Acoustic and volumetric properties of aqueous solution of levofloxacin nickel complexes at 308K

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Abstract

The density and ultrasonic velocity were measured for aqueous solutions of nickel complex and its ternary complex with 1,10-phenanthroline at 308 K. Using the experimental data, adiabatic compressibility, acoustic impedance, intermolecular free length and hydration number, apparent molar volume, limiting apparent molar volume, apparent molar compressibility, limiting apparent molar compressibility and their associated constants were calculated. These parameters were used to study the ion-solvent interaction in each solution.

Keywords: Ultrasonic Velocity, Hydration Number, Adiabatic Compressibility, Apparent Molar Volume, Apparent Molar Compressibility.

1. Introduction

Ultrasonic investigation in aqueous solutions of electrolytes and non-electrolytes provides useful information in understanding the degree and nature of interaction because intra molecular and intermolecular association related structural changes affect the ultrasonic velocity. By ultrasonic measurements, the molecular interactions in pure liquids1,2, aqueous solutions5,7 and liquid mixtures8-11 have also been studied. Iqbal et al12 have studied the apparent molar volume and adiabatic compressibility of aqueous solutions of drugs such as sodium salicylate, methyl orange, L-tryptophan, phenol and hydrochloride salts of procaine and pilocarpene and ephedrine. Naidu et al13 have reported the ultrasonic velocity, density and viscosity studies in aqueous solution of levofloxacin hemi hydrates, tacrolimus monohydrate and lisinopril dehydrate. The interaction between oral levofloxacin and multivalent cations has been described by pharmacokinetic studies14. In the present paper levofloxacin is selected for the study as it is effective against diarrhea caused by Escherichia Coli, campylobacter Jejune and shigella bacteria. It is used for testing infections of the sinuses, skin, lungs, ears, airways, bones and joints caused by susceptible bacteria. It is also used to treat urinary infections. It has been reported15-18 that the levofloxacin (quinolones) act as a monoionic bidentate ligand through their carboxyate and carboxyl groups. The interaction between quinoline and metal cations was based on chelation. Since the functional groups like carbonyl and carboxyl groups are required for antibacterial activity, it could be anticipated that all the quinolones could be interacting with metal ions19. The density and partial molar volume measurements of aqua-organic liquids at infinite dilution20 have been found to be highly useful in understanding the structure of molecular interaction between water and organic molecules. However there are rare reports on acoustic behaviour of metal complexes of drugs. The present paper represents the acoustical and volumetric proper ties of nickel complexes of levofloxacin and its ternary complex with 1,10-phenanthroline at 308 K.

2. Experimental

The hydrated salt NiCl2.6H2O was Anal R grade. Levofloxacin were obtained from a local pharmaceutical company. Water used in this study was doubled distilled water prepared by distilling water over alkaline potassium permanganate in all glass distillation flasks. All the complexes were prepared from reported methods21. These complexes were characterized by elemental analysis and spectroscopic methods. The ultrasonic velocity was measured by single crystal interferometer (Mittal, model-81) operating at a frequency of 2MHz. The temperature was maintained constant at 308.05K in a thermostat. The density of solutions was determined accurately using specific gravity bottle and electronic balance of accuracy (±0.1 mg).

3. Result and discussion

The desired parameters such as adiabatic compressibility (β), inter molecular free length (Lf), acoustic impedance (Z), hydration number (nH), limiting apparent molar compressibility (Kn), apparent molar volume (Vn), limiting apparent molar compressibility (Kn), limiting apparent molar volume (Vn) and their constants (S1 and S2) had been studied at 308 K. Density is known to be a measure of ion-solvent and solvent-solvent interactions. The ultrasonic velocity22,23, adiabatic compressibility, acoustic impedance, intermolecular free length and hydration number24 calculated with equations (1)-(4) are given as,

\[ U = (\beta d)^{1/2} \]  
\[ \beta = d^{-2}U^{-2} \]
The density was found to decrease for both the nickel complexes with increase in concentration. Decrease in density indicated the decrease in solvent-solvent or ion-solvent or structure breaking property of metal complexes. The variation of ultrasonic velocity with molar concentration was shown by Figure 1.

![Graph 1](image1)

**Fig. 1:** Variation of Ultrasonic Velocity (U) with Concentration for [Ni(Levo)2(H2O)2]2H2O and [Ni(Levo)(1,10-phenanthroline)]Cl Complexes At 308K.

The ultrasonic velocity increased smoothly with concentration in [Ni (lev) 2(H2O) 2]2H2O. But increase in ultrasonic velocity occurred steadily in case of [Ni (lev) (1, 10-phenanthroline)] Cl. The increase in ultrasonic velocity for both the nickel complexes may be due to molecular association caused by cohesive forces.

The adiabatic compressibility (β) is a measure of intermolecular association or repulsion calculated from the measured ultrasonic velocity (U) and density (d). The β values were found to increase in [Ni(lev)2(H2O)2]2H2O and decrease in [Ni(lev)(1,10-phenanthroline)]Cl (Figure 2).

![Graph 2](image2)

**Fig. 2:** Variation of Adiabatic Compressibility (β) with Concentration for [Ni(Levo)2(H2O)2]2H2O and [Ni(Levo)(1,10-phenanthroline)]Cl Complexes At 308K.

Decrease in adiabatic compressibility in [Ni (lev) (1, 10-phenanthroline)] Cl might be due to close association between water molecules i.e. solvent-solvent interaction and also electrostriction. The increase in β values for [Ni (lev) 2(H2O) 2]2H2O complex with increase in concentration of solution may be due to molecular association or repulsion calculated from the measured ultrasonic velocity (U) and density (d).
collection of water molecules around ions. This implies significant solute-solvent interaction in [Ni (levo)2(H2O)2]2H2O.

