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Theoretical evaluation of ultrasonic velocities in binary liquid mixtures at different temperatures

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ABSTRACT

Ultrasonic velocities calculated from various theories and relations like Nomoto's relation, Van dael ideal mixing relation, Impedance relation, Rao's specific velocity relation and Jungie's theory are compared with experimental values in binary liquid mixtures o-anisidine with o-cresol at temperatures 303.15, 308.15, 313.15 and 318.15 K over the entire mole fraction range. The relative applicability of these theories to the present system is checked and discussed. A good agreement is observed between experimental and theoretical values. The results are explained in the light of molecular interactions occuring in these mixtures.

***Keywords*:** Binary liquid mixtures; o-anisidene, o-cresol; Nomoto; ultrasonic velocity

1. INTRODUCTION

Results of theoretical evaluation of ultrasonic velocities are used for the better understanding of molecular arrangements in liquid mixtures. In assessing the nature of molecular interactions and investigating the physico-chemical behaviour, ultrasonic study of liquid mixtures gained more importance during the last few decades. Several researchers [1-4] carried out ultrasonic investigations on binary and ternary liquid mixtures and compared the experimental values with theoretical relations [5-9] of Nomoto, Van Dael and Vangeel, Impedance dependence, Rao's specific velocity and Junjie's equations and the results are explained in terms of molecular interactions. o-anisidine is mainly used in the manufacture of dyes for tattooing and coloration of paper. Cresols are used to dissolve other chemicals, as disinfectants and deodorizers, and to make specific chemicals that kill insect pests. Ultrasonic velocities calculated in binary liquid mixture o-anisidine with o-cresol using the above relations are compared with the experimental values at temperatures 303.15, 308.15, 313.15 and 318.15 K for the entire mole fraction range.

2. EXPERIMENTAL

The chemicals used in this work are obtained from Loba (o-anisidine, purity 98 %) and SDFCL (o-cresol, purity 99 %) and were used as such without further purification. The purity of the samples was checked by comparing the experimental values of density with the values reported in literature [10]. The mixtures of required proportions are prepared by using Job's method of continuous variation and are preserved in well-stoppared conical flasks. The flasks are left free to allow them to attain thermal equilibrium after they are prepared.

Using ultrasonic interferometer (Mittal enterprises, India; Model: F-80X) ultrasonic velocities were measured. It consists of a high frequency generator and a measuring cell and the measurements were made at a fixed frequency of 3MHz. The calibration of the equipment was done by measuring the velocity in water and benzene, and the results were compared with the literature values [11]. The ultrasonic velocity has an accuracy of ±0.5 %. Temperature was controlled by circulating water around the liquid cell from thermostatically controlled constant temperature water bath. Using specific gravity bottle, the densities of pure liquids and liquid mixtures were measured. Weights were measured with an electronic balance (Shimadzu AUY220, Japan) capable of measuring up to 0.1mg. An average of 4-5 measurements was taken for each sample.

3. RESULTS AND DISCUSSION

Theoretical values of ultrasonic velocities were calculated using different theories and empirical relations. Comparison of theoretical values of ultrasonic velocities with those obtained experimentally in the present binary liquid mixtures is expected to reveal the nature of interaction between the component molecules in the mixture. Such theoretical study is useful in building the comprehensive theoretical model for the liquid mixtures. Theoretical values of ultrasonic velocities in the mixtures o-anisidine + o-cresol at different mole fractions of o-anisidine for different temperatures were calculated using the following theories and relations:

Nomoto relation for ultrasonic velocity in binary liquid mixtures,

$$U_N = [(x_1R_1+x_2R_2)/(x_1V_1+x_2V_2)]^3 \quad (1)$$

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.

Van Dael and Vangeel Ideal mixing relation,

$$U_{imx} = [(x_1/M_1U^2_1 + x_2/M_2U^2_2)(x_1M_1+x_2M_2)]^{-1/2} \quad (2)$$

where U_{imx} is the ideal mixing ultrasonic velocity in liquid mixture. U_1 and U_2 are ultrasonic velocities of the individual compounds.

Impedance dependent relation,

$$U_{Im} = \Sigma x_iZ_i / \Sigma\, x_i\rho_i \quad (3)$$

where x_i is the mole fraction, ρ_i the density of the mixture and Z_i is the acoustic impedance.
Rao's specific velocity,

$$U_R = (\Sigma x_i\, r_i\, \rho_i)^3 \quad (4)$$

where x_i is the mole fraction, ρ_i the density of the mixture and r_i is the Rao's specific sound velocity.
Jungie equation,

$$U_J = (x_1M_1/\rho_1 + x_2M_2/\rho_2)/\ [\{x_1M_1+x_2M_2\}^{1/2}\ \mathbf{x}\ \{x_1M_1/\rho_1U^2{}_1+x_2M_2/\rho_2U^2{}_2\}]^{1/2} \quad (5)$$

