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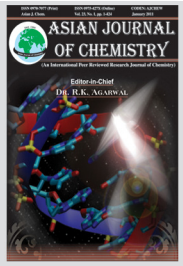

Interaction Studies in Binary Liquid Mixture of Alkanes and Aromatic Compounds Ultrasonically at 313.15 K

M.C. SAXENA[1], POONAM DUBEY[2,*], ASHUTOSH TRIPATHI[3] and AMARJEET KAUR[4]

[1]Chemical Laboratories K.S. Saket Post Graduate College, Ayodhya-224 001, India
[2]Department of Chemistry, Gurunanak Girls Post Graduate College, Faizabad-224 001, India
[3]Department of Chemistry, P.B. Post Graduate College, Pratapgarh-230 002, India
[4]Department of Chemistry, Jhunjhunwala Post Graduate College, Faizabad-224 133, India

*Corresponding author: E-mail: poonam_dubey28@rediffmail.com

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The present investigation deals with the evaluation of ultrasonic velocity theoretically in six binary liquid mixtures hexane + benzene, hexane + toluene, hexane + ethyl benzene, heptane + benzene, heptane + toluene and heptane + ethyl benzene at 313.15 K, using Nomoto relation and ideal mixing relation, testing their validity and their comparison. Molecular interactions has also been assessed directly in terms of ultrasonic velocity.

Key Words: Nomoto, Ideal mixing, Non-ideality, Interaction, Binary mixture.

INTRODUCTION

Assuming the linearity of the molecular sound velocity, Nomoto[1] established the following empirical relation for the sound velocity in the binary liquid mixutre:

$$R = x_1R_1 + x_2R_2 \quad (1)$$

where x represents the mole fraction and R molecular sound velocity which is related to molecular weight M and density ρ by relation:

$$R = \frac{M}{\rho}\cdot U^{1/3} = V.U^{1/3} \quad (2)$$

The molar volume (V) which was supposed to be additive, is given by:

$$V = x_1V_1 + x_2V_2 \quad (3)$$

On the basis of above equations, the ultrasonic velocity is given by:

$$U = \left(\frac{R}{V}\right)^3 = \left(\frac{x_1R_1 + x_2R_2}{x_1V_1 + x_2V_2}\right)^3 \quad (4)$$

The deviation of molecular sound velocity, ultrasonic velocity and molecular volume from linearly are represented as:

$$\begin{aligned} \Delta R &= R_{cal} - R_{exp} \\ \Delta U &= U_{cal} - U_{exp} \\ \Delta V &= V_{cal} - V_{exp} \end{aligned} \quad (5)$$

Van Dael and Vangeel[2,3] using the assumption made by Richardson[4] and Blandamer *et al.*[5] that the adiabatic compressibility (βs) of the mixture should be given by:

$$\beta s = \phi_1(\beta s)_1 + \phi_2(\beta s)_2 \quad (6)$$

and suggested the following relation for sound velocity in homogenous liquid mixture:

$$\beta s_{(im)} = \phi_1\frac{\gamma_1}{\gamma_{(im)}}(\beta s)_1 + \phi_2\frac{\gamma_2}{\gamma_{(im)}}(\beta s)_2 \quad (7)$$

where ϕ is the volume fraction and γ represents the specific heat ratio.

The eqn. 6 holds true if the mixture is an ideal one and $\gamma_1 = \gamma_2 = \gamma_{(im)}$ eqn. 6 can be transformed in to linear combination of the mole fraction (x). If the assumptions $\gamma_1 = \gamma_2$ is made.

$$\beta s_{(im)} = x_1(\beta s)_1 + x_2(\beta s)_2 \quad (8)$$

on the basis of above equations, Van Dael and Vangeel[2,3] gave the following equations for sound velocity in mixture:

$$\frac{1}{x_1M_1 + x_2M_2}\cdot\frac{1}{U^2_{(im)}} = \frac{x_1}{M_1U_1^2} + \frac{x_2}{M_2U_2^2} \quad (9)$$

In all the above expressions suffix 1 and 2 refer to component liquids first and second, respectively.

RESULTS AND DISCUSSION

In the present work, ultrasonic velocity has been evaluated by Nomoto relation and ideal mixing relation (Van Dael's

relation) to test their validity and comparison with the experimental results. The interactions in the system, taken for study, has also been studied, using sound velocity values.

The necessary data required for the calculation has been collected from the work of Calvar *et al.*[6].

The percentage deviation from linearly for Nomoto relation, molar volume, molar sound velocity has been evaluated and has been tabulated in the second, third and fourth column of the Table-1. Experiment sound velocity, Nomoto's sound velocity and ideal mixing sound velocities are given in fifth, sixth, seventh column fo the Table-1. The last column of the table includes the ratio of U_{exp}^2/U_{ideal}^2.

