Theoretical based studies of ultrasonic velocities in dioxane -water mixtures of 4-bromo-2-{(e)-[(4-chlorophenyl) imino] methyl}phenol at different temperatures

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ABSTRACT

Ultrasonic velocity examined from Nomoto's relation, Van Dael ideal mixing relation, impedance relation, Rao's specific velocity relation and Junjie's theory has been compared in the mixtures of 4-bromo-2-{(e)-[(4-chlorophenyl)imino]methyl}phenol as a common component with different percentage of dioxane- water mixture at 305.15, 310.15, 315.15 and 320.15 K . A good agreement has been justified between experimental and theoretical ultrasonic velocities.U^2_{exp}/U^2_{mix} has also been evaluated for non-ideality in the mixtures. The relative applicability of above theories to the present systems has been compared and discussed. The results are highlighted on the basis of molecular interactions occurring in these liquid mixtures.

Key words: Ultrasonic velocity, 4-bromo-2-{(e)-[(4-chlorophenyl) imino] methyl} phenol, dioxane- water mixture.

INTRODUCTION

Acoustics parameter like ultrasonic dealing with sound above the audible range and frequencies are higher than 20,000 Hz and their wavelengths are small. The results was showed in terms of molecular interactions, ultrasonic investigations on liquid mixtures and compared the experimental results of ultrasonic velocity with theoretical relations of Nomoto [1], Van dael and Vangeel [2],impedence relation [3], Rao's specific velocity [4] and Junjie [5] carried out by some scholars[6-10].Ultrasonic velocities in dioxane- water mixtures of 4-bromo-2-{(e)-[(4-chlorophenyl)imino]methyl}phenol(L) by using the above theoretical relations are compared with the experimental values of ultrasonic velocities at different temperatures 305.15, 310.15and 315.15 K and study the molecular interaction from the deviation in the values of U^2_{exp}/U^2_{mix} on the basis of earlier studies. Studies of acoustic behavior of 3-(2-benzimidazol)-3-nitro-6-methylchromen-4-one (BNMC) in a different solvents system by using ultrasonic interferometer[11].

EXPERIMENTAL PROCEDURE

All chemicals are analytical reagent (AR) grade with were obtained from Sd Fine chemicals, India which is used as such without further purification. After literature survey [12,13]the purity of samples was checked. The mixtures were prepared of required proportions by Job's method of continuous variation. Weighing was made on Mechaniki Zaktady Precyzyjnej Gdansk Balance, made in Poland (± 0.001 gm). The speed of sound waves was obtained by using variable path, single crystal interferometer (Mittal Enterprises, Model MX-3) with accuracy of ± 0.03% and frequency 1 MHz A special thermostatic arrangement was done for density and ultrasonic velocity measurements. Elite thermostatic water bath was used; in which continuous stirring of water was carried out with the help of electric stirrer and temperature variation was maintained within ± 0.1°C.

THEOROTICAL RELATION FOR ULTRASONIC VELOCITY

1. Nomoto relation

$$U_N = [(x_1R_1+x_2R_2) / (x_1V_1+x_2V_2)]^3 \text{……..1}$$

Where, R- molar sound velocity

$x_1$and x_2 - mole fractions of liquid mixture

V- is molar volume.

2. Van Dael and Vangeel relation

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

Where, U_{mix}- mixing ultrasonic velocity in liquid mixture

U_1 and U_2 -ultrasonic velocities of individual compounds.

3. Impedance relation

$$U_{Imp} = x_i Z_i / x_i \quad _i \ldots\ldots\ldots\ldots\ldots\ldots 3$$

Where, x_i - mole fraction,

$_i$ - density of the mixture

Z_i -acoustic impedance

4. Rao's velocity

$$U_R = (x_i r_i \quad _i)^3 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 4$$

Where, x_i - mole fraction

U_i -ultrasonic velocity,

i - density of the mixture

r_i -Rao's specific sound velocity = $U^{1/3}{}_i / \quad _i$

Z_i -acoustic impedance

5. Jungie equation

$$U_J = (x_1M_1/ \quad _1 + x_2M_2/ \quad _2)/ [\{x_1M_1+x_2M_2\}^{1/2} \mathbf{x} \{x_1M_1/ \quad _1U^2{}_1+x_2M_2/ \quad _2U^2{}_2\}]^{1/2} \ldots 5$$

Where, M_1, M_2 - molecular weights of constituent components,

$_1$ and $\quad _2$ -densities of constituent components.

