = 395.5$	$B_{21} = -2.5710$	$B_{22} = 0.0043$	$\sigma = 0.15$	$B_{20} = -1253.7$	$B_{21} = 8.3186$	$B_{22} = -0.0138$	$\sigma = 0.31$
$B_{30} = -1305.3$	$B_{31} = 8.4642$	$B_{32} = -0.0137$		$B_{30} = -1904.9$	$B_{31} = 12.5984$	$B_{32} = -0.0208$	
$B_{40} = -327.4$	$B_{41} = 2.1359$	$B_{42} = -0.0036$		$B_{40} = -80.6$	$B_{41} = 0.3370$	$B_{42} = -0.0003$	
Butyl acetate + p-xylene				*Butyl acetate + isobutylbenzene*			
$B_{00} = 110.4$	$B_{01} = -0.7374$	$B_{02} = 0.0011$		$B_{00} = -254.1$	$B_{01} = 1.8558$	$B_{02} = -0.0036$	
$B_{10} = 336.5$	$B_{11} = -2.2865$	$B_{12} = 0.0039$		$B_{10} = -11.5$	$B_{11} = 0.0931$	$B_{12} = -0.0002$	
$B_{20} = 268.0$	$B_{21} = -1.8870$	$B_{22} = 0.0033$	$\sigma = 0.20$	$B_{20} = 929.1$	$B_{21} = -6.2387$	$B_{22} = 0.0105$	$\sigma = 0.19$
$B_{30} = -349.9$	$B_{31} = 2.1740$	$B_{32} = -0.0033$		$B_{30} = 2288.8$	$B_{31} = -15.3294$	$B_{32} = 0.0257$	
$B_{40} = -1364.4$	$B_{41} = 9.1681$	$B_{42} = -0.0154$		$B_{40} = -117.1$	$B_{41} = 0.6196$	$B_{42} = -0.0007$	
Butyl acetate + mesitylene				*Butyl acetate + t-butylbenzene*			
$B_{00} = -39.6$	$B_{01} = 0.4462$	$B_{02} = -0.0012$		$B_{00} = 162.9$	$B_{01} = -0.9015$	$B_{02} = 0.0008$	
$B_{10} = -401.2$	$B_{11} = 2.7409$	$B_{12} = -0.0046$		$B_{10} = 550.8$	$B_{11} = -3.6469$	$B_{12} = 0.0060$	
$B_{20} = -2464.3$	$B_{21} = 16.3796$	$B_{22} = -0.0272$	$\sigma = 0.18$	$B_{20} = 2417.5$	$B_{21} = -15.9883$	$B_{22} = 0.0264$	$\sigma = 0.30$
$B_{30} = -647.0$	$B_{31} = 4.0387$	$B_{32} = -0.0062$		$B_{30} = 1373.6$	$B_{31} = -9.5347$	$B_{32} = 0.0166$	
$B_{40} = 3801.4$	$B_{41} = -25.2075$	$B_{42} = 0.0417$		$B_{40} = -2762.2$	$B_{41} = 17.6363$	$B_{42} = -0.0280$	

