International Journal for Pharmaceutical Research Scholars (IJPRS)

V-3, I-3, 2014 ISSN : 2277 - 7873

RESEARCH ARTICLE

Ultrasonic Velocity and Allied Parametrs of 1, 1'-bis (4-benzoyloxy-R_1, R_2-Phenyl) Cyclohexane in 1,4-Dioxane at 30°C

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Manuscript No: IJPRS/V3/I3/00366, Received On: 16/08/2014, Accepted On: 18/09/2014

ABSTRACT

Ultrasonic velocity (3MHz) and density of 1,1'-bis (4-benzoyloxy-R_1, R_2 – phenyl) Cyclohexane in 1, 4-dioxane at 30^0C have been determined and several acoustical parameters have been calculated and correlated with concentration. These desired Parameters are interpreted in terms of solvent – solute and solute – solute interactions.

KEYWORDS

Ultrasonic Velocity; Correlation Coefficients(V) (acoustical parameters) for aromatic ester)

INTRODUCTION

Molecular properties in liquid state are very useful in chemical analysis where the knowledge of thernio-dynamic and physical properties are essential for design calculations involving separations, heat transfer, mass transfer and fluid flow. Thermodynamic properties and their temperature dependence are potentially rich source of information's about type and extent of molecular interactions occurring in the solution. With this consideration and in continuation with our recent work , the present piece of work reports sound velocity studies on 1,1 '-bis (4-benzoyloxy – R_1, R_2 -phenyl)cyclohexane-dioxane solutions at 30°C.

EXPERIMENTAL

1,4-Dioxane was purified by fractional distillation. Esters 1-4 were synthesized and purified according to our recent publication.[6-8] The ester solutions (W/V) of different molarities were prepared in 1,4- dioxane

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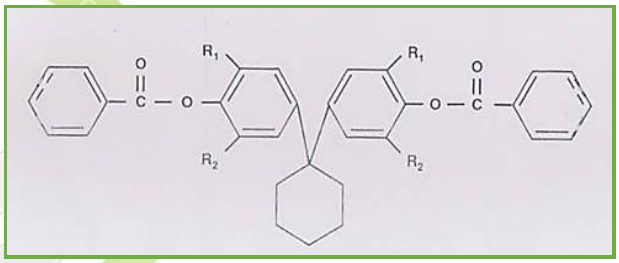

Ester-1: R_1 = H and R_2 = H

Ester-2: R_1 = Br and R_2 = Br

Ester-3: R_1 = Cl and R_2 = Cl

Ester-4: R_1 = CH_3 and R_2 = Cl

The density (ρ), viscosity (η) and sound velocity (U) measurements[2] of pure solvent and solutions were carried out at 30 ± 0.1° C using a specific gravity bottle, a suspended level Ubbelohde viscometer and a Single Crystal Multifrequency Inerferometer (M-82) operating at 3 MHz with accuracies of ± 0.0001 g/cm^3, ± 0.1 % and ±0.06 % respectively.

RESULT AND DISCUSSION

The variation of ρ, η and U (Scheme-1) of esters 1-4 with concentration (C) are reported in Table 1. In order to understand the effect of

substituents on solvent -solute and solute - solute interactions, several acoustical parameters were calculated and correlated with concentration Table-2. It is clear from Table-2 that an excellent correlation is observed between a given parameter and concentration.

From Table 1 it is clear that the change in viscosity is more compared to density and velocity which indicates that the viscosity is more susceptible to structural changes due to apparent structural change. Jone-Dole constants A and B were determined from the intercept and slope of $(\eta_r - 1) / \sqrt{C}$ against $\sqrt{C}$ plots. The least squared values of A and B along with correlation coefficient (γ) are reported in Table 3. The positive values of A and B suggest strong solvent- solute and solute - solute interactions. An increase in velocity and acoustical impedance (Z) and decrease in isentropic compressibility[5] (Ks) with increasing concentration suggested the presence of solvent - solute interaction and it is further confirmed by increase in Rao's molar sound function (R), vander Waals constant[9] (b) and decrease in relaxation strength (r), intermolecular free path length (L_f) and internal pressure (π) with concentration[3-4]. The decrease in π with C suggests decrease in cohesive forces which again confirms change in structural arrangement. As dioxane has two lone pairs of electrons which may interact with electronegative halogen and lone pairs of ester group and also with electropositive methyl group. It is likely that lone pair lone- pair interaction and dipole- dipole interaction of the same type disrupt the structure formed due to opposite dipole- dipole interaction. Thus solvophobicity is due to electrostatic repulsion between lone pairs of solvent with lone pairs of solute whereas solvophilicity is due to electrostatic attraction between lone pairs of solvent and electropositive solute which results in the formation of rigid structure of solvent molecules around the solute molecules. In conclusion solvent- solute and solute- solute interactions exist in the ester solutions and esters 1 and 3 have more structure forming tendency compared to esters 2 and 4.

