Studies on acoustic properties of some substituted pyrazole, isoxazole and pyrazoline in dioxane at 303 K

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Ultrasonic velocities and densities of 3-(2-hydroxy-3-bromo-5-methylphenyl)-5-phenyl isoxazole, 1-phenyl-3-(2-hydroxy-3-bromo-5-methylphenyl)-5-(4-methoxyphenyl) pyrazole (L1), 1-phenyl-3-(2-hydroxy-3-bromo-5-methylphenyl)-5-phenyl pyrazoline and 1-phenyl-3-(2-hydroxy-3-bromo-5-methylphenyl)-5-(4-methoxy-phenyl) pyrazoline at different concentration in dioxane have been carried out at 303 K. Different acoustic properties like partial molal volume, adiabatic compressibility, apparent molal compressibility, intermolecular free length, specific acoustic impedance and relative association, etc., have been determined. These parameters obtained have been interpreted in terms of solute-solvent and solute-solute interactions.

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Ultrasonic wave propagation in liquid has been the subject of exhaustive research, which have been carried out theoretically and practically. Ultrasonic parameters are being extensively used to study molecular interaction in pure liquid\(^1\), liquid mixture\(^6\), electronic solutions\(^7\).

Ultrasonic velocity and adsorption studies in case of electrolyte-solution have led to new insight into the process of ion association and complex formation\(^8,9\). Sondawale and Narwade\(^10\) have studied ultrasonic velocity of peptide in binary mixture. Rohankar\(^11\) has investigated the ultrasonic velocity of monochloro acetic acid and trichloro acetic acid in THF-water and dioxane water mixture. Ultrasonic velocity of substituted acrylonaphene and its complexes in acetone\(^12\) and of substituted thiazole and carboxylate at different liquid mixture has been studied\(^13\).

Looking at the important role of substituted 3-(2-hydroxy-3-bromo-5-methylphenyl)-5-phenyl isoxazole(L1), 1-phenyl-3-(2-hydroxy-3-bromo-5-methylphenyl)-5-(4-methoxyphenyl) pyrazole(L2), 1-phenyl-3-(2-hydroxy-3-bromo-5-methylphenyl)-5-phenyl pyrazoline (L3) and 1-phenyl-3-(2-hydroxy-3-bromo-5-methylphenyl)-5-(4-methoxyphenyl) pyrazoline(L4) as antibiotic drugs, it was thought worthwhile to study the 2 mg acoustic properties of L1, L2, L3 and L4 in 0.01, 0.005, 0.0025, 0.0015 M in solutions dioxane at 303 K.

Experimental
The solvent used was purified by standard procedure\(^14\). Solutions of different concentration were prepared by dissolving known weight of substances. All weighing were made on Mechaniki Zaktady Precyzyjnej Gdansk Balance (± 0.001 g).

Density measurements were performed with a precalibrated bicapillary pyknometer. The accuracy in density measurement was found to be ± 0.001 cm\(^3\).

The speed of sound waves was obtained using variables path, single crystal interferometer (Mittal Enterprises, Model MX-3) with accuracy of ± 0.03% and frequency 1 MHz. The temperature was maintained at 303 ± 0.1 K by using thermostat bath.

Results and discussion
The apparent molal volume and apparent molal compressibility has been calculated from Eqs 1 and 2 (Ref. 15).

\[ \phi_v = \frac{1000(d_0 - d_s)}{md_0} + \frac{M}{d} \] \hspace{1cm} ... (1)

\[ \phi_k = \frac{1000(\beta_1 d_0 - \beta_s d_s)}{md_0} + \frac{\beta_0 M}{d} \] \hspace{1cm} ... (2)

where, \(d_0\) and \(d_s\) represent densities of solvent and solution respectively, \(m\) is the molality, \(M\) is the molecular weight of solute; \(\beta_1\) and \(\beta_0\) are the adiabatic compressibilities of solution and solvent respectively. Specific acoustic impedance (\(Z\)), relation association (\(R_a\)) and free length (\(L_f\)) are the functions of ultrasonic velocity and are computed by Eqs 3-5 (ref. 16).

\[ Z = U_d d_b \] \hspace{1cm} ... (3)

\[ R_a = \frac{d_b}{d_0} \left( \frac{U_b}{U_s} \right)^{1/3} \] \hspace{1cm} ... (4)
where $U_a$ and $U_s$ are velocity of ultrasonic wave in solvent and solution and $k$ is Jacobson's constant $(6.0186 \times 10^4)$.

The value of $\psi$, $\phi_{(s)}$, $\beta_s$, $d_s$, $L_s$, $Z$, and $R_A$ obtained in the present investigation at different concentration are presented in Table 1. It could be seen from Table 1 that intermolecular free length increase linearly with decrease in concentration of $L_1$, $L_2$, $L_3$, and $L_4$ in dioxane and hence increase in ultrasonic velocity with the concentration of $L_1$, $L_2$, $L_3$, and $L_4$.

This indicate that there is strong interaction between ion and solvent molecules, suggesting a structure promoting behaviour of the added solute. This may also imply that there is decrease in number of free ions, showing the occurrence of ionic association due to strong ion-ion interactions.

The increase of $\beta_s$ with decrease in concentration of solution may be due to aggregation of solvent molecule around ions supporting ionic solvent interactions.

It is observed from Table 1 that apparent molal volume and apparent adiabatic compressibility increase with decrease in concentration. The positive value of $\phi_{(s)}$ shows strong electrostatic force in the vicinity of ions, causing electrostatic solution of ions. The relative association is influence by two factors, (i) the breaking up of the solvent and (ii) the increase of $\psi$ with decrease in concentration.
molecule on addition of electrolyte to it; and, (ii) solvated ions that are simultaneously present.

The increase of \( R_A \) with concentration suggests that solvation of ions predominates over the breaking up of the solvent aggregates on addition of substance. It is observed from Table 1 that there is a linear variation of \( R_A \) and \( Z \) values with respect to the concentration of solution. The lower the values of \( R_A \) signifies the weak association between the solvent and solute.

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References