where M_1, M_2 are molecular weights of constituent components, ρ_1 and ρ_2 are the densities of constituent components. The theoretical evaluation of sound velocity based on different models in liquid mixtures has been used to correlate with the experimental findings. The theoretical values of ultrasonic velocities calculated by using the Equations (1-5) along with the experimental values for the binary mixtures at temperatures of 303.15, 308.15, 313.15 and 318.15K are given in Table 1. The validity of these theories is checked by percentage deviation for the mixtures at all the temperatures and is given in Tables 2. It can be observed from Table 1 that the theoretical values of ultrasonic velocity calculated by using various theories show deviation from experimental values. The limitations and approximation incorporated in these theories are responsible for the deviations of theoretical values from experimental values. In Nomoto's theory, it is supposed that the volume does not change on mixing. But on mixing two liquids, the interaction between the molecules of the two liquids takes place because of the presence of various types of forces such as dispersive forces, charge transfer, hydrogen bonding, dipole-dipole and dipole-induced dipole interactions.

Thus, the observed deviation of theoretical values of velocity from the experimental values shows that the molecular interactions are taking place [12,13] between the unlike molecules in the liquid mixture. From Table 2, more deviations are observed in case of Nomoto theory and less deviation are observed in case of Van dael ideal mixing relation. On increasing temperature, it was observed that the ultrasonic velocity values decrease in the liquid mixtures chosen. This is probably due to the fact that the thermal energy activates the molecule, which would increase the rate of association of unlike molecules.

Table 1. Experimental and theoretical values of velocities in o-anisidine + o- cresol system at different temperatures

x_1	U_{exp}	U_N	U_{imx}	U_{Im}	U_R	U_J
303.15K						
0.0000	1485.26	1485.26	1485.26	1485.26	1485.26	1459.09
0.0929	1492.10	1496.28	1494.85	1496.18	1495.49	1465.52
0.1872	1500.00	1507.35	1504.77	1507.18	1505.93	1472.13
0.2831	1509.47	1518.47	1515.02	1518.25	1516.58	1478.94
0.3805	1521.42	1529.65	1525.62	1529.39	1527.47	1485.95
0.4795	1527.36	1540.89	1536.60	1540.61	1538.58	1493.16
0.5802	1542.00	1552.18	1547.97	1551.91	1549.93	1500.59

0.6825	1552.46	1563.52	1559.76	1563.29	1561.53	1508.23
0.7865	1564.21	1574.92	1571.99	1574.74	1573.39	1516.10
0.8924	1579.47	1586.38	1584.69	1586.28	1585.50	1524.21
1.0000	1597.89	1597.89	1597.89	1597.89	1597.89	1532.56
308.15 K						
0.0000	1466.84	1466.84	1466.84	1466.84	1466.84	1444.62
0.0929	1474.52	1477.51	1476.12	1477.39	1476.74	1450.92
0.1872	1482.36	1488.24	1485.70	1488.01	1486.84	1457.40
0.2831	1491.63	1499.01	1495.62	1498.71	1497.15	1464.06
0.3805	1503.05	1509.83	1505.87	1509.49	1507.68	1470.91
0.4795	1509.36	1520.70	1516.49	1520.34	1518.43	1477.95
0.5802	1522.84	1531.62	1527.49	1531.27	1529.41	1485.19
0.6825	1533.05	1542.59	1538.90	1542.28	1540.63	1492.63
0.7865	1543.84	1553.60	1550.73	1553.36	1552.09	1500.29
0.8924	1559.31	1564.67	1563.01	1564.53	1563.80	1508.17
1.0000	1575.78	1575.78	1575.78	1575.78	1575.78	1516.28
313.15K						
0.0000	1452.11	1452.11	1452.11	1452.11	1452.11	1433.59
0.0929	1460.89	1462.48	1461.11	1462.35	1461.72	1439.69
0.1872	1469.26	1472.89	1470.41	1472.66	1471.53	1445.96
0.2831	1478.21	1483.35	1480.03	1483.04	1481.54	1452.39
0.3805	1489.42	1493.85	1489.99	1493.50	1491.75	1459.01
0.4795	1495.57	1504.40	1500.29	1504.03	1502.19	1465.81
0.5802	1508.36	1515.00	1510.97	1514.64	1512.85	1472.80
0.6825	1517.36	1525.64	1522.04	1525.32	1523.73	1479.99
0.7865	1527.84	1536.33	1533.52	1536.08	1534.86	1487.38
0.8924	1543.47	1547.06	1545.45	1546.92	1546.22	1494.98
1.0000	1557.84	1557.84	1557.84	1557.84	1557.84	1502.80
318.15K						
0.0000	1437.06	1437.06	1437.06	1437.06	1437.06	1422.13
0.0929	1446.31	1447.28	1445.91	1447.10	1446.51	1428.35
0.1872	1455.31	1457.54	1455.06	1457.22	1456.16	1434.73
0.2831	1464.73	1467.84	1464.52	1467.42	1466.00	1441.27
0.3805	1475.89	1478.18	1474.31	1477.70	1476.06	1447.98
0.4795	1481.52	1488.56	1484.45	1488.05	1486.32	1454.88
0.5802	1494.21	1498.98	1494.95	1498.49	1496.80	1461.95
0.6825	1502.45	1509.44	1505.83	1509.01	1507.51	1469.22
0.7865	1512.84	1519.94	1517.13	1519.60	1518.45	1476.68
0.8924	1527.90	1530.47	1528.86	1530.28	1529.62	1484.34
1.0000	1541.05	1541.05	1541.05	1541.05	1541.05	1492.21

