



Available online at www.sciencedirect.com





Karbala International Journal of Modern Science 4 (2018) 126–133 http://www.journals.elsevier.com/karbala-international-journal-of-modern-science,

# Theoretical assessment of ultrasonic velocities of binary liquid mixtures containing p-chloroacetophenone with 1-alcohols at temperatures from 303.15 K to 318.15 K

Radha Sirija Maganti<sup>a</sup>, Gayatri Devi Nanduri<sup>a</sup>, Raghu Sai Sarath Dittakavi<sup>b</sup>, Ramachandran Dittakavi<sup>a,\*</sup>

<sup>a</sup> Physico-Chemical Laboratory, Department of Chemistry, Acharya Nagarjuna University, Guntur 522510, AP, India <sup>b</sup> V.R.Siddhartha College of Engineering, Vijayawada, AP, India

> Received 30 August 2017; revised 12 December 2017; accepted 13 December 2017 Available online 9 February 2018

#### Abstract

Ultrasonic velocities and densities and viscosities of parachloroacetophenone with alcohols have been measured at temperatures range from 303.15 K to 318.15 K over the entire composition range of mole fraction. Theoretical ultrasonic velocities were correlated by using Nomoto's relation ( $U_{NOM}$ ), Impedance relation ( $U_{IR}$ ), Ideal mixing relation ( $U_{IMR}$ ), Junjie's relation ( $U_J$ ) and Rao's specific velocity ( $U_R$ ). The theoretical and experimental values found good agreement with molecular interaction parameter ( $\alpha$ ) and chi square Goodness-of-fit test ( $X^2$ ).

© 2017 The Authors. Production and hosting by Elsevier B.V. on behalf of University of Kerbala. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Keywords: Molecular interaction parameter; Chi square test; Theoretical velocities; Ultrasonic velocity

# 1. Introduction

The ultrasonic velocity and density are vital parameters used in understanding the nature of molecular association emanating from intermolecular interactions between liquid components mixtures. The experimental and theoretical values of ultrasonic velocities in binary liquid mixtures show deviations [1,2]. The interpretation of ultrasonic velocities has been widely useful for understanding the molecular interactions between polar and non-polar groups between component molecules [3]. Similar kind of research work has been done by earlier workers. In the present paper, the theoretical ultrasonic velocities of binary liquid mixtures containing Parachloroacetophenone (PclAp) and 1-Alcohols (1-Propanol, 1-Butanol, 1-Pentanol) over the entire mole fraction range and temperatures from 303.15 K to 318.15 K have been correlated with Nomoto [4], Van Dael and Vangeel ideal mixing relations [5], impedance relation [6], junjie [7], and Rao's specific velocity [8]. Proper applicability of the theories of present work has been discussed. The results were evaluated in terms of molecular interaction parameter ( $\alpha$ ) and chi square Goodness-of-fit test (X<sup>2</sup>). The deviation of molecular interaction parameter from unity has also been calculated for explaining the non-ideality in the liquid mixtures.

https://doi.org/10.1016/j.kijoms.2017.12.003

<sup>\*</sup> Corresponding author. *E-mail address:* dittakavirc@gmail.com (R. Dittakavi). Peer review under responsibility of University of Kerbala.

<sup>2405-609</sup>X/© 2017 The Authors. Production and hosting by Elsevier B.V. on behalf of University of Kerbala. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

#### R.S. Maganti et al. / Karbala International Journal of Modern Science 4 (2018) 126-133

#### 2. Materials and methods

Parachloroacetophenone (pclAp), is taken as the main component and 1-Alcohols (1-Propanol, 1-Butanol, 1-Pentanol) are taken as secondary components as three binary systems. These chemicals purchased from S.D. Fine chemicals Ltd. India are used in the present work. The selected solvents were purified by adopting the methods as described in the literature [13,14]. The mixtures were prepared by mixing weighed amounts of the pure liquids by adopting the method of a closed system by using Mettler Toledo (ME204) balance with the precision of  $\pm 0.1$  mg. Mixtures were allowed to stand for some time before every measurement so as to avoid air bubbles. Ultrasonic velocities (u) and densities were determined by using an Ultrasonic Interferometer Model

 $R_1$  and  $R_2$  are the molar sound velocity of 1st and 2nd components.

#### (2) Impedance relation

The specific acoustic impedance relation is used for evaluating the ultrasonic velocity in the liquid mixtures  $U_{IR} = \Sigma X_i Z_i / \Sigma X_i \rho_i$  (4)

Where  $X_i$  is the mole fraction,  $\rho_i$  is the density of the mixture,  $Z_i$  is the acoustic impedance.

