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ScienceDirect
Karbala International Journal of Modern Science 1 (2015) 172–177
http://www.journals.elsevier.com/karbala-international-journal-of-modern-science/

Comparative study of theoretical ultrasonic velocities of binary liquid mixtures containing quinoline and mesitylene at temperatures T = (303.15,308.15,313.15 and 318.15) K

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Received 22 October 2015; revised 9 November 2015; accepted 16 November 2015
Available online 17 December 2015

Abstract

Ultrasonic velocities and densities of binary liquid mixtures containing quinoline and mesitylene have been measured at temperatures T = (303.15,308.15,313.15 and 318.15) K over the entire molefraction range of quinoline under frequency of 3 MHz. Theoretical velocities have been evaluated by using Nomoto (U_{NOM}), Impedance (U_{IMP}), Van-Dael and Vangeel (U_{VDV}), Junjie (U_{JUN}) and Rao's specific velocity (U_{RAO}) models. A good agreement has been found between experimental and theoretical values. U^2_{EXP}/U^2_{IMX} has also been evaluated for non-ideality in the liquid mixtures. The results are discussed in terms of intermolecular interactions between the component molecules of the binary liquid mixtures.

Keywords: Ultrasonic velocity; Density; Binary liquid mixture; Mesitylene; Quinoline

1. Introduction

Measurement of ultrasonic velocity has been adequately employed in understanding the molecular interactions in pure, binary, and higher order multi component liquid mixtures [1–3]. The propagation of ultrasonic velocity in a medium is a thermodynamic property and has come to be recognized as a very specific and unique tool for predicting and estimating various physico -chemical properties of the liquid mixtures under consideration [4–10]. Ultrasonic velocity measurement data proves to be a very simple and convenient tool to determine various thermodynamic properties of liquid and liquid mixtures. In the present paper the theoretical values of ultrasonic velocity in binary liquid mixtures containing quinoline and mesitylene at temperatures T = (303.15,308.15,313.15 and 318.15) K over the entire molefraction range of quinoline have been evaluated by using Nomoto [11], impedance relation [12], Van Dael and Vangeel ideal mix relations [13], Junjie [14] and Rao's Specific velocity relations [15] and are compared with the experimental values. Quinoline is a heterocyclic aromatic organic compound with the chemical formula

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Peer review under responsibility of University of Kerbala.

http://dx.doi.org/10.1016/j.kijoms.2015.11.003

C_9H_7N. Quinoline is a colorless liquid with strong odor and widely useful in manufacturing of dyes, pesticides and solvent for resins and terpenes. Quinoline is often reported as an environmental contaminant associated with facilities processing oil shale or coal, and has also been found at legacy wood treatment sites. Owing to high water solubility quinoline has significant potential for mobility in the environment, which may promote water contamination. Mesitylene is a colorless liquid with sweet aromatic odor with the chemical formula $C_6H_3(CH_3)_3$ and it is a component of coal tar, which is its traditional source. In the electronics industry, mesitylene has also been used as a developer for photopatternable silicones due to its solvent properties and also it is precursor to diverse fine chemicals. Comparison of theoretical values of ultrasonic velocities with the experimentally measured values in the present binary liquid mixtures is expected to reveal the nature of interactions between the component molecules of the liquid mixtures. The deviation in the variation of U^2_{EXP}/U^2_{IMX} from unity has also been evaluated for explaining the non-ideality in the liquid mixtures.

2. Materials and methods

The chemicals used in the present investigation are of AnalaR grade and are obtained from SDFCL chemicals (quinoline) and MERCK chemicals (mesitylene). The chemicals are purified by standard procedure [16]. The different concentrations of the liquid mixture are prepared by varying mole fractions with respect to Job's method of continuous variation. Stoppard conical flasks are used for preserving the prepared mixtures and the flasks are left undisturbed to attain thermal equilibrium. Ultrasonic pulse echo interferometer (Mittal enterprises, India, Model: F-80X) is used for ultrasonic velocities measurements and all these measurements are done at a fixed frequency of 3 MHz. The temperature of the pure liquids or liquid mixtures is done by using temperature controlled water bath by circulating water around the liquid cell which is present in interferometer. Specific gravity bottle is used for the measurement of densities of pure liquids and liquid mixtures with an accuracy of + or − 0.5%. An electronic weighing balance (Shimadzu AUY220, Japan), with a precision of + or − 0.1 mg is used for the measurements of mass of pure liquids or liquid mixtures. Average of 4–5 measurements is taken for each sample. Ostwald's viscometer is used for the measurement of viscosity of pure liquids or liquid mixtures. The time of flow of liquid in the viscometer is measured with an electronic stopwatch with a precision of 0.01 s.