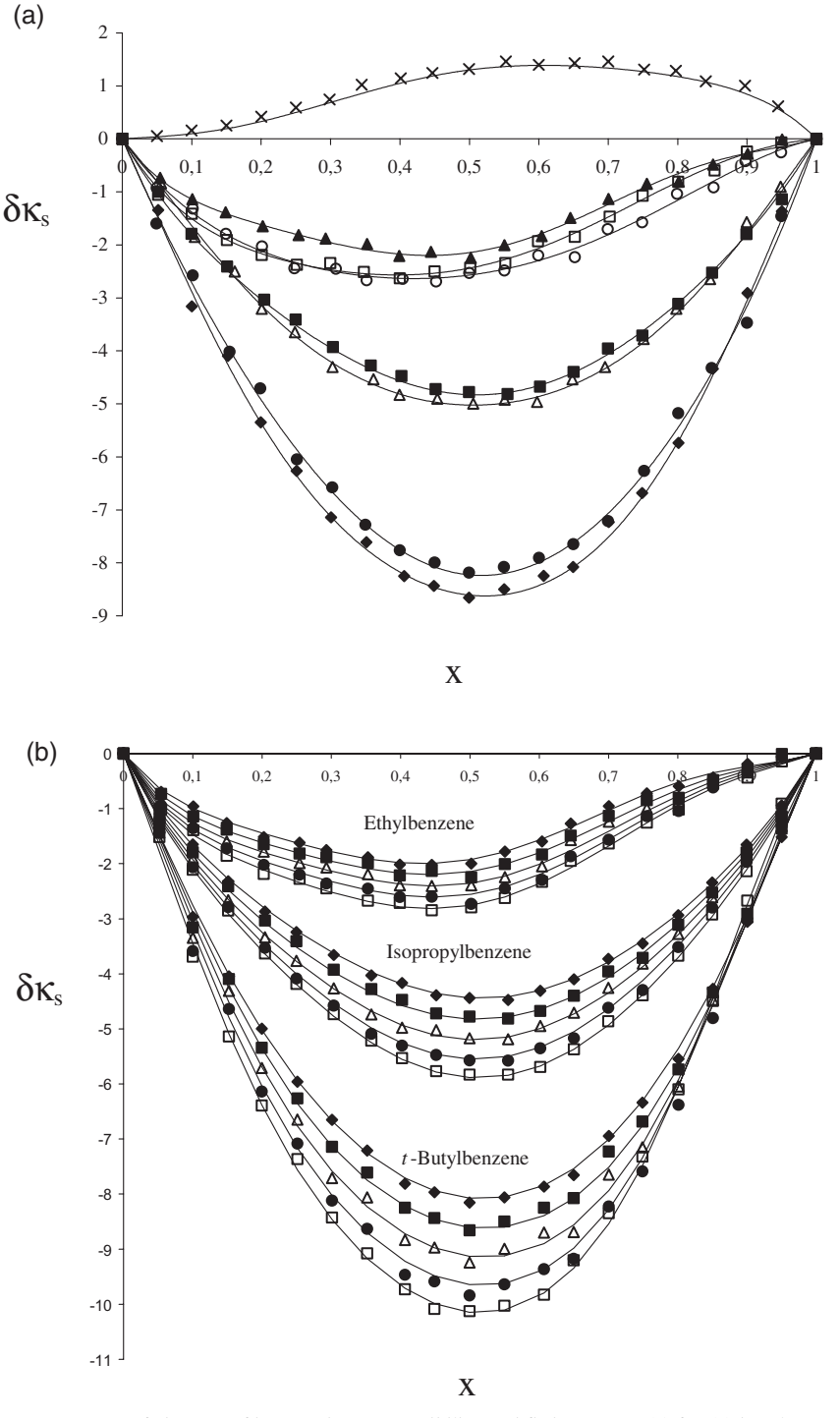

FIGURE 1 Curves of changes of isentropic compressibility and fitting curves (–) for (a) butyl acetate + (×) toluene, (▲) ethylbenzene, (○) *p*-xylene, (□) mesitylene, (■) isopropylbenzene, (●) butylbenzene, (△) isobutylbenzene or (◆) *t*-butylbenzene) at 298.15 K, and (b) butyl acetate + (ethylbenzene, isopropylbenzene and *t*-butylbenzene) at (◆) 293.15 K, (■) 298.15 K, (△) 303.15 K, (●) 308.15 K and (□) 313.15 K.

intermolecular free length (L_f), the van der Waals' constant (b), molecular radius (r), geometrical volume (B), molar surface area (Y), available volume (V_a), volume at absolute zero (V_0), molar sound velocity (R), collision factor (S), specific acoustic impedance (Z), relative association (R_A), and molecular association (M_A), attending to the following set of equations

$$L_f = \left(\frac{K}{\rho^{1/2} \cdot u}\right) \tag{5}$$

$$b = \left(\frac{M}{\rho}\right) - \left(\frac{RT}{\rho \cdot u^2}\right) \cdot \left(\left[1 + \frac{M \cdot u^2}{3RT}\right]^{1/2} - 1\right) \tag{6}$$

$$r = \left(\frac{3b}{16\Pi N}\right)^{1/3} \tag{7}$$

$$B = \left(\frac{4}{3}\right)\Pi r^3 N \tag{8}$$

$$Y = \left(36\Pi N B^2\right)^{1/3} \tag{9}$$

$$\kappa_s = \left(\frac{L_f^2}{K^2}\right) \tag{10}$$

$$V_0 = V - V_a \tag{11}$$

$$R = \frac{M \cdot u^{1/3}}{\rho} \tag{12}$$

$$S = \frac{u \cdot V}{B \cdot u_\infty} \tag{13}$$

$$Z = u \cdot \rho \tag{14}$$

$$R_A = \left(\frac{\rho_{mix}}{\rho}\right) \cdot \left(\frac{u}{u_{mix}}\right)^{1/3} \tag{15}$$