Table 2. Percentage deviation between experimental and theoretical values of velocities in o-anisidine + o-cresol system at varying temperatures

x_1	$\%U_N$	$\%U_{imx}$	$\%U_{Im}$	$\%U_R$	$\%U_J$	$\%U_N$	$\%U_{imx}$	$\%U_{Im}$	$\%U_R$	$\%U_J$
	303.15 K					308.15 K				
0.0000	0.0000	0.0000	0.0000	0.0000	-1.7623	0.0000	0.0000	0.0000	0.0000	-1.5149
0.0929	0.2799	0.1845	0.2736	0.2271	-1.7816	0.2031	0.1083	0.1946	0.1504	-1.6004
0.1872	0.4899	0.3177	0.4785	0.3952	-1.8577	0.3965	0.2256	0.3814	0.3021	-1.6837
0.2831	0.5963	0.3672	0.5813	0.4712	-2.0226	0.4948	0.2673	0.4749	0.3700	-1.8483
0.3805	0.5412	0.2760	0.5240	0.3975	-2.3314	0.4511	0.1878	0.4284	0.3078	-2.1385
0.4795	0.8858	0.6048	0.8678	0.7347	-2.2390	0.7513	0.4725	0.7275	0.6008	-2.0812
0.5802	0.6601	0.3872	0.6428	0.5145	-2.6857	0.5764	0.3055	0.5536	0.4313	-2.4725
0.6825	0.7127	0.4703	0.6975	0.5845	-2.8490	0.6218	0.3812	0.6018	0.4941	-2.6365
0.7865	0.6849	0.4976	0.6734	0.5867	-3.0756	0.6323	0.4462	0.6170	0.5343	-2.8207
0.8924	0.4374	0.3307	0.4309	0.3820	-3.4987	0.3435	0.2375	0.3349	0.2882	-3.2795
1.0000	0.0000	0.0000	0.0000	0.0000	-4.0886	0.0000	0.0000	0.0000	0.0000	-3.7758
	313.15 K					318.15 K				
0.0000	0.0000	0.0000	0.0000	0.0000	-1.2752	0.0000	0.0000	0.0000	0.0000	-1.0386
0.0929	0.1086	0.0152	0.0998	0.0568	-1.4512	0.0671	0.0275	0.0548	0.0139	-1.2419
0.1872	0.2469	0.0786	0.2312	0.1542	-1.5862	0.1534	0.0171	0.1315	0.0583	-1.4144
0.2831	0.3475	0.1234	0.3268	0.2250	-1.7465	0.2126	0.0142	0.1838	0.0870	-1.6017
0.3805	0.2974	0.0381	0.2738	0.1568	-2.0417	0.1554	0.1070	0.1225	0.0112	-1.8907
0.4795	0.5904	0.3157	0.5656	0.4426	-1.9898	0.4754	0.1975	0.4410	0.3239	-1.7983
0.5802	0.4399	0.1729	0.4161	0.2974	-2.3573	0.3194	0.0493	0.2864	0.1733	-2.1588
0.6825	0.5455	0.3082	0.5247	0.4200	-2.4628	0.4652	0.2252	0.4363	0.3366	-2.2119
0.7865	0.5554	0.3719	0.5395	0.4591	-2.6481	0.4691	0.2836	0.4471	0.3705	-2.3905
0.8924	0.2326	0.1281	0.2236	0.1783	-3.1415	0.1684	0.0628	0.1560	0.1128	-2.8513
1.0000	0.0000	0.0000	0.0000	0.0000	-3.5330	0.0000	0.0000	0.0000	0.0000	-3.1696

4. CONCLUSIONS

Theoretical evaluations of ultrasonic velocities in binary liquid mixtures are determined, and the validity of different theories is checked. It is observed that out of all the theories Van Dael ideal mixing relation gives best results followed by Rao's theory.

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