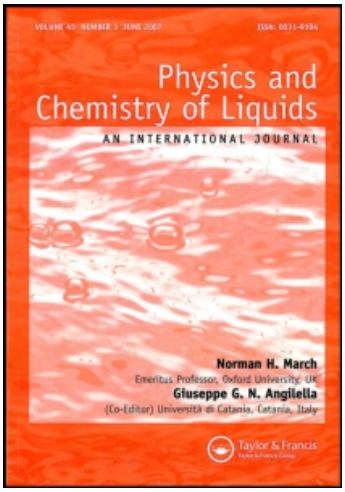

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D. Ramachandran[a]; K. Rambabu[b]; P. Venkateswarlu[b]; G. K. Raman[b]
[a] Department of Chemistry, NUPG centre, Nuzvid, A.P., India [b] Department of Chemistry, S. V. University, Tirupati, A.P., India

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SPEED OF SOUND AND ISENTROPIC COMPRESSIBILITIES OF TERNARY MIXTURES CONTAINING BUTYLACETATE (1) + PROPANOL(2) + AROMATIC HYDROCARBONS AND BUTYLACETATE (1) + BUTANOL(2) + AROMATIC HYDROCARBONS(3) RESPECTIVELY AT 303.15 K

D. RAMACHANDRAN[a*], K. RAMBABU[b]
P. VENKATESWARLU[b] and G. K. RAMAN[b]

[a] **Department of Chemistry, NUPG centre, Nuzvid-521 201, A.P., India;*
[b] *Department of Chemistry, S.V.University, Tirupati-517 502, A.P., India*

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Isentropic compressibilities of ten ternary mixtures butylacetate(1) + propanol(2) + benzene(3), + toluene(3), + chlorobenzene(3), + bromobenzene(3), + nitrobenzene and butylacetate(1) + butanol(2) + benzene(3), + toluene(3), chlorobenzene(3), + bromobenzene(3) and + nitrobenzene(3) respectively were determined from speed of sound measurements at 303.15 K.

The deviations in the isentropic compressibility were also computed. Values of dKs_{123} are positive in mixtures of butylacetate(1) + propanol(2) + benzene(3) and + toluene(3) and butylacetate(1) + butanol(2) + benzene(3) + toluene(3) and + chlorobenzene(3). dKs_{123} is negative in the systems, butylacetate(1) + propanol(2) + chlorobenzene(3), + bromobenzene(3), + nitrobenzene(3) and butylacetate(1) + butanol(2) + bromobenzene(3) and + nitrobenzene(3) correspondingly. An attempt has also been made to throw light on the nature of intermolecular interactions via these deviations in isentropic compressibility.

Keywords: Ternary mixtures; sound velocity

*Address for correspondence

1. INTRODUCTION

This work forms part of a study of thermodynamic properties of ternary mixtures [1,2]. Thermodynamic properties of pure liquids and liquid mixtures are of interest both to chemists and to chemical engineers for processing of petroleum and petrochemical products. The present study was undertaken to determine the isentropic compressibility from speed of sound measurements and the density evaluated from excess volumes. Further, the third component brings a change in both the nature and degree of interaction between pairs of molecules. We present here experimental data for the isentropic compressibility often ternary mixtures, butylacetate(1) + propanol(2) + benzene(3), + toluene(3), + chlorobenzene(3), + bromobenzene(3) + nitrobenzene(3) and butylacetate(1) + butanol(2) + benzene(3), + toluene(3) + chlorobenzene(3), + bromobenzene(3), + nitrobenzene(3) respectively. The aim of this programme is to characterize the effect of the chain of the alkanols on isentropic compressibility.

2. EXPERIMENTAL SECTION

Apparatus and Procedure: Isentropic compressibilities were computed from the measured speed of sound and the density, evaluated from excess volume measurements. Excess volumes as a function of composition were measured directly by a dialatometric method described earlier [3]. The speed of sound were measured using a variable path interferometer technique [4] at a frequency of 3MHz and the values are accurate to ±0.015%. All the measurements were made at a constant temperature employing a thermostat that could maintain the temperature of 303.15 + 0.01K. Isentropic compressibilities calculated from the speed of sound and density are accurate t ± 2 TPa^{-1}.