Table 1: The density, the viscosity and ultrasonic velocity of 1, 4-dioxane and ester solutions at 30^0C

Conc. mol/lit	**Density ρ x 10^{-3} kg/m^3**	**Viscosity η, m Pas**	**Velocity U ms^{-1}**
Ester-1			
0.0000	1.0263	1.0675	1332.6
0.0105	1.0280	1.0861	1333.6
0.0210	1.0283	1.1039	1335.2
0.0315	1.0286	1.1228	1338.1
0.0420	1.0290	1.1395	1341.1
0.0524	1.0294	1.1605	1343.5
0.0629	1.0299	1.1898	1346.2
Ester-2			
0.0000	1.0263	1.0675	1332.6
0.0063	1.0293	1.0933	1334.5
0.0126	1.0306	1.1122	1336.4
0.0189	1.0320	1.1311	1338.5
0.0252	1.0340	1.1567	1340.3
0.0316	1.0360	1.1727	1343.0
0.0379	1.0384	1.1916	1345.9

Ester-3			
0.0000	1.0263	1.0675	1332.6
0.0081	1.0273	1.0962	1332.4
0.0163	1.0282	1.1045	1333.3
0.0244	1.0289	1.1169	1333.6
0.0326	1.0302	1.1338	1334.3
0.0407	1.0313	1.1499	1336.2
0.0488	1.0325	1.1636	1339.1
Ester-4			
0.0000	1.0263	1.0675	1332.6
0.0099	1.0294	1.0760	1335.2
0.0198	1.0297	1.0996	1338.2
0.0297	1.0299	1.1231	1340.8
0.0396	1.0304	1.1458	1342.8
0.0495	1.0309	1.1661	1345.3
0.0594	1.0321	1.1888	1351.3

Table 2: The correlation coefficients (ν) and correlation equations for aromatic esters 1,2,3 and 4

Parameter Y	**Correlation Coefficient (ν)**	**Correlation Equation**
Ester-1		
U_1 ms^{-1}	0.9973	U + 247.58C = 1030.5
$Zx10^{-3}$, $Kgm^{-2}S^{-1}$	0.9991	Z – 371.37C = 994.98
Ks, TPa^{-1}	-0.9881	Ks + 561.81C = 918.25
$Rx10^4$, $m^{10/3}$ $S^{-1/3}$ Mol^{-1}	0.9952	R+10.625C = 9.4290
$bx10^6$, m^3	0.9898	b+92.32C = 80.49
ν	-0.9986	ν - 0.2595C = 0.3085
L_f	-0.9938	L_f -0.074C = 0.4669
π 10^{-8}, Pa	-0.9953	π - 2.428C = 5.1100
Ester-2		
U_1 ms^{-1}	0.9948	U + 355.69C =1331.5
$Zx10^{-3}$, $Kgm^{-2}S^{-1}$	0.9939	Z + 745.74C = 1368.10
Ks, TPa^{-1}	-0.9846	Ks – 435.23C =548.51
$Rx10^4$, $m^{10/3}$ $S^{-1/3}$ Mol^{-1}	0.9991	R+15.029C = 9.5030
$bx10^6$, m^3	0.9998	b+124.45C = 80.73
ν	-0.9914	ν - 0.3713C = 0.3070
L_f	-0.9957	L_f -0.1883C = 0.4675
π 10^{-8}, Pa	-0.9901	π - 2.9553C = 5.1198

Ester-3		
U_1 ms^{-1}	0.9956	U + 150.62C =1330.5
$Zx10^{-3}$, $Kgm^{-2}S^{-1}$	0.9876	Z + 328.62C = 1365.14
Ks, TPa^{-1}	-0.9675	Ks – 191.24C =550.50
$Rx10^4$, $m^{10/3}$ $S^{-1/3}$ Mol^{-1}	0.9999	R+12.351C = 9.4460
$bx10^6$, m^3	0.9997	b+105.70C = 80.773
ν	-0.9836	ν - 0.1573C = 0.3074
L_f	-0.9921	L_f -0.1273C = 0.4683
π 10^{-8}, Pa	-0.9989	π - 3.94203C = 5.1340
Ester-4		
U_1 ms^{-1}	0.9829	U + 299.37C =1331.90
$Zx10^{-3}$, $Kgm^{-2}S^{-1}$	0.9798	Z + 374.94C = 1370.1
Ks, TPa^{-1}	-0.9822	Ks – 266.04C =547.91
$Rx10^4$, $m^{10/3}$ $S^{-1/3}$ Mol^{-1}	0.9918	R+0.9000C = 0.9445
$bx10^6$, m^3	0.9998	b+90.800C = 80.600
ν	-0.9968	ν - 0.3148C = 0.3068
L_f	-0.9951	L_f -0.1141C = 0.4660
π 10^{-8}, Pa	-0.9815	π - 1.8650C = 5.0860

Table 3: Jore – Dole Constants A and B for Esters 1-4 at 30^0C

Ester	**A**	**B**	**ν**
1	-0.064	1.499	0.9843
2	0.061	2.788	0.9894
3	0.066	1.541	0.9917
4	-0.122	2.426	0.9981

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