#### (3) Junjie equation

This equation is given by Junjie, which depends on mole fraction, molecular weight and density of the mixture is given as

$$U_{J} = \left(\frac{X_{1}M_{1}}{\rho_{1}} + \frac{X_{2}M_{2}}{\rho_{2}}\right) \left/ \left[ \left\{ X_{1}M_{1} + X_{2}M_{2} \right\}^{1/2} \left\{ \frac{X_{1}M_{1}}{\rho_{1}U_{1}^{2}} + \frac{X_{2}M_{2}}{\rho_{2}U_{2}^{2}} \right\} \right]^{1/2}$$
(5)

DSA-5000M, from Anton Paar India Pvt. Ltd. The densities were measured by taking the sample of 2 ml.

#### 3. Theory

Explanation and evaluation of various ultrasonic theories are as follows:

#### (1) Nomoto theory

It is based on the additivity of molar sound velocity( $\mathbf{R}$ ) and no volume change on mixing.

$$R = M/\rho U^2 \tag{1}$$

Where U and  $\rho$  are ultrasonic velocity and density which are evaluated experimentally. M is the mean molecular weight

$$M = (X_1 M_1 + X_2 M_2) \tag{2}$$

Where  $M_1$  and  $M_2$  are the molecular weights of constituent components

$$U_{Nom} = \left[\frac{X_1 R_1 + X_2 R_2}{X_1 V_1 + X_2 V_2}\right]^3$$
(3)

 $X_1$  and  $X_2$  are the mole fractions of 1st and 2nd components.  $V_i$  is the molar volume of component i.

#### (4) Rao's specific velocity relation

Rao's specific velocity relation is the ratio of molar sound velocity or Rao's constant (R) and molar volume (V)

$$U_R = \left(\frac{R}{V}\right)^3 \tag{6}$$

#### (5) Ideal mixing relation

Van Dael and Vangeel suggested the ideal mixing relation

$$\frac{1}{X_1 M_1 + X_2 M_2} \frac{1}{U_{imr}^2} = \frac{X_1}{M_1 U_1^2} + \frac{X_2}{M_2 U_2^2}$$
(7)

Where  $U_{imr}$  is the ideal mixing relation of ultrasonic velocity,  $U_1$  and  $U_2$  are the velocities of the individual components.

#### (6) Molecular interaction parameter ( $\alpha$ ) is given by

$$\alpha = \left( U_{exp}^2 / U_{imr}^2 \right) - 1 \tag{8}$$

Table 1

Experimental and Theoretical values of ultrasonic velocities along with percentage deviations and molecular interaction parameter of parachloroacetophenone+1-Propanol at temperatures from 303.15 K to 318.15 K.