Materials: The methods of purifying the various components and checking their purity have been described earlier [1,2].

3. RESULTS AND DISCUSSION

Isentropic compressibilities of ternary mixtures, $K_{s_{123}}$; were calculated using the expression

$$K_{s_{123}} = U^{-2}\rho^{-1} \tag{1}$$

where U and ρ denote the speed of sound and density respectively.

The densities for ternary mixtures were calculated from the relation

$$\rho = \frac{x_1 M_1 + x_2 M_2 + x_3 M_3}{V + V^E_{123}} \tag{2}$$

where x_1, x_2 and x_3 and M_1, M_2 and M_3 denote the molefractions and molecular weights of butylacetate, propanol, aromatic hydrocarbons and butylacetate, butanol, aromatic hydrocarbons respectively.

$$V = \Sigma\, x_i V^0_i \tag{2a}$$

where V^0_i is the molar volume of pure component i and V^E_{123} is the experimental excess molar volume.

The deviation in isentropic compressibility, $K_{s_{123}}$, for a ternary mixtures was computed employing the relation

$$K_{s_{123}} = K_{s_{123}} - K^{id}_{s_{123}} \tag{3}$$

where $K_{s_{123}}$ and $K^{id}_{s_{123}}$ are isentropic compressibilities of the real and an ideal mixtures respectively. The ideal isentropic compressibility was assumed to be additive in terms of volume fraction and was calculated using the relation,

$$K^{id}_{s_{123}} = \phi_1 K_{s_1} + \phi_2 K_{s_2} + \phi_1 K_{s_3} \tag{4}$$

where ϕ_1, ϕ_2 and ϕ_3 and K_{s_1}, K_{s_2} and K_{s_3} are volume fractions and isentropic compressibilities of butyl acetate, propanol, aromatic hydrocarbons and butyl acetate, butanol, aromatic hydrocarbons respectively.

The quantity $dK_{s_{123}}$ the difference between the measured value and that computed from constituent binary data was calculated as shown below:

$$dK_{s_{123}} = K_{s_{123}} - K^{1}_{s_{123}} \tag{5}$$

where $K_{s_{123}}$ is the deviation in isentropic compressibility calculated from experimental data and $K^{1}_{s_{123}}$ is the deviation calculated from binary data. The latter quantity was calculated using the relation

$$K_{s_{123}} = K_{s_{12}} + K_{s_{13}} + K_{s_{23}} \tag{6}$$

where $K_{s_{12}}$, $K_{s_{13}}$ and $K_{s_{23}}$ denote deviations in isentropic compressibility of the binary data. $K_{s_{ij}}$ for a binary mixture was estimated using the smoothing equation

$$K_{sij} = \phi_i\phi_j[a_0 + a_1(\phi_i - \phi_j) + a_2(\phi_i - \phi_j)^2] \tag{7}$$

where a_0, a_1 and a_2 are constants obtained by the method of least squares.

Further the binary parameters for the deviation in isentropic compressibility to compute ternary data for mixtures of butylacetate with aromatic hydrocarbons, butylacetate with alcohols and alcohols with aromatic hydrocarbons were taken from the literature [5–9]. These parameters are given in Table II along with the standard deviation σ (ΔK_s).

The experimental isentropic compressibility, $K_{s_{123}}$ and the deviation in isentropic compressibility, $K_{s_{123}}$, for the ternary mixtures are given in columns 5 and 6 of Table I. Finally, the quantity $dK_{s_{123}}$ is given in column 8 of Table I.