$$M_A = \left[\left(\frac{u_{mix}}{\sum_i x_i u_i}\right)^2 - 1\right], \tag{16}$$

where L_f is the free length of ideal mixing, K is a temperature-dependent constant ($K = (93.875 + 0.375 \cdot T) \times 10^{-8}$), u_∞ is taken as $1600\,\mathrm{ms}^{-1}$ [9], and R and Π are common universal constants. These parameters are given in Table IV for the pure compounds in the temperature range 293.15–313.15 K. The variation of the magnitudes L_f and Z (by means of Eq. (1)) are shown in the Figs. 2(a) and 3(a) for the whole set of binary mixtures at 298.15 K, and Figs. 2(b) and 3(b) show these magnitudes as a function of temperature for the three binary systems. The Fig. 2(a,b) point out an analogous effect for molecular structure and temperature, showing the lowest values for the highest molecules and slight effect of temperature. As expected, this fact increases the nonideality of the mixture. At any case, increasing temperatures produces

TABLE IV Acoustic parameters for the pure compounds enclosed into the studied mixtures in the range 293.15–313.15 K

Temperature (K)	$L_f \times 10^9$ (m)	b ($m^3\,mol^{-1}$)	$r \times 10^{12}$ (m)	B ($m^3\,mol^{-1}$)	$Y \times 10^{13}$ (m^2)	V_a ($m^3\,mol^{-1}$)	V_0 ($m^3\,mol^{-1}$)	R ($m^3\,mol^{-1}$)·($m\,s^{-1}$)$^{1/3}$	S	Z ($kg\,m^{-2}\,s^{-1}$)	R_A
Butyl acetate											
293.15	1.792	122.729	4.800	30.682	1.918	31.976	99.849	1405.471	3.254	1067.877	1.0000
298.15	1.845	123.195	4.806	30.799	1.923	33.869	98.713	1405.466	3.205	1043.718	1.0000
303.15	1.900	123.671	4.812	30.918	1.927	35.787	97.572	1405.498	3.156	1019.666	1.0000
308.15	1.957	124.159	4.818	31.040	1.933	37.720	96.441	1405.649	3.107	995.832	1.0000
313.15	2.016	124.648	4.825	31.162	1.938	39.649	95.323	1405.838	3.059	972.494	1.0000
Toluene											
293.15	1.651	98.764	4.465	24.691	1.659	18.202	88.089	1167.733	3.568	1149.468	0.9546
298.15	1.698	99.093	4.470	24.773	1.663	19.752	87.099	1167.427	3.516	1124.664	0.9547
303.15	1.747	99.412	4.474	24.853	1.666	21.303	86.104	1167.003	3.465	1100.327	0.9550
308.15	1.798	99.737	4.479	24.934	1.67	22.876	85.105	1166.598	3.413	1076.044	0.9552
313.15	1.851	100.059	4.484	25.015	1.674	24.483	84.079	1166.057	3.361	1051.723	0.9557
Ethylbenzene											
293.15	1.637	114.449	4.689	28.612	1.830	19.911	102.532	1349.84	3.583	1161.713	0.9516
298.15	1.679	114.827	4.695	28.707	1.834	21.631	101.429	1349.492	3.533	1137.729	0.9519
303.15	1.726	115.205	4.700	28.801	1.838	23.354	100.328	1349.127	3.483	1114.088	0.9522
308.15	1.774	115.591	4.705	28.898	1.843	25.080	99.240	1348.854	3.434	1090.714	0.9525
313.15	1.824	115.975	4.710	28.994	1.847	26.800	98.164	1348.594	3.386	1067.798	0.9528
p-Xylene											
293.15	1.651	115.228	4.700	28.807	1.839	20.796	102.543	1356.463	3.560	1145.033	0.9470
298.15	1.697	115.608	4.705	28.902	1.843	22.515	101.445	1356.14	3.510	1121.438	0.9472
303.15	1.745	115.989	4.710	28.997	1.847	24.244	100.345	1355.794	3.461	1098.101	0.9475
308.15	1.794	116.370	4.716	29.093	1.851	25.981	99.247	1355.432	3.411	1075.049	0.9478
313.15	1.845	116.750	4.721	29.187	1.855	27.767	98.109	1354.89	3.361	1051.795	0.9483
Mesitylene											
293.15	1.615	130.495	4.899	32.624	1.998	21.158	117.758	1537.698	3.610	1173.513	0.9458
298.15	1.659	130.911	4.904	32.728	2.002	23.030	116.543	1537.218	3.561	1150.498	0.9460
303.15	1.704	131.325	4.909	32.831	2.006	24.902	115.333	1536.722	3.513	1127.83	0.9464
308.15	1.750	131.749	4.915	32.937	2.011	26.783	114.132	1536.321	3.465	1105.339	0.9467
313.15	1.797	132.169	4.920	33.042	2.015	28.644	112.952	1535.935	3.418	1083.414	0.9471