3. Theory

Various theories used for evaluating ultrasonic velocities in binary liquid mixtures and their equations are as follows.

(1). **Nomoto** established an empirical relation for ultrasonic velocity in binary liquid mixtures as:

$$U_{NOM} = \left[(X_1R_1 + X_2R_2)/(X_1V_1 + X_2V_2)\right]^3 \quad (1)$$

where R is molar sound velocity, X_1 and X_2 are the mole fractions of 1st and 2nd components of the liquid mixture and V is molar volume.

(2). **Impedance** dependent relation:

$$U_{IMP} = \sum X_i Z_i \Big/ \sum X_i \rho_i \quad (2)$$

where X_i is the mole fraction, ρ_i the density of the mixture and Z_i is the acoustic impedance.

(3). **Van Dael and Vangeel** Ideal mixing relation:

$$U_{VDV} = \left[\left(X_1/M_1U_1^2 + X_2/M_2U_2^2\right)\left(X_1M_1 + X_2M_2\right)\right]^{-1/2} \quad (3)$$

where M_1, M_2 are molecular weights of constituent components. U_1 and U_2 are ultrasonic velocities of individual compounds.

(4). **Junjie** equation:

$$U_{JUN} = \left(X_1M_1/\rho_1 + X_2M_2/\rho_2\right) \Big/ \left[\left\{X_1M_1 + X_2M_2\right\}^{1/2}\left\{X_1M_1/\rho_1U_1^2 + X_2M_2/\rho_2U_2^2\right\}\right]^{1/2} \quad (4)$$

Table 1
The values of densities (ρ) and ultrasonic velocities (u) of pure liquids with literature values at temperature T = 303.15 K.

Liquids	Density ρ (Kg m^{-3})		Ultrasonic velocity u (m s^{-1})	
	Exp	Lit	Exp	Lit
quinoline	1085.4	1085.7 [17]	1553.68	1547 [17]
mesitylene	856.3	856.9 [18]	1314.15	1316.82 [18]

where ρ_1 and ρ_2 are the densities of constituent components.

(5). **Rao's** specific velocity:

$$U_{RAO} = \left(\sum X_i\, r_i\, \rho_i\right)^3 \quad (5)$$

Table 2
Experimental and theoretical values of ultrasonic velocities in the binary liquid mixtures containing (quinoline + mesitylene) over the entire molefraction range of quinoline at four temperatures T = (303.15,308.15,313.15 and 318.15) K.