X1	U <sub>m/s</sub>	Unom	U <sub>imr</sub>	U <sub>ir</sub>	U <sub>rao</sub>	Uj	%U <sub>nom</sub>	%U <sub>imr</sub>	$\% U_{ir}$	$\% U_r$	$\% U_j$	$U_{exp}{}^2/U_{imr}{}^2$	α
pclAp+	1-Propano	l at 303.15	5 K										
0.0000	1201.1	1201.1	1201.1	1201.1	1201.1	1201.1	0.00	0.00	0.00	0.00	0.00	1.00	0.00
0.0587	1194.7	1217.2	1174.3	1219.1	1313.0	1204.0	1.88	-1.71	2.04	9.90	0.78	1.04	0.04
0.1233	1190.9	1237.5	1151.5	1237.8	1418.9	1209.9	3.91	-3.31	3.94	19.14	1.59	1.07	0.07
0.1943	1190.9	1258.1	1133.4	1257.1	1514.1	1218.9	5.65	-4.83	5.56	27.14	2.35	1.10	0.10
0.3423	1202.1	1296.3	1115.4	1293.6	1643.6	1244.2	7.83	-7.21	7.61	36.73	3.50	1.16	0.16
0.4384	1216.8	1318.0	1116.8	1315.0	1681.9	1264.1	8.32	-8.22	8.07	38.23	3.89	1.19	0.19
0.5395	1238.2	1338.8	1129.3	1335.7	1688.3	1287.3	8.12	-8.80	7.87	36.35	3.97	1.20	0.20
0.6457	1267.5	1358.6	1156.0	1355.8	1663.1	1313.7	7.18	-8.80	6.97	31.21	3.64	1.20	0.20
0.7576	1306.1	1377.5	1202.6	1375.4	1607.3	1343.3	5.47	-7.92	5.31	23.07	2.85	1.18	0.18
0.8756	1355.0	1395.6	1280.1	1394.4	1522.9	1376.3	2.99	-5.53	2.91	12.39	1.57	1.12	0.12
1.0000	1412.8	1412.8	1412.8	1412.8	1412.8	1412.8	0.00	0.00	0.00	0.00	0.00	1.00	0.00
308.15 H	K												
0	1200.8	1200.8	1200.8	1200.8	1200.8	1200.8	0.00	0.00	0.00	0.00	0.00	1.00	0.00
0.0587	1195.9	1221.1	1174.1	1219.5	1313.3	1204.0	2.11	-1.82	1.98	9.82	0.68	1.04	0.04
0.1233	1192.8	1241.8	1151.5	1238.9	1419.9	1210.2	4.11	-3.46	3.87	19.04	1.46	1.07	0.07
0.1943	1193.4	1262.8	1133.5	1259.0	1515.8	1219.7	5.82	-5.02	5.50	27.02	2.21	1.11	0.11
0.3423	1205.4	1301.7	1115.9	1296.9	1646.8	1246.0	7.99	-7.42	7.59	36.62	3.37	1.17	0.17
0.4384	1220.7	1323.9	1117.6	1319.1	1686.0	1266.6	8.45	-8.45	8.06	38.12	3.76	1.19	0.19
0.5395	1243.2	1345.1	1130.6	1340.6	1693.3	1290.5	8.19	-9.06	7.83	36.20	3.80	1.21	0.21
0.6457	1273.6	1365.3	1157.9	1361.5	1669.0	1317.8	7.20	-9.08	6.90	31.05	3.47	1.21	0.21
0.7576	1313.3	1384.6	1205.5	1381.8	1614.1	1348.5	5.43	-8.20	5.22	22.91	2.68	1.19	0.19
0.8756	1362.6	1403.0	1284.7	1401.5	1530.4	1382.7	2.96	-5.72	2.85	12.31	1.47	1.13	0.13
1	1420.6	1420.6	1420.6	1420.6	1420.6	1420.6	0.00	0.00	0.00	0.00	0.00	1.00	0.00
313.15 H	K												
0	1200.3	1200.3	1200.3	1200.3	1200.3	1200.3	0.00	0.00	0.00	0.00	0.00	1.00	0.00
0.0587	1195.2	1220.3	1173.6	1218.8	1313.2	1203.3	2.10	-1.80	1.98	9.87	0.68	1.04	0.04
0.1233	1192.7	1240.7	1150.9	1237.9	1420.0	1209.4	4.03	-3.50	3.79	19.06	1.40	1.07	0.07
0.1943	1193.4	1261.5	1132.9	1257.7	1515.9	1218.6	5.70	-5.07	5.38	27.02	2.11	1.11	0.11
0.3423	1205.5	1299.8	1115.2	1295.1	1646.4	1244.5	7.83	-7.49	7.43	36.57	3.24	1.17	0.17
0.4384	1220.9	1321.7	1116.8	1317.0	1685.3	1264.9	8.26	-8.53	7.87	38.03	3.60	1.20	0.20
0.5395	1243.2	1342.6	1129.6	1338.2	1692.3	1288.5	8.00	-9.14	7.64	36.12	3.64	1.21	0.21
0.6457	1273.7	1362.6	1156.7	1358.8	1667.6	1315.5	6.98	-9.19	6.69	30.93	3.28	1.21	0.21
0.7576	1313.2	1381.6	1203.9	1378.8	1612.2	1345.8	5.20	-8.33	5.00	22.76	2.48	1.19	0.19
0.8756	1362.1	1399.8	1282.4	1398.3	1527.8	1379.6	2.76	-5.85	2.65	12.16	1.28	1.13	0.13
1	1417.1	1417.1	1417.1	1417.1	1417.0	1417.1	0.00	0.00	0.00	-0.01	0.00	1.00	0.00
318.15 H	K												
0	1194.0	1194.0	1194.0	1194.0	1194.0	1194.0	0.00	0.00	0.00	0.00	0.00	1.00	0.00
0.0587	1189.5	1214.2	1167.4	1212.7	1306.8	1197.1	2.08	-1.85	1.95	9.86	0.64	1.04	0.04
0.1233	1187.0	1234.9	1144.9	1232.2	1413.6	1203.3	4.04	-3.54	3.81	19.09	1.37	1.07	0.07
0.1943	1187.9	1256.0	1127.1	1252.2	1509.6	1212.7	5.73	-5.12	5.42	27.08	2.09	1.11	0.11
0.3423	1200.7	1294.9	1109.7	1290.2	1640.4	1238.9	7.85	-7.58	7.46	36.62	3.19	1.17	0.17
0.4384	1216.3	1317.1	1111.5	1312.4	1679.6	1259.5	8.29	-8.62	7.91	38.10	3.56	1.20	0.20
0.5395	1239.2	1338.3	1124.4	1334.0	1687.1	1283.5	8.00	-9.26	7.65	36.14	3.58	1.21	0.21
0.6457	1270.4	1358.6	1151.8	1354.9	1662.9	1310.8	6.94	-9.34	6.65	30.90	3.18	1.22	0.22
0.7576	1310.8	1377.9	1199.2	1375.2	1608.2	1341.6	5.12	-8.51	4.91	22.68	2.34	1.19	0.19
0.8756	1360.7	1396.4	1278.3	1394.9	1524.2	1375.9	2.62	-6.06	2.51	12.01	1.11	1.13	0.13
1	1414.0	1414.0	1414.0	1414.0	1413.9	1414.0	0.00	0.00	0.00	-0.01	0.00	1.00	0.00