Isopropylbenzene											
293.15	1.653	130.824	4.903	32.706	2.001	23.694	115.763	1532.927	3.539	1144.71	0.9487
298.15	1.699	131.260	4.909	32.815	2.006	25.625	114.523	1532.476	3.490	1121.307	0.9490
303.15	1.746	131.688	4.914	32.922	2.010	27.564	113.274	1531.898	3.441	1098.236	0.9494
308.15	1.795	132.125	4.919	33.031	2.014	29.506	112.039	1531.424	3.392	1075.422	0.9497
313.15	1.844	132.569	4.925	33.142	2.019	31.426	110.841	1531.117	3.344	1053.164	0.9501
Butylbenzene											
293.15	1.624	147.096	5.099	36.774	2.164	24.053	132.015	1726.326	3.590	1163.959	0.9407
298.15	1.667	147.566	5.104	36.892	2.168	26.089	130.700	1725.878	3.543	1141.783	0.9410
303.15	1.711	148.036	5.109	37.009	2.173	28.130	129.388	1725.412	3.496	1119.88	0.9412
308.15	1.756	148.516	5.115	37.129	2.178	30.172	128.092	1725.054	3.450	1098.239	0.9415
313.15	1.803	148.995	5.120	37.249	2.182	32.232	126.786	1724.626	3.404	1076.76	0.9419
Isobutylbenzene											
293.15	1.676	148.074	5.110	37.019	2.173	27.886	129.488	1724.803	3.498	1122.803	0.9416
298.15	1.722	148.543	5.115	37.136	2.178	29.971	128.139	1724.141	3.451	1100.791	0.9419
303.15	1.768	149.019	5.121	37.255	2.183	32.070	126.791	1723.515	3.403	1078.933	0.9423
308.15	1.816	149.506	5.126	37.377	2.187	34.169	125.463	1723.023	3.357	1057.343	0.9426
313.15	1.865	150.001	5.132	37.500	2.192	36.250	124.166	1722.691	3.311	1036.207	0.9430
tert-Butylbenzene											
293.15	1.639	145.924	5.085	36.481	2.152	25.577	129.370	1706.508	3.546	1157.189	0.9517
298.15	1.684	146.392	5.090	36.598	2.157	27.708	127.971	1705.682	3.497	1133.942	0.9521
303.15	1.730	146.856	5.096	36.714	2.161	29.837	126.577	1704.8	3.448	1111.085	0.9526
308.15	1.778	147.326	5.101	36.831	2.166	31.963	125.198	1703.997	3.399	1088.545	0.9532
313.15	1.828	147.796	5.107	36.949	2.171	34.149	123.774	1702.988	3.350	1065.816	0.9539