An examination of results included in Table I shows that the values of $dK_{s_{123}}$ are non zero. This suggests that the ternary mixtures are not ideal interms of constituent binaries. This shows that the third component modifies both the nature and degree of interaction between molecular of components. The algebraic values of $dK_{s_{123}}$ fall in the order nitrobenzene > bromobenzene > chlorobenzene > benzene > toluene in case of both butylacetate + propanol + aromatic hydrocarbons and butylacetate + butanol + aromatic hydrocarbon systems respectively. This order indicates that $dK_{s_{123}}$ becomes more negative

TABLE I Experimental values for Isentropic Compressibilities of Ternary systems: butylacetate (1) + Propanol (2) + aromatic hydrocarbons (3) and butylacetate (1) + butanol (2) + aromatic hydrocarbons at 303.15 K respectively

ϕ_1	ϕ_3	$\frac{\rho}{(g.cm^{-3})}$	$\frac{U}{(m.s^{-1})}$	$\frac{K_{S123}}{TPa^{-1}}$	$\frac{K_{S123}}{TPa^{-1}}$	$\frac{K'_{S123}}{TPa^{-1}}$	$\frac{dK_{S123}}{TPa^{-1}}$
butylacetate (1) + propanol (2) + benzene (3)							
0.1330	0.0787	0.81015	1180	886	22	10	12
0.1548	0.2399	0.82266	1186	864	30	12	18
0.1604	0.3340	0.82984	1194	845	29	10	19
0.1553	0.4720	0.83978	1196	832	32	13	19
0.2000	0.5038	0.84249	1201	823	40	19	21
0.1630	0.6179	0.85152	1207	806	42	22	20
0.1483	0.6584	0.85358	1213	796	39	20	19
0.1391	0.8065	0.87649	1225	760	29	13	16
0.1112	0.8349	0.86447	1241	751	24	9	15
butylacetate (1) + Propanol (2) + toluene (3)							
0.1516	0.0376	0.80904	1184	882	11	6	5
0.1388	0.2354	0.82068	1202	843	7	8	−1
0.1318	0.3673	0.82819	1209	826	13	9	4
0.1395	0.4909	0.83594	1213	813	22	11	11
0.1429	0.6160	0.84369	1220	796	28	13	15
0.1431	0.6769	0.84749	1224	788	30	14	16
0.1260	0.7604	0.85156	1235	770	26	12	14
0.1507	0.7594	0.85352	1236	767	24	11	13
0.0655	0.8249	0.85095	1248	754	18	5	13
butylacetate (1) propanol (2) + chlorobenzene (3)							
0.1361	0.0956	0.83547	1204	826	−24	−11	−13
0.1400	0.1243	0.84461	1210	809	−32	−15	−17
0.1488	0.3741	0.92183	1220	729	−36	−17	−19
0.1383	0.4810	0.95294	1222	703	−30	−19	−11
0.1839	0.5502	0.97732	1215	693	−17	−14	−3
0.1451	0.6353	0.99942	1218	674	−12	−11	−1
0.1407	0.6814	1.01273	1223	660	−12	−9	−3
0.0888	0.8189	0.04921	1238	622	−12	−6	−6
0.0794	0.8661	0.06242	1240	612	−8	−4	−4
butyl acetate (1) + propanol (2) + bromobenzene (3)							
0.0746	0.1055	0.87442	1190	808	−35	−2	−33
0.1494	0.1672	0.92269	1181	777	−40	−8	−32
0.1464	0.3647	1.05905	1160	702	−43	−11	−32
0.1278	0.4625	1.12466	1150	672	−38	−12	−26
0.1284	0.5431	1.17995	1144	648	−33	−14	−19
0.1475	0.6586	1.26033	1143	607	−30	−17	−13
0.1496	0.6979	1.28981	1141	596	−27	−15	−12
0.0819	0.8309	1.35936	1144	562	−16	−8	−8
0.0923	0.8597	1.39296	1138	554	−13	−5	−8
butylacetate (1) + propanol (2) + nitro benzene (3)							
0.0634	0.0743	0.87346	1180	822	−25	−5	−20
0.1467	0.1748	0.87825	1234	748	−46	−10	−36
0.1560	0.2995	0.92985	1272	665	−68	−18	−50
0.1317	0.4508	0.98744	1316	585	−77	−20	−57

TABLE I Experimental values for Isentropic Compressibilities of Ternary systems: butylacetate (1) + Propanol (2) + aromatic hydrocarbons (3) and butylacetate (1) + butanol (2) + aromatic hydrocarbons at 303.15 K respectively