# (7) Percentage deviation is expressed as

# (8) Chi square test for goodness-of-fit $(X^2)$

 $(\Delta U/U)\% = [(\text{Uexp} - \text{U theoretical})/\text{Uexp}]*100$  (9)

According to Karl Pearlson, the Chi square is calculated by using the expression

Table 2

Experimental and Theoretical values of ultrasonic velocities along with percentage deviations and molecular interaction parameter of parachloroacetophenone+1-Butanol at temperatures from 303.15 K to 318.15 K.

X1	U <sub>m/s</sub>	Unom	U <sub>imr</sub>	U <sub>ir</sub>	U <sub>rao</sub>	Uj	%U <sub>nom</sub>	%U <sub>imr</sub>	%U <sub>ir</sub>	%U <sub>r</sub>	%Uj	$U_{exp}^{2}/U_{imr}^{2}$	α
PclAp+1	l-Butanol	303.15 K											
0.0000	1231.4	1231.4	1231.4	1231.3	1231.3	1231.4	0.00	0.00	0.00	-0.01	0.00	1.00	0.00
0.0708	1228.0	1248.2	1214.2	1249.7	1326.4	1233.2	1.65	-1.12	1.77	8.01	0.42	1.02	0.02
0.1467	1227.6	1265.5	1201.0	1268.1	1413.7	1237.8	3.09	-2.16	3.30	15.16	0.83	1.04	0.04
0.2278	1230.3	1283.0	1192.3	1286.4	1489.4	1245.4	4.28	-3.09	4.56	21.06	1.22	1.06	0.06
0.3889	1244.8	1315.1	1190.1	1319.3	1586.0	1267.2	5.65	-4.39	5.99	27.41	1.80	1.09	0.09
0.4884	1259.8	1333.4	1198.8	1337.5	1611.1	1284.5	5.85	-4.84	6.17	27.89	1.96	1.10	0.10
0.5888	1279.8	1350.9	1215.9	1354.6	1612.1	1304.7	5.55	-4.99	5.84	25.96	1.94	1.11	0.11
0.6902	1305.2	1367.5	1242.8	1370.5	1590.4	1327.6	4.77	-4.78	5.00	21.85	1.72	1.10	0.10
0.7926	1336.1	1383.3	1281.7	1385.5	1548.3	1353.3	3.53	-4.07	3.70	15.88	1.29	1.09	0.09
0.8959	1372.3	1398.4	1336.4	1399.6	1488.3	1381.6	1.90	-2.62	1.99	8.45	0.68	1.05	0.05
1.0000	1412.8	1412.8	1412.8	1412.8	1412.8	1412.8	0.00	0.00	0.00	0.00	0.00	1.00	0.00
308.15 K													
0.0000	1221.3	1221.3	1221.3	1221.3	1221.3	1221.3	0.00	0.00	0.00	0.00	0.00	1.00	0.00
0.0708	1220.0	1239.7	1204.7	1241.5	1316.9	1223.9	1.62	-1.25	1.76	7.94	0.32	1.03	0.03
0.1467	1220.4	1258.6	1192.2	1261.7	1404.7	1229.5	3.13	-2.32	3.38	15.10	0.74	1.05	0.05
0.2278	1224.1	1277.8	1184.1	1281.8	1481.4	1238.1	4.39	-3.27	4.72	21.02	1.15	1.07	0.07
0.3889	1240.5	1313.1	1183.4	1317.9	1580.5	1262.1	5.85	-4.60	6.24	27.41	1.74	1.10	0.10
0.4884	1257.0	1333.2	1193.2	1338.0	1607.6	1281.0	6.06	-5.08	6.44	27.89	1.91	1.11	0.11
0.5888	1279.1	1352.4	1211.6	1356.7	1610.6	1303.0	5.73	-5.28	6.07	25.92	1.87	1.11	0.11
0.6902	1306.6	1370.7	1240.2	1374.2	1591.3	1327.8	4.91	-5.08	5.18	21.79	1.63	1.11	0.11
0.7926	1339.8	1388.1	1281.4	1390.7	1551.6	1355.7	3.60	-4.36	3.79	15.81	1.18	1.09	0.09
0.8959	1378.7	1404.8	1339.3	1406.1	1493.9	1386.6	1.89	-2.86	1.99	8.36	0.57	1.06	0.06
1.0000	1420.6	1420.6	1420.6	1420.6	1420.6	1420.6	0.00	0.00	0.00	0.00	0.00	1.00	0.00
313.15 K													
0.0000	1194.6	1194.6	1194.6	1194.6	1194.7	1194.6	0.00	0.00	0.01	0.01	0.00	1.00	0.00
0.0708	1194.4	1215.0	1179.0	1217.2	1289.9	1198.3	1.73	-1.29	1.91	8.00	0.33	1.03	0.03
0.1467	1196.0	1236.0	1167.4	1239.7	1377.7	1205.0	3.34	-2.40	3.65	15.19	0.75	1.05	0.05
0.2278	1200.7	1257.3	1160.3	1262.2	1454.7	1214.9	4.71	-3.37	5.12	21.15	1.18	1.07	0.07
0.3889	1219.6	1296.6	1161.6	1302.5	1556.1	1241.8	6.31	-4.76	6.80	27.59	1.82	1.10	0.10
0.4884	1238.1	1319.1	1172.8	1324.9	1585.7	1262.7	6.55	-5.28	7.01	28.08	1.99	1.11	0.11
0.5888	1262.2	1340.6	1192.8	1345.8	1591.9	1286.8	6.21	-5.49	6.62	26.13	1.95	1.12	0.12
0.6902	1292.4	1361.0	1223.5	1365.3	1576.2	1314.2	5.31	-5.33	5.65	21.97	1.69	1.12	0.12
0.7926	1328.9	1380.6	1267.5	1383.7	1540.4	1345.0	3.89	-4.62	4.12	15.92	1.21	1.10	0.10
0.8959	1371.2	1399.3	1329.4	1400.9	1486.6	1379.2	2.05	-3.05	2.17	8.41	0.58	1.06	0.06
1.0000	1417.1	1417.1	1417.1	1417.1	1417.0	1417.1	0.00	0.00	0.00	-0.01	0.00	1.00	0.00
318.15 K													
0.0000	1183.0	1182.9	1183.0	1182.9	1182.8	1183.0	0.00	0.00	0.00	-0.01	0.00	1.00	0.00
0.0708	1183.6	1204.2	1167.7	1206.3	1277.9	1187.1	1.74	-1.34	1.92	7.96	0.29	1.03	0.03
0.1467	1186.1	1225.9	1156.5	1229.8	1365.6	1194.2	3.35	-2.49	3.69	15.14	0.69	1.05	0.05
0.2278	1191.7	1248.0	1149.8	1253.2	1442.8	1204.6	4.72	-3.52	5.16	21.07	1.08	1.07	0.07
0.3889	1212.1	1288.8	1151.9	1295.0	1545.1	1232.4	6.33	-4.97	6.84	27.48	1.68	1.11	0.11
0.4884	1231.4	1312.1	1163.5	1318.2	1575.6	1254.0	6.55	-5.51	7.05	27.95	1.84	1.12	0.12
0.5888	1256.4	1334.4	1184.2	1339.9	1583.0	1279.0	6.20	-5.75	6.64	25.99	1.79	1.13	0.13
0.6902	1288.0	1355.7	1215.5	1360.2	1568.7	1307.3	5.25	-5.63	5.61	21.79	1.50	1.12	0.12
0.7926	1326.1	1376.0	1260.5	1379.3	1534.4	1339.1	3.76	-4.94	4.01	15.71	0.98	1.11	0.11
0.8959	1369.5	1395.5	1323.9	1397.2	1482.1	1374.6	1.90	-3.33	2.02	8.23	0.38	1.07	0.07
1.0000	1414.0	1414.0	1414.0	1414.0	1413.9	1414.0	0.00	0.00	0.00	-0.01	0.00	1.00	0.00