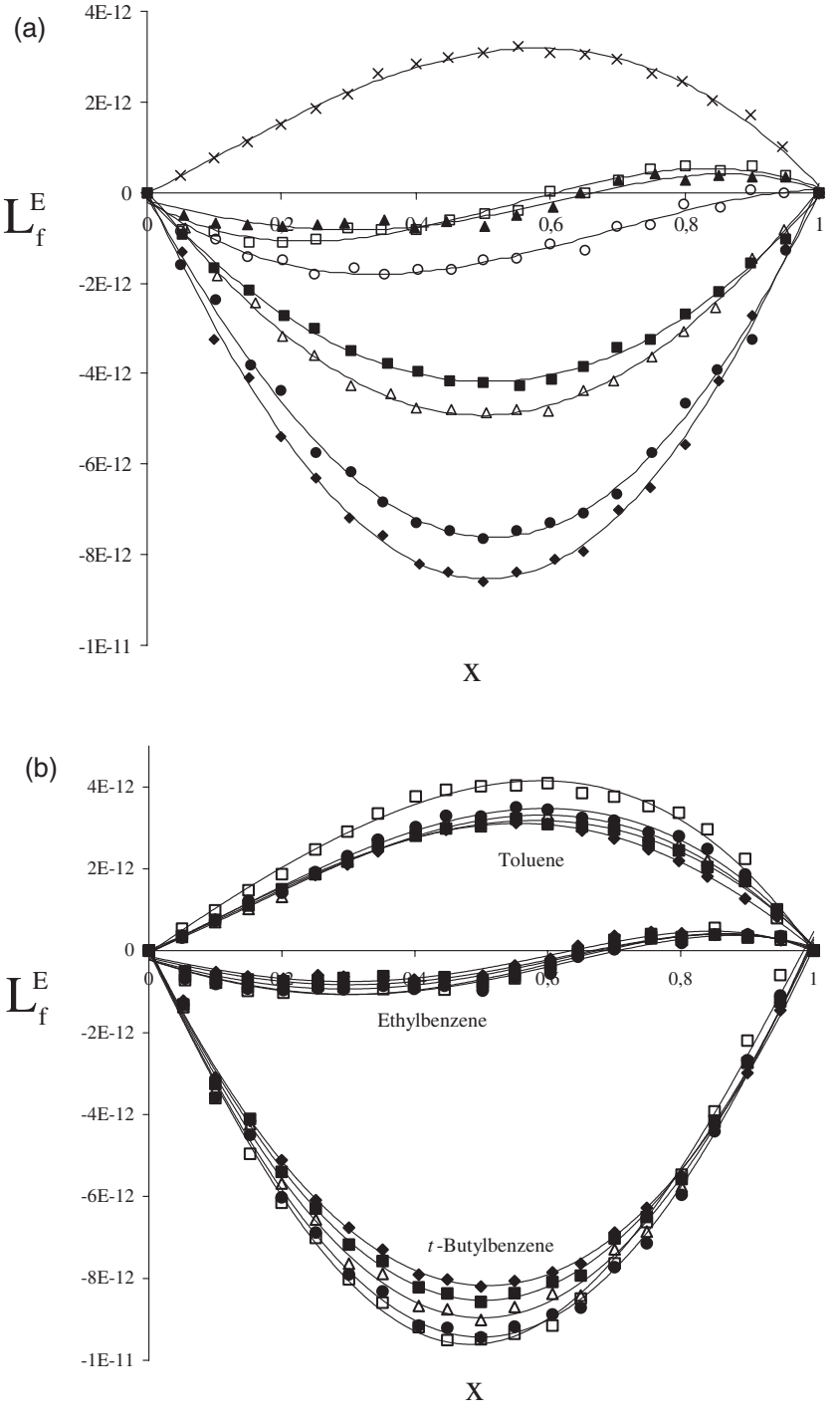

FIGURE 2 Curves of excess intermolecular free length for (a) butyl acetate + (×) toluene, (▲) ethylbenzene, (○) *p*-xylene, (□) mesitylene, (■) isopropylbenzene, (●) butylbenzene, (△) isobutylbenzene or (◆) *t*-butylbenzene) at 298.15 K, and (b) butyl acetate + (toluene, ethylbenzene and *t*-butylbenzene) at (◆) 293.15 K, (■) 298.15 K, (△) 303.15 K, (●) 308.15 K and (□) 313.15 K.