ϕ_1	ϕ_3	$\frac{\rho}{(g.cm^3)}$	$\frac{U}{(m.s^{-1})}$	$\frac{K_{S123}}{TPa^{-1}}$	$\frac{K_{S123}}{TPa^{-1}}$	$\frac{K'_{S123}}{TPa^{-1}}$	$\frac{dK_{S123}}{TPa^{-1}}$
0.1347	0.5858	1.02364	1365	524	−73	−22	−51
0.1411	0.6469	1.06071	1366	502	−65	−19	−46
0.1705	0.7088	1.09402	1381	479	−57	−17	−40
0.0861	0.8087	1.12586	1399	454	−38	−10	−28
0.0689	0.8805	1.15251	1407	438	−21	−4	−17
		butylacetate (1) + butanol (2) + benzene (3)					
0.0678	0.0787	0.81111	1217	832	11	4	7
0.1378	0.2005	0.82313	1210	830	25	9	16
0.1552	0.2335	0.82627	1208	829	28	11	17
0.1362	0.3639	0.83335	1214	814	30	11	19
0.1337	0.4661	0.83984	1216	805	34	13	21
0.1452	0.6177	0.85094	1224	784	32	12	20
0.1484	0.6565	0.85391	1227	778	31	12	19
0.1154	0.7497	0.85822	1237	762	27	11	16
0.0802	0.8231	0.86111	1249	744	18	5	13
		butylacetate (1) + butanol (2) + toluene (3)					
0.0946	0.0662	0.81207	1217	831	8	1	7
0.1529	0.1625	0.82127	1211	830	19	7	12
0.1252	0.3322	0.82852	1218	814	24	8	16
0.1553	0.5056	0.83987	1222	797	28	9	19
0.1578	0.5289	0.84125	1223	795	29	10	19
0.1063	0.5801	0.84055	1226	792	32	12	20
0.1494	0.6636	0.84837	1230	779	30	11	19
0.1219	0.8045	0.85487	1246	754	22	9	13
0.1001	0.8336	0.85797	1253	743	15	3	12
		butylacetate (1) + butanol (2) + chlorobenzene (3)					
0.1071	0.0435	0.82233	1205	837	17	11	6
0.1451	0.1506	0.85732	1177	842	48	38	10
0.1321	0.3412	0.91324	1189	774	27	19	8
0.1291	0.4599	0.94791	1201	731	14	8	6
0.1514	0.4878	0.95766	1206	718	7	3	4
0.1412	0.5835	0.98504	1217	685	−2	−4	2
0.1561	0.6326	1.00052	1222	669	−6	−6	3
0.1046	0.7895	1.04269	1231	633	−3	−2	−1
0.0604	0.8669	1.06176	1237	616	−1	−8	−2
		butylacetate (1) + butanol (2) + bromobenzene (3)					
0.0796	0.0638	0.85138	1208	865	−6	−2	−4
0.1435	0.1920	0.94402	1186	753	−18	−7	−11
0.1298	0.2605	0.99003	1180	726	−24	−10	−14
0.1344	0.4842	1.14253	1155	656	−25	−11	−14
0.1480	0.5229	1.16984	1153	643	−26	−13	−13
0.1428	0.6284	1.24082	1150	609	−27	−16	−11
0.1421	0.6626	1.26399	1146	602	−24	−14	−10
0.1321	0.7337	1.31170	1139	588	−16	−7	−9
0.0951	0.8344	1.37695	1138	561	−11	−4	−7

TABLE I (Continued)

ϕ_1	ϕ_3	$\frac{\rho}{(g.cm^3)}$	$\frac{U}{(m.s^{-1})}$	$\frac{K_{s123}}{TPa^{-1}}$	$\frac{K_{s123}}{TPa^{-1}}$	$\frac{Kt_{s123}}{TPa^{-1}}$	$\frac{dK_{s123}}{TPa^{-1}}$
butylacetate (1) + butanol (2) + nitrobenzene (3)							
0.0600	0.0899	0.84208	1248	763	−30	−6	−24
0.1389	0.1858	0.88612	1265	705	−47	−11	−36
0.1286	0.3558	0.95295	1311	611	−68	−19	−49
0.1405	0.4674	0.99777	1338	560	−72	−22	−50
0.1302	0.5156	1.01587	1351	539	−72	−23	−49
0.1385	0.6104	1.05358	1371	505	−66	−21	−45
0.1349	0.6832	1.08166	1385	482	−58	−18	−40
0.1210	0.7916	1.12268	1402	453	−41	−12	−29
0.0628	0.8664	1.14668	1414	436	−26	−6	−20