Perusal of the Table-1 shows that all the quantities varies with the composition of the mixture in every system. Deviation

TABLE-1
MAXIMUM PERCENTAGE DEVIATION OF THE MOLECULAR SOUND VELOCITY (R), THE MOLAR VOLUME (V) FROM LINEARLY, THE MAXIMUM PERCENTAGE DEVIATION OF THE SOUND VELOCITY (U) FROM NOMOTO'S EMPIRICAL RELATION AND THE RATIO U_{exp}^2/U_{im}^2

x_1 (Ref. 6)	ΔU/U (%) (eqn. 5)	ΔV/V (%) (eqn. 5)	ΔR/R (%) (eqn. 5)	U_{exp} (m/s) (Ref. 6)	U_{nom} (m/s) (eqn. 4)	U_{im} (m/s) (eqn. 9)	U_{exp}^2/U_{im}^2
Hexane (x_1) + Benzene (x_2)							
0.0000	0.0000	0.0000	0.0000	1230.0	1230.0	1230.0	1.0000
0.0378	0.1984	-0.0320	0.0341	1214.8	1217.2	1221.6	0.9887
0.1009	0.4957	-0.1123	0.0533	1191.1	1197.0	1207.8	0.9724
0.1986	0.8439	-0.2115	0.0711	1158.5	1168.3	1186.3	0.9535
0.2979	1.0701	-0.2671	0.0917	1129.8	1142.0	1164.5	0.9412
0.4020	1.1392	-0.2898	0.0924	1104.3	1117.0	1141.6	0.9355
0.6024	1.0476	-0.2665	0.0848	1063.9	1075.1	1097.6	0.9394
0.7014	0.8823	-0.2304	0.0652	1047.7	1057.06	1075.9	0.9482
0.8010	0.6741	-0.1700	0.0555	1033.2	1040.2	1054.0	0.9608
0.9083	0.3244	-0.0518	0.0565	1020.2	1023.5	1030.4	0.9802
0.9464	0.1982	-0.0290	0.0371	1015.9	1017.9	1022.0	0.9879
1.0000	0.0000	0.0000	0.0000	1010.3	1010.3	1010.3	1.0000
Hexane (x_1) + Toluene (x_2)							
0.0000	0.0000	0.0000	0.0000	1240.7	1240.7	1240.7	1.0000
0.1032	0.1458	0.0772	0.1259	1208.5	1210.2	1216.9	0.9862
0.1980	0.2679	0.1023	0.1916	1180.8	1183.9	1195.0	0.9762
0.2997	0.3359	0.1280	0.2399	1153.5	1157.3	1171.6	0.9692
0.4027	0.4007	0.1363	0.2699	1127.5	1132.0	1147.9	0.9647
0.5005	0.4246	0.1261	0.2677	1104.6	1109.3	1125.3	0.9634
0.5998	0.4021	0.1247	0.2587	1083.1	1087.4	1102.5	0.9651
0.6987	0.3344	0.0977	0.2092	1063.3	1066.8	1079.7	0.9698
0.7984	0.2546	0.0835	0.1684	1044.5	1047.1	1056.7	0.9769
0.9042	0.1020	0.0600	0.0940	1026.3	1027.3	1032.3	0.9882
1.0000	0.0000	0.0000	0.0000	1010.3	1010.0	1010.0	1.0000
Hexane (x_1) + Ethyl benzene (x_2)							
0.0000	0.0000	0.0000	0.0000	1256.9	1256.9	1256.9	1.0000
0.0465	-0.0031	0.0653	0.0642	1243.8	1243.7	1245.4	0.9973
0.0771	0.0173	0.0863	0.0921	1235.0	1235.2	1237.8	0.9953
0.2010	0.0494	0.1888	0.2053	1200.8	1201.3	1207.3	0.9892
0.3015	0.0814	0.2353	0.0262	1173.9	1174.8	1182.5	0.9854
0.3990	0.1174	0.2649	0.3039	1148.5	1149.8	1158.5	0.9828
0.5092	0.1184	0.2761	0.3155	1121.1	1122.4	1131.3	0.9819
0.6010	0.1222	0.2559	0.2965	1098.9	1100.2	1108.6	0.9824
0.7012	0.0919	0.2277	0.2583	1075.7	1076.6	1083.9	0.9847
0.7999	0.0034	0.1852	0.1863	1054.1	1054.1	1059.6	0.9895
0.8993	0.0244	0.1044	0.1126	1031.8	1032.0	1035.1	0.9935
0.9534	-0.0010	0.0553	0.0550	1020.3	1020.2	1021.7	0.9970
1.0000	0.0000	0.0000	0.0000	1010.3	1010.3	1010.3	1.0000
Heptane (x_1) + Benzene (x_2)							
0.0000	0.0000	0.0000	0.0000	1230.0	1230.0	1230.0	1.0000
0.0511	0.4252	-0.1225	0.0196	1210.9	1216.0	1221.6	0.9824
0.1025	0.8090	-0.2359	0.0351	1193.3	1203.0	1213.2	0.9673
0.1998	1.2860	-0.3918	0.0403	1165.5	1180.6	1197.3	0.9475
0.2987	1.5366	-0.4713	0.0458	1142.8	1160.6	1181.1	0.9360
0.3972	1.6183	-0.4923	0.0526	1124.4	114.8	1165.0	0.9314
0.5013	1.5343	-0.4718	0.0446	1108.9	1126.1	1148.0	0.9329
0.5998	1.3661	-0.4370	0.0224	1096.8	1111.9	1131.9	0.9388
0.6980	1.1639	-0.3607	0.0308	1086.4	1099.1	1115.8	0.4786
0.8043	0.8141	-0.2496	0.0232	1077.8	1086.6	1098.4	0.9626
0.9013	0.4298	-0.1143	0.0292	1071.6	1076.2	1082.6	0.9797
0.9518	0.2190	-0.0568	0.0162	1068.8	1071.1	1074.3	0.9896
1.0000	0.0000	0.0000	0.0000	1066.5	1066.5	1066.5	1.0000