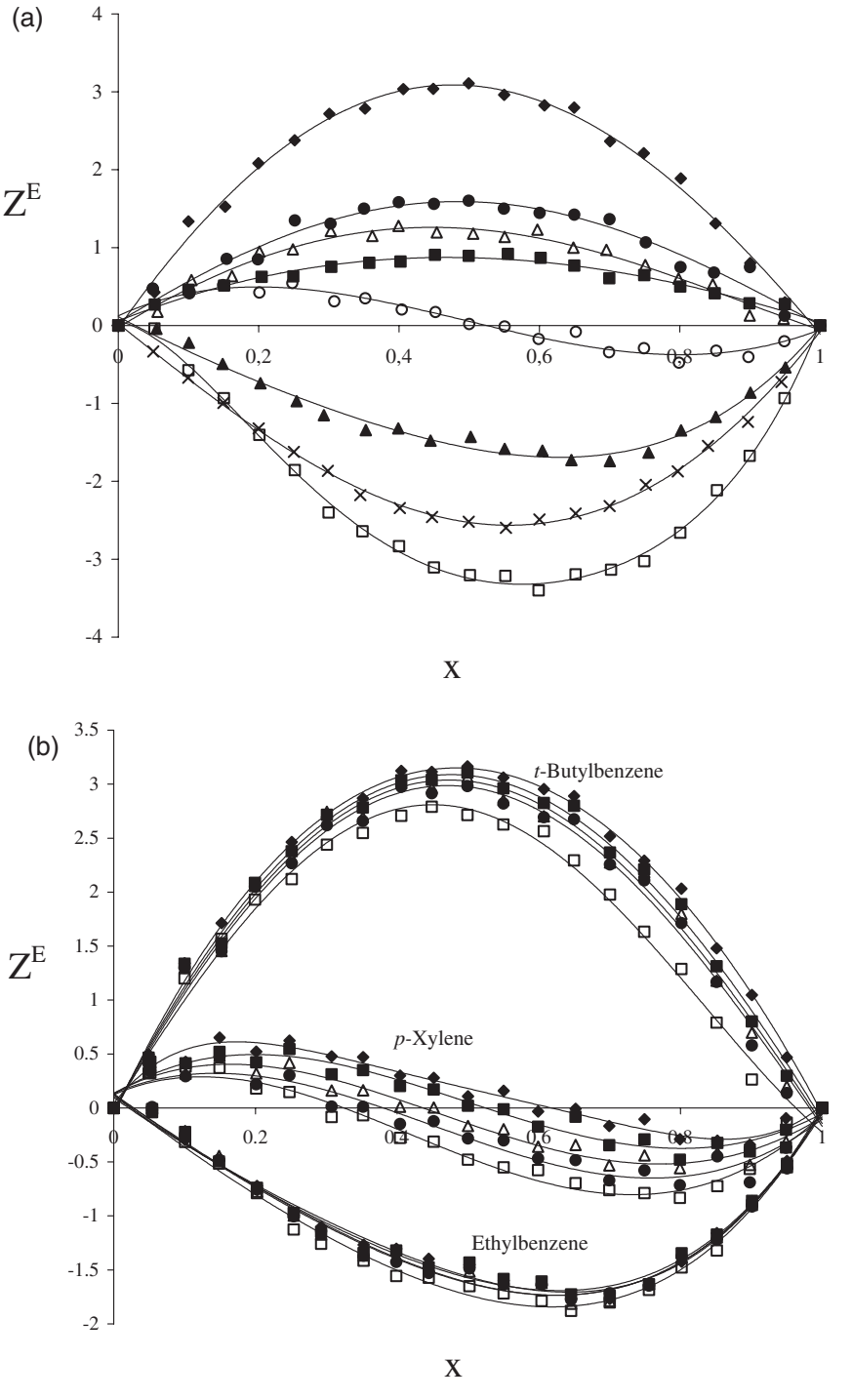

FIGURE 3 Curves of excess specific acoustic impedance for (a) butyl acetate + (×) toluene, (▲) ethylbenzene, (○) *p*-xylene, (□) mesitylene, (■) isopropylbenzene, (●) butylbenzene, (△) isobutylbenzene or (◆) *t*-butylbenzene) at 298.15 K, and (b) butyl acetate + (ethylbenzene, *p*-xylene and *t*-butylbenzene) at (◆) 293.15 K, (■) 298.15 K, (△) 303.15 K, (●) 308.15 K and (□) 313.15 K.