The value of acoustic impedance (Z) decreased with increase in concentration for both the complexes in water. When concentration of solute increases, the thickness of oppositely charged ionic atmosphere may increase due to decrease in ionic strength. This is suggested by decrease in acoustic impedance with increase in concentration in both the systems investigated.

It was found that intermolecular free length increased on increasing the concentration of [Ni (levo)2(H2O)2]2H2O and decreased in [Ni (levo) (1, 10-phenanthroline)]Cl. The increase in Lf values was due to greater force of interaction between complex and water molecule by forming hydrogen bonding.

The hydration number was increasing with increase in concentration due to strong solute-solvent interaction. There was regular increase in hydration number with increase in concentration in case of [Ni (levo) (1, 10-phenanthroline)]Cl which indicates the increase in size of secondary layer of hydration i.e. the solvent molecules forms strong co-ordination bond in primary layer. The hydration number in primary layer corresponds to co-ordination number and it is concentration independent. But the hydration number in secondary layer is concentration dependent. So increase in hydration with concentration indicated that water molecules are strongly attached in secondary layer.

Table 2: The Values of Concentration, Apparent Molar Volume (V p).

<table>
<thead>
<tr>
<th>Concentration (c) mol dm⁻³</th>
<th>Apparent molar volume (V p) x 10⁻³ m³ mol⁻¹</th>
<th>Limiting apparent molar volume (V p) x 10⁻³ m³ mol⁻¹</th>
<th>S l m² kg⁻¹ mol⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Ni(levo)2(H2O)2]2H2O</td>
<td>0.0099 0.6803</td>
<td>0.6874</td>
<td>0.6083</td>
</tr>
<tr>
<td>[Ni(levo)(1,10-phenanthroline)]Cl</td>
<td>0.0291 0.7530</td>
<td>0.578</td>
<td>0.3443</td>
</tr>
<tr>
<td>[Ni(levo)(1,10-phenanthroline)]Cl</td>
<td>0.0385 0.8285</td>
<td>0.8654</td>
<td>0.6083</td>
</tr>
<tr>
<td>[Ni(levo)(1,10-phenanthroline)]Cl</td>
<td>0.0477 0.8654</td>
<td>0.6083</td>
<td>0.3443</td>
</tr>
</tbody>
</table>

From Table 2 it was observed that apparent molar volume increased with concentration in both systems indicating the existence of solute-solvent interaction. The value of limiting apparent molar volume and experimental slope were positive in both systems shown by Figure 3.

It indicates the ion-dipolar interaction in both aqueous solutions. The lower positive value of S l in [Ni (levo) (1, 10-phenanthroline)]Cl indicated strong solute-solvent interaction.

Table 3: The Values of Concentration, Apparent Molar Compressibility (K p), Limiting Apparent Molar Compressibility (K p) and Experimental Slope (S l) of [Ni(levo)2(H2O)2]2H2O and [Ni(levo)(1,10-phenanthroline)]Cl Complexes In Water At 308K.

<table>
<thead>
<tr>
<th>Concentration (c) mol dm⁻³</th>
<th>Apparent molar compressibility (K p) x 10⁻¹ m² mol⁻¹</th>
<th>Limiting apparent molar compressibility (K p) x 10⁻¹ m² mol⁻¹</th>
<th>S l m² kg⁻¹ mol⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Ni(levo)2(H2O)2]2H2O</td>
<td>0.0099 1.9801</td>
<td>0.0196 2.3523</td>
<td>0.0291 2.7682 1.832 0.6248</td>
</tr>
<tr>
<td>[Ni(levo)(1,10-phenanthroline)]Cl</td>
<td>0.0385 3.0297</td>
<td>0.0477 3.4035</td>
<td>0.0197 1.8621</td>
</tr>
<tr>
<td>[Ni(levo)(1,10-phenanthroline)]Cl</td>
<td>0.0481 2.5901</td>
<td>0.0284 2.1233</td>
<td>0.0388 2.3381</td>
</tr>
<tr>
<td>[Ni(levo)(1,10-phenanthroline)]Cl</td>
<td>0.0643 3.4301</td>
<td>0.0980 3.5301</td>
<td>0.0841 2.5901</td>
</tr>
</tbody>
</table>

The value of apparent molar compressibility (K p) was increased with increase in concentration in both systems shown Table 3. It shows strong electrostatic attractive force in the vicinity of ions. It may be concluded that strong molecular association was found in [Ni (levo)2(H2O)2]2H2O with higher positive K p values.

![Fig. 3: Variation of Apparent Molar Volume (V p) with C²/³ for [Ni(levo)2(H2O)2]2H2O and [Ni(levo)(1,10-phenanthroline)]Cl Complexes At 308K.](image)

![Fig. 4: Variation of Apparent Molar Compressibility (K p) with C²/³ For [Ni(levo)2(H2O)2]2H2O and [Ni(levo)(1,10-phenanthroline)]Cl Complexes 308K.](image)

The value of K p and S l were obtained in Figure 4. The higher positive K p and S l value also indicates strong solute-solute interaction. The solute-solvent interaction is enhanced with chelation.

4. Conclusion:

Acoustical and volumetric properties of aqueous solutions of [Ni (levo)2(H2O)2]2H2O and [Ni (levo) (1, 10-phenanthroline)]Cl at 308K was studied. From the experimental data solute-solvent and solute-solute interaction were studied. It was concluded that there was weak solute-solvent interaction in [Ni (levo)2(H2O)2]2H2O system and strong solute-solvent interaction in [Ni (levo) (1, 10-phenanthroline)]Cl system.
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References