Molefraction of quinoline (X_1)	U_{EXP} m s^{-1}	U_{NOM} m s^{-1}	U_{IMP} m s^{-1}	U_{VDV} m s^{-1}	U_{JUN} m s^{-1}	U_{RAO} m s^{-1}
T = 303.15 K						
0.0000	1314.2	1314.2	1314.2	1314.2	1314.2	1314.2
0.1160	1340.3	1336.9	1348.3	1337.5	1322.5	1340.6
0.2280	1369.4	1359.9	1379.4	1361.0	1325.1	1366.4
0.3361	1399.5	1383.2	1407.8	1384.6	1328.8	1391.7
0.4405	1427.6	1406.8	1433.8	1408.3	1333.6	1416.4
0.5415	1452.7	1430.6	1457.8	1432.2	1339.4	1440.5
0.6392	1476.8	1454.7	1479.9	1456.2	1346.4	1464.2
0.7337	1500.9	1479.0	1500.4	1480.3	1354.6	1487.3
0.8253	1523.0	1503.6	1519.4	1504.6	1364.1	1509.9
0.9140	1541.1	1528.5	1537.1	1529.1	1374.8	1532.0
1.0000	1553.7	1553.7	1553.7	1553.7	1553.7	1553.7
T = 308.15 K						
0.0000	1299.0	1299.0	1299.0	1299.0	1299.0	1299.0
0.1160	1324.2	1322.8	1334.9	1323.3	1273.6	1326.7
0.2280	1353.3	1346.9	1367.6	1347.7	1277.0	1353.8
0.3361	1383.4	1371.3	1397.5	1372.3	1281.5	1380.3
0.4405	1411.5	1396.0	1424.8	1397.1	1287.0	1406.2
0.5415	1436.6	1421.0	1450.0	1422.2	1293.7	1431.6
0.6392	1460.7	1446.3	1473.2	1447.4	1301.6	1456.4
0.7337	1483.8	1472.0	1494.7	1472.9	1310.8	1480.8
0.8253	1506.9	1497.9	1514.7	1498.5	1321.4	1504.6
0.9140	1528.0	1524.1	1533.3	1524.5	1333.3	1527.9
1.0000	1550.7	1550.7	1550.7	1550.7	1550.7	1550.7
T = 313.15 K						
0.0000	1282.7	1282.7	1282.7	1282.7	1282.7	1282.7
0.1160	1308.2	1307.6	1320.5	1307.8	1192.3	1311.7
0.2280	1337.3	1332.9	1354.8	1333.3	1196.4	1340.1
0.3361	1367.4	1358.5	1386.2	1359.0	1201.7	1367.9
0.4405	1395.5	1384.5	1415.0	1384.9	1208.0	1395.2
0.5415	1420.6	1410.8	1441.4	1411.2	1215.5	1421.9
0.6392	1444.7	1437.4	1465.9	1437.8	1224.3	1448.0
0.7337	1467.8	1464.4	1488.5	1464.7	1234.3	1473.6
0.8253	1491.9	1491.7	1509.5	1491.9	1245.8	1498.7
0.9140	1517.0	1519.4	1529.1	1516.9	1258.8	1523.3
1.0000	1547.4	1547.4	1547.4	1547.4	1547.4	1547.4
T = 318.15 K						
0.0000	1266.4	1266.4	1266.4	1266.4	1266.4	1266.4
0.1160	1292.0	1292.3	1305.6	1291.0	1212.4	1296.5
0.2280	1321.2	1318.5	1341.3	1318.4	1217.5	1325.9
0.3361	1351.3	1345.0	1373.8	1344.9	1223.7	1354.7
0.4405	1379.4	1371.9	1403.7	1371.7	1231.1	1383.0
0.5415	1404.5	1399.2	1431.1	1398.9	1239.8	1410.7
0.6392	1428.6	1426.8	1456.5	1426.5	1249.8	1437.8
0.7337	1452.7	1454.8	1480.0	1452.6	1261.3	1464.4
0.8253	1477.8	1483.2	1501.8	1477.0	1274.3	1490.5
0.9140	1505.9	1511.9	1522.1	1504.2	1289.1	1516.0
1.0000	1541.1	1541.1	1541.1	1541.1	1541.1	1541.1

Table 3
Percentage deviations between experimental and theoretical values of ultrasonic velocities in the binary liquid mixtures containing (quinoline + mesitylene) over the entire molefraction range of quinoline at four temperatures T = (303.15, 308.15, 313.15 and 318.15) K.

Molefraction of quinoline (X_1)	$\%U_{NOM}$	$\%U_{IMP}$	$\%U_{VDV}$	$\%U_{JUN}$	$\%U_{RAO}$
T = 303.15 K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1160	−0.2499	0.6006	−0.2046	−1.3267	0.0236
0.2280	−0.6892	0.7311	−0.6114	−3.2307	−0.2160
0.3361	−1.1622	0.5920	−1.0635	−5.0491	−0.5578
0.4405	−1.4588	0.4347	−1.3497	−6.5857	−0.7855
0.5415	−1.5229	0.3479	−1.4127	−7.7975	−0.8373
0.6392	−1.5000	0.2077	−1.3974	−8.8291	−0.8562
0.7337	−1.4600	−0.0367	−1.3729	−9.7481	−0.9087
0.8253	−1.2740	−0.2381	−1.2096	−10.4380	−0.8623
0.9140	−0.8191	−0.2602	−0.7838	−10.7911	−0.5915
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T = 308.15 K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1160	−0.1021	0.8145	−0.0681	−3.8164	0.1907
0.2280	−0.4697	1.0608	−0.4119	−5.6355	0.0373
0.3361	−0.8719	1.0182	−0.7996	−7.3675	−0.2241
0.4405	−1.0957	0.9446	−1.0169	−8.8185	−0.3736
0.5415	−1.0836	0.9322	−1.0052	−9.9451	−0.3480
0.6392	−0.9834	0.8570	−0.9115	−10.8897	−0.2921
0.7337	−0.7989	0.7362	−0.7388	−11.6586	−0.2062
0.8253	−0.5995	0.5172	−0.5559	−12.3144	−0.1569
0.9140	−0.2555	0.3460	−0.2321	−12.7422	−0.0111
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T = 313.15 K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1160	−0.0416	0.9392	−0.0253	−8.8578	0.2687
0.2280	−0.3260	1.3118	−0.2998	−10.5318	0.2115
0.3361	−0.6468	1.3760	−0.6160	−12.1200	0.0404
0.4405	−0.7879	1.3957	−0.7567	−13.4359	−0.0215
0.5415	−0.6907	1.4670	−0.6621	−14.4373	0.0905
0.6392	−0.5046	1.4654	−0.4809	−15.2598	0.2298
0.7337	−0.2336	1.4098	−0.2161	−15.9086	0.3964
0.8253	−0.0150	1.1798	−0.0041	−16.4990	0.4553
0.9140	0.1532	0.7951	−0.0099	−17.0253	0.4123
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T = 318.15 K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1160	0.0174	1.0503	−0.0789	−6.1643	0.3415
0.2280	−0.2034	1.5214	−0.2073	−7.8494	0.3582
0.3361	−0.4620	1.6682	−0.4709	−9.4434	0.2561
0.4405	−0.5395	1.7601	−0.5539	−10.7512	0.2617
0.5415	−0.3760	1.8964	−0.3953	−11.7282	0.4408
0.6392	−0.1229	1.9519	−0.1457	−12.5151	0.6452
0.7337	0.1469	1.8766	−0.0062	−13.1764	0.8055
0.8253	0.3648	1.6216	−0.0562	−13.7689	0.8564
0.9140	0.3997	1.0736	−0.1122	−14.3999	0.6701
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