greater values of L_f^E which may be understood as a weaker molecular interaction by steric hindrance. It is interesting to point out the sigmoid trend of ethylbenzene and mesitylene as a function of composition, showing negative values for low concentration of ester. As a conclusion from Table IV and as the evolution of the acoustic parameters as a function of composition points out, a clearly different trend exists between light and heavy compounds as solvents of butyl acetate. The lightest compounds show increasing values of these parameters when diluted (for rising concentration of ester). As an exception, the collision factor is obviously decreasing as a consequence of this trend. On the other hand, the heaviest solvents (mesitylene, isopropylbenzene, butylbenzene, isobutylbenzene, or *t*-butylbenzene) show decreasing values of these parameters as a function of concentration. An interpretation of these facts may be of two different characters. Firstly geometrical—each solvent is increased molecular-size for strong concentrations of ester due to the small volume of light solvents and the slight polar interactions among butyl acetates. For higher solvents (ethylbenzene and so on), the molecular size is key for diminishing probable interactions among ester molecules, these bonds being mismatched by steric hindrance and produce positive excess molar volumes [6]. Secondly, the interaction character must be taken into account, the parameters L_f, S and Z are closely related to interaction and probable bonds. At each case an aweakening of interactions as a function of composition (higher free length and then lower collision factor) is observed. In what is referred to Fig. 3(a,b), an analogous interpretation may be made. We observe a decreasing tendency of the excess specific acoustic impedance with temperature which suggest, as above, an aweakening interaction between solvent and ester due to the dispersive relation among these molecules. This fact is noted for any binary mixture and temperature. These conclusions are reinforced by the evolution of the other parameters, increasing Van der Waals constant, geometrical parameters (area, volume and radio) which are increased for rising temperatures and compositions when the compounds are light, as explained above, and as expected, a diminution of the collision factor under the same conditions.

3.3. Theoretical Models

The estimation of different thermodynamic properties of binary or multicomponent mixtures have been the subject of study in recent years, applying different empirical or semiempirical models due to their interest to optimize industrial equipment and understanding the mixing liquids trend. In the last few years, the CFT and FCT have proved their applicability for multicomponent estimation and accurate results for molecules of different nature. Empirical models are also used but their simplicity sometimes leads to poorer results. In this work the empirical models of Danusso and Nomoto are also enclosed [7–8]. Experimental data for the isentropic compressibility of the mixtures were compared with values determined by different mixing procedures. The models of Danusso and Nomoto (Eqs. (17) and (18)) equations are in accordance with the following expressions

$$\kappa_S = \left(\frac{1}{M \cdot \rho}\right) \cdot \left(\sum_{i=1}^{N} \frac{n_i M_i}{\rho_i^2 u_i^2}\right) \tag{17}$$

$$\kappa_S = \left(\frac{1}{\rho}\right) \cdot \left(\frac{\sum_i^N n_i R_i}{\sum_i^N n_i u_i}\right)^{-6}, \tag{18}$$

where $R = u^{1/3} \cdot \sum_i^N n_i V_i$ and theories CFT, FLT [9–11]; (Eqs. (19) and (20)) for the isentropic compressibilities were applied

$$\kappa_S = \left(\frac{1}{\rho^3}\right) \cdot \left(\frac{M}{u_\infty \cdot \sum_i^N x_i S_s \cdot \sum_i^N x_i B_s}\right)^2 \tag{19}$$

$$\kappa_S = \left(\frac{L_f^2}{K^2}\right). \tag{20}$$

The Collision Factor Theory is dependent on the collision factors among molecules as a function of temperature in pure solvent or mixture. The pertinent relations in these calculations and their theoretical basis are described in the literature cited. The collision factors (S) and the characteristic molecular volumes (B) of the pure solvents used in the CFT calculations were estimated by using the experimental ultrasonic velocities, enclosed in this article, and the molar volumes [6]. These values could be also evaluated by means of the group contribution method proposed by Schaaffs [16], when no experimental ones are disposable.

The Free Length Theory estimates the isentropic compressibility of a mixture attending to the free displacement of molecules as a main function of temperature. The deviations of each procedure for the studied mixtures are given in Table V by means of Eq. (4) and as expected they increase as a consequence of rising temperatures. Attending to the deviation computed data, we arrive at the conclusion that the application of the FLT predicts experimental data extremely well for all the studied mixtures, proving this procedure as an accurace tool for isentropic compressibility data in these kinds of systems. In the second term the model proposed by Nomoto also presents slight deviations (except for mesitylene), while on the other hand, the Danusso and CFT methods present greater deviations, specially for toluene.