$$X^{2} = \sum_{i=1}^{n} \frac{\left(U_{(obs)} - U_{(cal)}\right)^{2}}{U_{(cal)}}$$
(10)

Where n is the number of data used,  $U_{obs}$  is the experimental values of ultrasonic velocities,  $U_{cal}$  is the calculated values of ultrasonic velocities.

Table 3

Experimental and Theoretical values of ultrasonic velocities along with percentage deviations and molecular interaction parameter of parachloroacetophenone+1-Pentanol at temperatures from 303.15 K to 318.15 K.

$\mathbf{X}_1$	U <sub>m/s</sub>	Unom	$U_{imr}$	$U_{ir}$	U <sub>rao</sub>	$U_j$	$\% U_{nom}$	$\% U_{imr}$	$\% U_{ir}$	$\% U_r$	$\% U_j$	$U_{exp}^{2}/U_{imr}^{2}$	α
pclAp+	1-Pentano	l 303.15 K											
0.0000	1253.9	1253.9	1253.9	1253.9	1253.9	1253.9	0.00	0.00	0.00	0.00	0.00	1.00	0.00
0.0830	1253.5	1268.9	1245.2	1272.6	1383.7	1270.0	1.23	-0.66	1.52	10.39	1.32	1.01	0.01
0.1696	1255.8	1284.1	1240.1	1290.6	1507.5	1286.5	2.25	-1.25	2.77	20.05	2.45	1.03	0.03
0.2594	1260.9	1299.5	1238.7	1307.9	1618.0	1303.1	3.06	-1.76	3.72	28.32	3.34	1.04	0.04
0.4305	1277.8	1327.7	1247.4	1337.5	1764.2	1333.5	3.91	-2.38	4.67	38.06	4.36	1.05	0.05
0.5314	1292.6	1343.8	1259.9	1353.2	1800.8	1350.3	3.96	-2.53	4.69	39.31	4.46	1.05	0.05
0.6297	1310.6	1359.0	1277.7	1367.4	1795.8	1365.6	3.69	-2.51	4.33	37.02	4.20	1.05	0.05
0.7257	1331.9	1373.5	1301.2	1380.3	1751.1	1379.6	3.12	-2.31	3.63	31.47	3.57	1.05	0.05
0.8193	1356.2	1387.2	1331.0	1392.0	1668.5	1391.9	2.29	-1.86	2.65	23.03	2.64	1.04	0.04
0.9107	1383.5	1400.3	1367.8	1402.8	1553.6	1403.0	1.22	-1.13	1.40	12.30	1.41	1.02	0.02
1.0000	1412.8	1412.8	1412.8	1412.8	1412.8	1412.8	0.00	0.00	0.00	0.00	0.00	1.00	0.00
308.15 H	K												
0.0000	1254.9	1254.9	1254.9	1254.8	1254.8	1254.9	0.00	0.00	0.00	-0.01	0.00	1.00	0.00
0.0830	1256.0	1270.5	1246.4	1274.3	1385.4	1271.3	1.15	-0.76	1.46	10.30	1.22	1.02	0.02
0.1696	1258.8	1286.3	1241.5	1293.1	1509.8	1288.2	2.18	-1.38	2.72	19.94	2.33	1.03	0.03
0.2594	1264.2	1302.4	1240.5	1311.1	1621.0	1305.2	3.01	-1.88	3.71	28.22	3.24	1.04	0.04
0.4305	1282.0	1331.8	1249.9	1342.1	1768.6	1336.6	3.89	-2.50	4.68	37.96	4.26	1.05	0.05
0.5314	1297.5	1348.6	1262.9	1358.4	1806.1	1354.0	3.94	-2.67	4.70	39.20	4.36	1.06	0.06
0.6297	1316.4	1364.4	1281.3	1373.2	1802.0	1370.0	3.65	-2.67	4.31	36.89	4.07	1.06	0.06