RESULTS AND DISCUSSION

Comparative study of theoretical values of ultrasonic velocities and which obtained experimentally in the present liquid mixtures is explained the nature of interaction between the component molecules in the mixture. Theoretical study is useful in building the comprehensive theoretical model for the liquid mixtures. The theoretical values of ultrasonic velocities calculated by using the above all equations i.e. 1-5. and the experimental values for mixtures at different temperatures of 305.15, 310.15 and315.15 K are given in below table. From table it is clear that the theoretical values of ultrasonic velocity calculated by using various theories show deviation from experimental values. Due to the limitations and approximation of 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. On mixing of liquids, the interaction between the molecules of liquids takes place due to the presence of various factors such as dispersive forces, charge transfer, hydrogen bonding, dipole-dipole and dipole-induced dipole interactions. The deviations of experimental values from theoretical values calculated using van Dael and Vangeel equation might be due to the compressibility of the component liquids in the present mixtures. The deviations of experimental values and calculated values from impedance relation and Rao's relation simply non-additively of acoustic impedance and Rao's velocity in the liquid mixtures. In case of Junjie's relation large deviations are observed.It is reveals that, the observed deviation of theoretical values of velocity from the experimental values shows that there are molecular interactions takes place. On rising the temperature, the ultrasonic velocity values decrease in the liquid mixtures.

Theoretical results of ultrasonic velocities in liquid mixtures are showed, it is observed that out of all five theories Nomoto's theory gives best results followed by Impedance dependence relation in all the systems studied.

Table-A : Experimental and theoretical values of velocities ($m.s^{-1}$) in L + water- dioxane system at 305.15K

X_1	U_{exp}	U_N	U_{mix}	U_{Imp}	U_R	U_J
0.0000	1585.27	1585.27	1585.27	1585.27	1585.27	1559.10
0.0889	1600.01	1592.02	1590.08	1591.61	1591.26	1561.95
0.1799	1609.48	1598.79	1595.24	1598.05	1597.42	1564.88
0.2733	1615.80	1605.58	1600.79	1604.60	1603.76	1567.89
0.3691	1625.27	1612.39	1606.75	1611.26	1610.28	1570.98
0.4673	1631.59	1619.23	1613.17	1618.03	1616.98	1574.16
0.5682	1634.22	1626.08	1620.08	1624.92	1623.89	1577.41
0.6718	1637.90	1632.95	1627.54	1631.93	1631.01	1580.75
0.7783	1644.22	1639.84	1635.59	1639.06	1638.34	1584.17
0.8877	1650.54	1646.76	1644.28	1646.31	1645.90	1587.68
1.0002	1653.69	1653.69	1653.69	1653.69	1653.69	1591.29

Table-B: Experimental and theoretical values of velocities ($m.s^{-1}$) in L + Water- dioxane system at 310.15 K

X_1	U_{exp}	U_N	U_{mix}	U_{Imp}	U_R	U_J
0.0000	1465.27	1565.27	1465.27	1465.27	1465.27	1439.10
0.0889	1580.08	1572.09	1570.15	1571.68	1571.34	1542.02
0.1799	1589.59	1578.88	1575.36	1578.15	1577.54	1544.98
0.2733	1575.87	1565.65	1560.84	1564.67	1563.83	1527.97
0.3691	1605.34	1592.41	1596.75	1591.28	1590.30	1550.98
0.4673	1611.59	1599.25	1593.17	1598.05	1596.98	1554.19
0.5682	1614.24	1606.08	1600.10	1604.92	1603.89	1557.43
0.6718	1617.90	1612.97	1617.56	1611.95	1611.04	1560.78
0.7783	1624.24	1619.84	1615.63	1619.08	1618.34	1564.19
0.8877	1630.56	1626.78	1624.29	1626.31	1625.92	1567.70
1.0002	1633.69	1633.69	1633.68	1633.70	1633.69	1571.31

Table-C: Experimental and theoretical values of velocities ($m.s^{-1}$) in L + Water- dioxane system at 315.15 K

X_1	U_{exp}	U_N	U_{mix}	U_{Imp}	U_R	U_J
0.0000	1460.25	1560.25	1460.25	1460.25	1460.25	1434.10
0.0889	1575.08	1567.04	1570.14	1566.66	1555.34	1546.06
0.1799	1584.57	1573.88	1570.36	1578.10	1572.55	1540.99
0.2733	1555.87	1545.65	1540.84	1544.67	1543.83	1507.99
0.3691	1585.34	1572.41	1576.75	1571.28	1570.30	1530.99
0.4673	1591.59	1579.25	1573.17	1578.05	1576.98	1534.21
0.5682	1594.24	1586.08	1580.10	1584.92	1583.89	1537.45
0.6718	1597.90	1592.97	1597.56	1591.95	1591.04	1540.79
0.7783	1604.24	1599.84	1595.63	1599.08	1598.34	1544.19
0.8877	1610.56	1606.78	1604.29	1606.31	1605.92	1547.72
1.0002	1613.69	1613.69	1613.68	1613.70	1613.69	1551.33

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