where X_i is the mole fraction and ρ_i the density of the mixture.

(6). **Percentage** deviation in ultrasonic velocity:

The percentage deviations in ultrasonic velocity between the experimental and theoretical values are calculated as

$$(\Delta U/U)\,\% = ((U_{EXP} - U_{THEORY})/(U_{EXP})) \times 100 \quad (6)$$

4. Results and discussion

The comparision of experimental values of densities (ρ) and ultrasonic velocities (u) with the literature values is given in Table 1.

The experimental values of ultrasonic velocities along with the theoretically evaluated values by using various theories in the binary liquid mixtures containing quinoline and mesitylene at temperatures T = (303.15,308.15,313.15 and 318.15) K are given in Table 2 and the percentage deviations in experimental and theoretical ultrasonic velocity values are given in Table 3. The values of U^2_{EXP}/U^2_{IMX}, molecular interaction parameter (α) and average molecular interaction parameter (α_{AVG}) are given in Table 4.

Generally study of thermo-acoustical and excess thermo-acoustical parameters [19,20] are useful to explain strength of the interactions between the component molecules of liquid mixtures in most of the cases. But in some cases where there is no possibility for the calculation of acoustical and excess acoustical parameters, these theoretical ultrasonic velocity studies play the major role. It can be seen from Table 2 that, the theoretical values of ultrasonic velocity evaluated by various theories show deviations from experimental values. The limitations and approximations incorporated in these theories are responsible for it [21]. It is assumed that all the molecules are spherical in shape, which is not true every time. In Nomoto's theory, it is supposed that the volume does not change on mixing. Therefore, no interaction between the components of liquid mixtures has been taken into account. The assumption for the formation of ideal mixing relation is that the ratio of specific heats of ideal mixtures and the volumes are also equal. Again, no molecular interaction is taken into account. But on mixing two liquids, the interactions between the molecules of the two liquids takes place because of presence of various types of forces such as dispersion forces, charge transfer, hydrogen bonding, dipole−dipole and dipole-

Table 4
Values of U^2_{EXP}/U^2_{IMX} and molecular interaction parameter (α) and average interaction Parameter (α_{AGV}) in the binary liquid mixture containing (quinoline + mesitylene) over the entire molefraction of quinoline at four temperatures T = (303.15, 308.15, 313.15 and 318.15) K.

Molefraction of quinoline (X_1)	U^2_{EXP}/U^2_{IMX}	Molecular interaction parameter (α)	U^2_{EXP}/U^2_{IMX}	Molecular interaction parameter (α)
	T = 303.15 K		**T = 308.15 K**	
0.0000	1.0000	0.0000	1.0000	0.0000
0.1160	1.0041	0.0041	1.0030	0.0030
0.2280	1.0123	0.0123	1.0088	0.0088
0.3361	1.0216	0.0216	1.0162	0.0162
0.4405	1.0276	0.0276	1.0207	0.0207
0.5415	1.0289	0.0289	1.0220	0.0220
0.6392	1.0275	0.0275	1.0206	0.0206
0.7337	1.0232	0.0232	1.0165	0.0165
0.8253	1.0155	0.0155	1.0112	0.0112
0.9140	1.0061	0.0061	1.0047	0.0047
1.0000	1.0000	0.0000	1.0000	0.0000
Average molecular interaction parameter (α_{AVG}) = 0.0152			(α_{AVG}) = 0.0112	
	T = 313.15 K		**T = 318.15 K**	
0.0000	1.0000	0.0000	1.0000	0.0000
0.1160	1.0020	0.0020	1.0011	0.0011
0.2280	1.0060	0.0060	1.0042	0.0042
0.3361	1.0124	0.0124	1.0090	0.0090
0.4405	1.0160	0.0160	1.0121	0.0121
0.5415	1.0168	0.0168	1.0130	0.0130
0.6392	1.0150	0.0150	1.0111	0.0111
0.7337	1.0113	0.0113	1.0076	0.0076
0.8253	1.0067	0.0067	1.0048	0.0048
0.9140	1.0031	0.0031	1.0022	0.0022
1.0000	1.0000	0.0000	1.0000	0.0000
Average molecular interaction parameter (α_{AVG}) = 0.0081			(α_{AVG}) = 0.0059	