0.7257	1339.0	1379.5	1305.6	1386.7	1758.1	1384.7	3.03	-2.49	3.56	31.30	3.42	1.05	0.05
0.8193	1364.1	1393.9	1336.3	1399.0	1676.0	1397.9	2.18	-2.04	2.55	22.86	2.48	1.04	0.04
0.9107	1392.3	1407.6	1374.2	1410.2	1561.4	1409.8	1.10	-1.30	1.29	12.15	1.26	1.03	0.03
1.0000	1420.6	1420.6	1420.6	1420.6	1420.6	1420.6	0.00	0.00	0.00	0.00	0.00	1.00	0.00
313.15 H	K												
0.0000	1228.2	1228.2	1228.2	1228.1	1228.0	1228.2	0.00	0.00	-0.01	-0.02	0.00	1.00	0.00
0.0830	1230.9	1245.8	1220.8	1250.3	1307.9	1245.5	1.21	-0.82	1.57	6.25	1.18	1.02	0.02
0.1696	1235.1	1263.8	1217.0	1271.7	1379.4	1263.4	2.33	-1.47	2.97	11.68	2.30	1.03	0.03
0.2594	1241.9	1282.0	1217.1	1292.3	1440.1	1281.7	3.23	-1.99	4.06	15.96	3.21	1.04	0.04
0.4305	1262.6	1315.6	1229.1	1327.5	1516.2	1316.1	4.20	-2.65	5.15	20.09	4.24	1.06	0.06
0.5314	1280.2	1334.6	1243.8	1346.2	1536.6	1335.6	4.26	-2.84	5.16	20.03	4.33	1.06	0.06
0.6297	1301.6	1352.8	1264.2	1363.1	1539.6	1354.0	3.93	-2.87	4.72	18.28	4.02	1.06	0.06
0.7257	1327.0	1370.0	1290.9	1378.4	1527.2	1371.4	3.24	-2.72	3.87	15.08	3.34	1.06	0.06
0.8193	1355.1	1386.5	1324.5	1392.4	1501.3	1387.5	2.31	-2.26	2.75	10.79	2.39	1.05	0.05
0.9107	1386.7	1402.1	1366.0	1405.3	1464.0	1402.7	1.11	-1.49	1.34	5.58	1.15	1.03	0.03
1.0000	1417.1	1417.1	1417.1	1417.1	1417.0	1417.1	0.00	0.00	0.00	-0.01	0.00	1.00	0.00
318.15 H	K												
0.0000	1214.1	1214.1	1214.1	1214.2	1214.3	1214.1	0.00	0.00	0.01	0.01	0.00	1.00	0.00
0.0830	1218.0	1232.7	1207.2	1237.6	1343.4	1231.8	1.21	-0.88	1.61	10.30	1.14	1.02	0.02
0.1696	1223.3	1251.7	1204.0	1260.3	1466.9	1250.2	2.32	-1.58	3.03	19.92	2.20	1.03	0.03
0.2594	1230.7	1271.0	1204.7	1282.1	1578.1	1269.1	3.27	-2.12	4.17	28.22	3.12	1.04	0.04
0.4305	1253.1	1306.4	1217.8	1319.3	1728.6	1304.8	4.26	-2.82	5.29	37.95	4.13	1.06	0.06
0.5314	1271.7	1326.6	1233.3	1339.1	1769.8	1325.3	4.32	-3.02	5.30	39.17	4.22	1.06	0.06
0.6297	1294.5	1345.8	1254.7	1356.9	1770.6	1344.8	3.97	-3.07	4.82	36.78	3.88	1.06	0.06
0.7257	1321.2	1364.1	1282.5	1373.1	1732.6	1363.4	3.24	-2.94	3.93	31.13	3.19	1.06	0.06
0.8193	1350.8	1381.5	1317.4	1387.9	1656.9	1381.0	2.27	-2.48	2.75	22.66	2.23	1.05	0.05
0.9107	1383.2	1398.1	1360.6	1401.5	1548.7	1397.8	1.08	-1.63	1.32	11.97	1.06	1.03	0.03
1.0000	1414.0	1414.0	1414.0	1414.0	1413.9	1414.0	0.00	0.00	0.00	-0.01	0.00	1.00	0.00