4. CONCLUSIONS

In this work we present a new experimental study of ultrasonic trend of binary mixtures, butyl acetate + (toluene, ethylbenzene, *p*-xylene, mesitylene, isopropylbenzene, butylbenzene, isobutylbenzene, or *t*-butylbenzene) at the range 293.15–313.15 K, as a continuation of previous papers for the studied mixtures in this work. From the experimental data a set of acoustic parameters were derived, the influence of size, molecular volume and temperature being analyzed. Attending to the the changes of isentropic compressibilities, these data were correlated by polynomial expressions which fitted well. All the systems exhibited negative values except for toluene. Due to ultrasonic velocities which diminish for increasing molar fractions at each system, the liquid structure looses rigidity. The observed negative values of the change of isentropic compressibility mean that the mixing structure is less compressible than the ideal mixture. As mentioned above, all the acoustic parameters increase with mole fraction for

TABLE V Root mean square deviations σ (TPa^{-1}) for predicted isentropic compressibilities from experimental data for the binary mixtures butyl acetate + aromatic hydrocarbons

Temperature (K)	*Nomoto* (*Eq.* (*18*))	*Danusso* (*Eq.* (*17*))	*CFT* (*Eq.* (*19*))	*FLT* (*Eq.* (*20*))
Toluene				
293.15	1.02	4.07	5.77	0.12
298.15	1.08	4.31	6.09	0.10
303.15	1.18	4.61	6.38	0.09
308.15	1.22	4.85	6.75	0.08
313.15	0.95	4.75	7.45	0.05
Ethylbenzene				
293.15	0.42	3.13	2.56	0.07
298.15	0.46	3.40	2.67	0.10
303.15	0.52	3.69	2.82	0.15
308.15	0.58	4.04	2.95	0.20
313.15	0.58	4.30	3.20	0.26
p-Xylene				
293.15	0.63	3.66	2.58	0.03
298.15	0.64	3.83	2.74	0.08
303.15	0.62	3.98	2.95	0.12
308.15	0.63	4.19	3.17	0.18
313.15	0.62	4.34	3.40	0.23
Mesitylene				
293.15	2.57	0.68	1.01	0.09
298.15	2.69	0.69	1.07	0.13
303.15	2.82	0.70	1.12	0.19
308.15	2.93	0.71	1.21	0.26
313.15	3.12	0.72	1.37	0.34
Isopropylbenzene				
293.15	0.09	2.07	0.52	0.02
298.15	0.10	2.25	0.50	0.06
303.15	0.12	2.46	0.49	0.14
308.15	0.11	2.71	0.47	0.24
313.15	0.23	2.83	0.28	0.35
Butylbenzene				
293.15	1.57	1.08	2.16	0.05
298.15	1.70	1.25	2.20	0.07
303.15	1.76	1.52	2.32	0.21
308.15	1.85	1.80	2.42	0.39
313.15	1.95	2.09	2.49	0.59
Isobutylbenzene				
293.15	1.18	0.35	1.74	0.05
298.15	1.34	0.33	1.80	0.03
303.15	1.49	0.36	1.81	0.12
308.15	1.63	0.44	1.82	0.22
313.15	1.95	0.49	1.69	0.34
t-Butylbenzene				
293.15	0.41	2.35	2.24	0.09
298.15	0.56	2.47	2.21	0.04
303.15	0.67	2.64	2.23	0.19
308.15	0.77	2.85	2.26	0.36
313.15	1.17	2.83	2.07	0.53

slight aromatic rings (toluene, ethylbenzene and *p*-xylene) and decrease for the rest of them. Only L_f increases at any system in the present investigation, which indicates slight interaction among butyl acetate and solvent molecules. As shown in Fig. 2(a), all the systems present negative values for the excess intermolecular free length, L_f^E,

except for the sigmoid trend presented by mesitylene and ethylbenzene, and positive values of toluene, which may be attributed to the size of these three molecules that allow relative molecular interactions between acetate molecules. Negative values indicate that sound wave covers smaller distance with respect to ideality.

In regard to the obtained values for the excess acoustic impedance at all concentrations of the mixtures, these are positive for large aromatic rings (isopropylbenzene, butylbenzene, isobutylbenzene, or *t*-butylbenzene), sigmoid for *p*-xylene, and negative for the others.

In what is referred to as theoretical estimation, the results of the comparison of predicted values with experimental data appear summarized in Table V. Here the σ of isentropic compressibility predicted are shown, the FLT model predicting experimental data to a good level of accuracy.

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