induced dipole interactions [21]. Thus, the observed deviation of theoretical values of ultrasonic velocity from the experimental values shows that the molecular interaction is taking place between the unlike molecules in the liquid mixtures [22]. From Table 3, it is observed that the percentage deviations of the ultrasonic velocity are both negative and positive. Such deviations indicate the non-ideal behavior of liquid mixtures. The ratio of U^2_{EXP}/U^2_{IMX} is used as an important tool to measure the non-ideality in the mixtures, especially in these cases where the properties other than sound velocity are not known [21]. A perusal of Table 4 indicates considerable deviations from ideality, which may be due to the existence of strong dipole–dipole interactions in liquid mixtures [22,23]. The variations of the ratio of U^2_{EXP}/U^2_{IMX} with the molefraction of quinoline at four temperatures are represented in Fig. 1. These variations clearly indicate that ratio of U^2_{EXP}/U^2_{IMX} increases from unity with the increase of molefraction from 0 to 0.5 and above the 0.5 molefraction range the ratio of U^2_{EXP}/U^2_{IMX} decreases and tends to unity at all the observed temperatures. Also the deviation of the ratio U^2_{EXP}/U^2_{IMX} from unity is a direct measure of non-ideality of the system as a consequence of association or other type of interactions which is called as molecular interaction parameter (α). The positive values of α in the present binary system clearly indicate the existence of strong

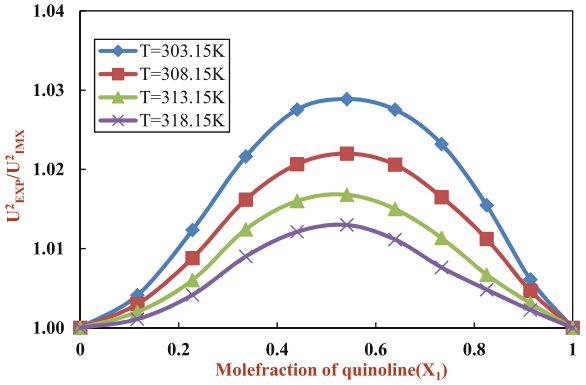

Fig. 1. The variations of ratio of U^2_{EXP}/U^2_{IMX} in the binary liquid mixtures containing (quinoline + mesitylene) over the entire molefraction range of quinoline at temperatures T = (303.15,308.15, 313.15 and 318.15) K.

interactions in the liquid mixtures [24]. From Table 4, it is also observed that α tends to decrease with the increase of temperature which clearly suggests that interactions become weak with the increase of temperature and this statement is also supported by the average value of molecular interaction parameter (α_{AVG}).

5. Conclusions

Theoretical ultrasonic velocities are evaluated in binary liquid mixture containing quinoline and mesitylene using Nomoto (U_{NOM}), impedance (U_{IMP}), Van-Dael and Vangeel (U_{VDV}), Junjie (U_{JUN}) and Rao's specific velocity (U_{RAO}) models and they are compared with the experimentally measured ultrasonic values at temperatures T = (303.15,308.15,313.15 and 318.15) K.From the comparision of these values, it may be concluded that Nomoto's relation, Van-Dael ideal mixing relation, Rao's and Impedance relation of ultrasound velocity have provided good results. The observed deviation of theoretical values of velocity from the experimental values is attributed to the presence of molecular interactions in the system studied. Also from the comparision, it is observed that out of all the theories Impedance relation gives best results followed by Rao's relation. Further the positive values of α and also from the magnitude of the ratio of U^2_{EXP}/U^2_{IMX} in the present system at all the temperatures clearly indicate the existence of strong association between the component molecules of the liquid mixture and also the strength of interaction between the component molecules in a liquid mixture decreases with the increase of temperature.

Acknowledgments

Authors are very much thankful to the Principal and Management authorities of V.R. Siddhartha Engineering College, Vijayawada, Andhra Pradesh, India for their cooperation in providing research facility.

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