# 4. Results and discussion

The experimental and theoretical ultrasonic velocities evaluated by Nomoto's relation  $(U_{NOM})$ , the

Impedence relation  $(U_{IR})$ , the Ideal mixing relation  $(U_{IMR})$ , Jungie's relation  $(U_J)$  and Rao's specific velocity  $(U_R)$  of all the three binary systems Parachloroacetophenone (PclAp), is taken as the main

Table 4 Values of chi square Goodness-of-fit test  $(X^2)$  for all the three systems at temperatures from 303.15 K to 318.15 K.

T(K)	U <sub>nom</sub>	U <sub>imr</sub>	U <sub>ir</sub>	U <sub>rao</sub>	Uj
PclAp+1-P	Propanol				
303.15 K	0.0000	0.0000	0.0000	0.0000	0.5259
308.15 K	0.0000	0.0000	0.0000	0.0000	0.6010
313.15 K	0.0000	0.0000	0.0001	0.0000	0.6787
318.15 K	0.0000	0.0000	0.0002	0.0000	0.7169
PclAp+1-B	Butanol				
303.15 K	0.0280	0.0672	0.0133	0.0000	0.9936
308.15 K	0.0195	0.0340	0.0077	0.0000	0.9958
313.15 K	0.0069	0.0207	0.0019	0.0000	0.9946
318.15 K	0.0078	0.0096	0.0020	0.0000	0.9978
PclAp+1-P	Pentanol				
303.15 K	0.4713	0.9236	0.1961	0.0000	0.2752
308.15 K	0.4992	0.8789	0.2043	0.0000	0.3292
313.15 K	0.3889	0.8174	0.1096	0.0000	0.3640
318.15 K	0.3818	0.7399	0.0931	0.0000	0.4311

component and 1-alcohols (1-Propanol, 1-Butanol, 1-Pentanol), along with molecular interaction parameter and percentage deviations are presented in the Tables 1-3 at the temperature range of 303.15 K to 318.15 K. The chi square goodness of fit is calculated and is presented in the Table 4.

The Figs. 1-3 show the extent of interaction that takes place between the component molecules. The positive deviation shows the strong interactions. The positive values of molecular interaction parameter show the existence of strong interaction for the formation of association between the component molecules, which shows the non-ideality in the mixture.

Finally, the chi square goodness of fit  $(X^2)$  determines the overall validity of the theory.