Heptane (x_1) + Toluene (x_2)							
0.0000	0.0000	0.0000	0.0000	1240.7	1240.7	1240.7	1.0000
0.0496	0.2616	-0.0101	0.0771	1225.2	1228.4	1232.0	0.9888
0.1037	0.3383	-0.0207	0.0921	1211.5	1215.6	1222.6	0.9818
0.2040	0.6451	-0.0398	0.1758	1185.7	1193.3	1205.1	0.9679
0.4060	0.7835	-0.0574	0.2045	1144.8	1153.8	1169.9	0.9574
0.5045	0.7825	-0.0558	0.2058	1127.8	1136.6	1152.8	0.9570
0.6016	0.7025	-0.0583	0.1765	1113.1	1220.9	1135.9	0.9602
0.7011	0.5933	-0.0468	0.1514	1099.4	1105.9	1118.5	0.9660
0.8029	0.4245	-0.0342	0.1075	1087.0	1091.6	1100.8	0.9750
0.9019	0.2511	-0.0180	0.0657	1075.9	1078.6	1083.5	0.9858
0.9517	0.1088	-0.0028	0.0334	1071.2	1072.3	1074.9	0.9931
1.0000	0.0000	0.0000	0.0000	1066.5	1066.5	1066.5	1.0000
Heptane (x_1) + Ethyl benzene (x_2)							
0.0000	0.0000	0.0000	0.0000	1256.9	1259.9	1256.9	1.0000
0.0494	0.0980	0.0046	0.0373	1243.9	1245.1	1247.4	0.9942
0.1039	0.2172	0.0050	0.0775	1229.8	1232.4	1237.1	0.9882
0.2025	0.3791	0.0259	0.1524	1205.9	1210.4	1218.3	0.9796
0.3022	0.4751	0.0159	0.1745	1183.7	1189.3	1199.3	0.9740
0.4038	0.5356	-0.0050	0.1734	1162.6	1168.8	1180.0	0.9706
0.5006	0.4919	-0.0263	0.1373	1144.6	1150.2	1161.5	0.9709
0.6003	0.4483	-0.0107	0.1388	1126.9	1131.9	1142.6	0.9727
0.7014	0.4023	-0.0065	0.1277	1109.8	1114.2	1123.3	0.9760
0.8048	0.2018	0.0069	0.0743	1094.8	1097.0	1103.6	0.9839
0.9028	0.1357	0.0136	0.0589	1079.9	1081.3	1085.0	0.9906
1.0000	0.0000	0.0000	0.0000	1066.5	1066.5	1066.5	1.0000

of the value of R has been observed in all the system. However the Δ % in molar volume are positive in the system II and III and negative in the system I, IV, V and VI.

A persual of the Table-1 also reveals that Nomoto's relation for sound velocity gave better agreement with the experiment values of sound velocity as compared to other relation, as observed by previous workers[7,8]. The calculated values obtained from both the relation follows the same trend as the experimental values, further confirms the validity of both the relation, *i.e.*, decreases regularly with higher concentration of the 1st component, alkane in the mixture.

The ratio of U_{exp}^2/U_{ideal}^2 given in the last column of the table reveals that the magnitude of U_{exp}^2/U_{ideal}^2 is appreciable and near to unity at higher concentration of aromatic compounds benzene, toluene and ethyl benzene in the mixture.

The variation of U_{exp}^2/U_{ideal}^2 with mole fraction of the components of the mixture is a clear indication of molecular interaction within the component, which may be attributed due to availability of π electrons of the aromatic hydrocarbon.

Thus the ratio of U_{exp}^2/U_{ideal}^2 can be used as important tool to measure the non-ideality of the mixture, especialloy when the data other than sound velocity and density are not available.

The negative values of percentage deviation of (Δv/V) further confirms the non-ideality of the system under present investigation.

Conclusion

Thus, it can be concluded that Nomot's empirical relation can be successfully used to predict sound velocity of binary liquid mixture, at wide range of composition and temperature, secondly the value of ratio of U_{exp}^2/U_{ideal}^2 can be used as important tool to assess the extent and magnitude of interaction within the component of the mixture, especially when the data other than sound velocity and density are not available, for the system.

Thus the study is two fold studyt, firstly testing the validity of various theoretical relations to evaluate sound velocity of the mixture and secondly interaction studies, using ultrasonic velocities data.

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