TABLE II Values Of The parameters a_0, a_1 and a_2 and the standard deviation σ (ΔKs) for binary systems at 303.15 K

System	$\frac{a_0}{TPa^{-1}}$	$\frac{a_1}{TPa^{-1}}$	$\frac{a_2}{TPa^{-1}}$	$\frac{\sigma(\Delta Ks)}{TPa^{-1}}$
butylacetate + benzene	80	−19	49	2
butylacetate + toluene	20	−15	35	1
butylacetate + chlorobenzene	−58	8	36	2
butylacetate + bromobenzene	−124	−54	−35	3
butylacetate + nitrobenzene	−220	36	157	2
butylacetate + propanol	84.965	−9.256	−17.672	0.5
butylacetate + butanol	63.237	4.619	−23.046	1
Propanol + benzene	44	1	35	1
Propanol + toluene	7	163	−31	1
Propanol + chlorobenzene	−92	280	4	1
Propanol + bromobenzene	−140	283	−156	3
Propanol + nitrobenzene	−261	106	−31	2
Butanol + benzene	64	−6	−12	1
Butanol + toluene	70	55	44	1
butanol + chlorobenzene	33	−23	19	1
butanol + bromobenzene	−64	90	25	3
butanol + nitrobenzene	−217	88	−79	1

with decreasing π electron density. The π electron density of the benzene ring decreases when the electron donating group(methyl) is replaced by an electron withdrawing substituent (halogen or nitro group). Further the replacement of propanol by butanol does not change the sign of deviation in isentropic compressibility except in case of chlorobenzene system. However, the algebric value of dK_{s123} is higher for the mixture containing propanol except in case of toluene system.

This reagent that structure breaking events are dominant in the series of butylacetate (1) + butanol (2) + aromatic hydrocarbons (3)

TABLE III Values Of Ternary Constants, A, B, and C and the standard deviation $\sigma(dKs_{123})$ of ternary systems at 303.15 K

System	*A*	*B*	*C*	$\sigma(dKs_{123})$
		TPa^{-1}		
butylacetate (1) + propanol (2) + benzene (3)	277	4523	137023	3
butylacetate (1) + propanol (2) + toluene (3)	425	89	69834	2
butylacetate (1) + propanol (2) + chlorobenzene	−684	2583	−39298	3
butylacetate (1) + propanol (2) + bromobenzene (3)	−499	−5310	−46035	3
butylacetate (1) + propanol (2) + nitrobenzene (3)	−984	−2811	5595	3
butylacetate (1) + butanol (2) + benzene (3)	501	1205	43439	2
butylacetate (1) + butanol (2) + toluene (3)	296	3128	45929	3
butylacetate (1) + butanol (2) + chlorobenzene (3)	382	−20079	117895	3
butylacetate (1) + butanol (2) + bromobenzene (3)	−505	−1846	−8828	2
butylacetate (1) + butanol (2) + nitrobenzene (3)	−960	−3169	−20471	3

with respect to the series butylacetate (1) + propanol (2) + aromatic hydrocarbons (3). This may be attributed to the difference in chain length of the alcohols.

The $dK_{s_{123}}$ values were fitted to the polynomial equation

$$dK_{s_{123}} = \phi_1\phi_2\phi_3[A + B\phi_1(\phi_2 - \phi_3) + C\phi_1^2(\phi_2 - \phi_3)^2] \qquad (8)$$

where ϕ_1, ϕ_2 and ϕ_3 are the volume fractions of components 1, 2 and 3 respectively. The values of adjustable parameters A, B and C are obtained by the least squares method and are given in Table III along with the standard deviations $\sigma(dK_{s_{123}})$

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