The evaluation and study of thermo-acoustical and its excess parameters are used to determine the strength and extent of intermolecular interactions between the constituent molecules of binary liquid mixtures [9,10]. There is no volume change on mixing so interactions are not possible in the case of Nomoto's theory. The ratio of specific heats of mixtures and the volumes are equal. No interactions took place for the Ideal Mixing Relation [11]. On mixing of two hetero components there is interactions between them due to some forces like dispersion forces, charge transfer, hydrogen bonding, dipole-dipole and dipole induced dipole interactions [12].

The molecular interaction parameter ( $\alpha$ ) is greater at larger temperature, because as the temperature increases, kinetic energy of the molecules increases, which leads to more bombardment of molecules than at the usual temperature, so that the more interaction between the unlike molecules takes place. Also, as the carbon chain length increases, the strength of interaction between the molecules decreases, due to the steric hindrance of long carbon chain length.

### 5. Conclusion

From the experimental and theoretical values of ultrasonic velocities in binary liquid mixture containing Parachloroacetophenone with alcohols, using Nomoto's relation ( $U_{NOM}$ ), Impedance relation ( $U_{IR}$ ), Ideal mixing relation ( $U_{IMR}$ ), Junjie's relation ( $U_J$ ) and



Fig. 1. Experimental and Theoretical values of ultrasonic velocities with molecular interaction parameter and mole fraction of parachloroacetophenone+1-Propanol at temperatures from 303.15 K to 318.15 K.



Fig. 2. Experimental and Theoretical values of ultrasonic velocities with molecular interaction parameter and mole fraction of parachloroacetophenone+1-Butanol at temperatures from 303.15 K to 318.15 K.



Fig. 3. Experimental and Theoretical values of ultrasonic velocities with molecular interaction parameter and mole fraction of parachloroacetophenone+1-Pentanol at temperatures from 303.15 K to 318.15 K.

Rao's specific velocity ( $U_R$ ) at temperatures from 303.15 K to 318.15 K. the Nomoto relation, impedance relation, ideal mixing relation, Rao's specific velocity relation, Junjie relation are in good agreement with molecular interaction parameter and chi square goodness of fit test ( $X^2$ ). According to Table 4, it is observed that Nomoto, Impedance relation and Rao's specific velocity relation are having minimum deviations, which are in best agreement with molecular interaction parameter and chi square goodness of fit test ( $X^2$ ). The ideal mixing relation and Junjie relations are showing larger deviations. Some of these larger deviations of theories from experimental and theoretical values are due to the molecular interactions between the mixing molecules.

#### Acknowledgements

The author M. Radha Sirija is grateful to U.G.C (New Delhi) for awarding BSR Fellowship and expresses gratitude to Research supervisor Dr. D. Ramachandran, Physico-Chemical laboratory, Department of chemistry, Acharya Nagarjuna University, Guntur for encouragement and support to carry out my research work.

## References

- [1] A. Bhattacharjee, M.N. Roy, J. Chem. Eng. Data 55 (2010) 5914–5920.
- [2] K. Rajagopal, S. Chenthilnath, Indian J. Pure Appl. Phys. 48 (2010) 326–333.

- [3] K.A. K RajKumar, G.R. Satyanarayana, G. Lakshmana Rao, Sk. Beebi, D. Bala, C. Rambabu, Chem. Sci. Trans. 6 (1) (2017) 87–96.
- [4] O. Nomoto, Empirical formula for sound velocity in liquid mixtures, J. Phys. Soc. Jpn. 13 (1958) 1528.
- [5] W. van Dael, E. Vangeel, in: Pro Int Conf on Calorimetry and Thermodynamics, Warsaw, 1955, p. 555.
- [6] B. Shipra, P.H. Persania, Asian J. Chem. 7 (1955) 417.
- [7] Z. Junjie, J. China Univ. Sci. Technol. 14 (1984) 298.
- [8] R. Rao, J. Chem. Phys. 9 (1941) 682.
- [9] K. Samatha, V.V. Hari Babu, J. Sreeeramamurthy, Acustica 84 (1998) 169.

- [10] M. Rita, P. Meenakshi, J. Indian Chem. Soc. 82 (2005) 791.
- [11] Sk. Fakruddin Babavali, P. Shakira, Ch. Srinivasu, K. Narendra, Karbala Int. J. Mod. Sci. 1 (2015) 172–177.
- [12] R. Bhaskaran, T.R. Kubendran, Int. J. Appl. Sci. Eng. 5 (2007) 115.
- [13] W.B. Bunger, J.A. Reddick, T.K. Sankano, Organic Solvents, fourth ed., vol. 3, Weissberger A, Wiley Interscience, New York, 1986.
- [14] Weissberger, E.S. Proskaner, Riddick, E.E. Toops, Organic Solvents, second ed., vol. 2, Weissberger A, Wiley Interscience, New York, 1955.