ACOUSTICAL STUDIES OF SOME PYRAZOLE DERIVATIVES IN DMF AND DMSO SOLUTIONS AT 298.15 K

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ABSTRACT

The density and ultrasonic velocity of some pyrazole derivatives have been studied in dimethyl formamide and dimethyl sulphoxide solutions at 298.15 K. From the experimental data, some acoustical parameters have been evaluated to understand the molecular interaction occurring in these solutions.

Keywords: Pyrazole derivatives, DMF, DMSO, acoustical parameters.

INTRODUCTION

Ultrasonic technology is known to have various applications in various fields (Zell et al., 2007; Datt et al., 2016) such as food (Rani et al., 2012), chemical (Levina et al., 2000; Pelegrinis et al., 2016), water treatment (Doosti et al., 2012), medicine (Sifras and Hirut, 2011) etc. Further, ultrasonic velocity measurements have been used in investigating various pure liquids (Gardas and Coutinho, 2008; Surayanarayana and Kuppusami, 1976), their mixtures (Naik and Bawankar 2016; Gutta, 2013; Dubey et al., 2009; Prasad et al., 2006) and solutions (Laux et al., 2009; Bhardwaj et al., 2014; Li et al., 2016) to study molecular interactions. Acoustical parameters obtained by density, viscosity and ultrasonic speed provide information about the nature and strength of these molecular interactions (Pandey et al., 1994; Chauhan et al., 2013). It also gives information about bonding between molecules and formation of complex at different temperatures through various interactions.

In continuation of our previous work (Baluja et al., 2008; Bhesaniya and Baluja, 2014; Baluja and Talaviya, 2015), in the present work, some new pyrazole derivatives have been synthesized and their density and sound velocity were measured in N, N, dimethylformamide and dimethyl sulfoxide solutions at 298.15 K. From these experimental data, some acoustical parameters such as isentropic compressibility ($\kappa_s$), intermolecular free length ($L_f$) and solvation number ($S_n$) have been evaluated in order to study molecular interactions in solutions.
EXPERIMENTAL
The solvents dimethyl formamide (DMF) and dimethyl sulfoxide (DMSO) used in present study were purified by standard method (Riddick et al., 1986).

The pyrazole derivatives have been synthesized in our laboratory and were purified by crystallization in ethanol. The structures of these compounds were confirmed by IR, NMR and mass spectral data. Figure 1 shows the structure of these compounds. The physical constants of these compounds are given in Table 1.

Apparatus and Procedure
Solutions of different concentrations (0.01 to 0.1M) were prepared in DMF and DMSO for the synthesized compounds and were kept at desired temperatures in air tight bottles. An electrical balance (Mettler Toledo AB204-S) with an accuracy of ±0.1 mg was used for the preparation of solutions.

Measurements of Density, and Ultrasound velocity
Ultrasonic velocity and density measurements of pure solvents and solutions of compounds have been done by using Anton Paar Density and Sound Velocity meter (DSC 5000M) with accuracy of ±0.5 m/s and ±0.000005 g/cm$^3$ respectively. The instrument was fully automated and the temperature was automatically controlled. Calibration was carried out using Milli-Q-water (Millipore Pvt. Ltd. Bangalore, India).

RESULTS AND DISCUSSION
The experimental data of density and ultrasonic velocity of pure solvents and solutions are reported in Table 2. Figure 2 shows the variation of ultrasonic velocity with concentration. It is observed from Table 2 and Figure 2 that velocity increases with concentration in both DMF and DMSO solutions for both the compounds.

From the experimental data of density and velocity, some acoustical parameters such as intermolecular free path length ($L_f$), isentropic compressibility ($\kappa_S$) and solvation number have been evaluated by equations reported earlier (Bhesaniya et al., 2014).

The variation of intermolecular free path length ($L_f$) and isentropic compressibility ($\kappa_S$) with concentration is shown in Figures 3 and 4 respectively. It is observed that both intermolecular free path length ($L_f$) and isentropic compressibility ($\kappa_S$) decrease with concentration. This might be due to the aggregation of solvent molecules around solute molecules, indicating there by the presence of solute-solvent interaction for both compounds in both the solvents DMF and DMSO. Thus, there exists strong interaction between solvent and compound molecules in both the solvents DMF and DMSO.

This is further confirmed by solvation number. The solvation number ($S_n$) is a measure of structure forming or structure breaking tendency of a solute in solutions. Figure 5 shows the variation of solvation number with concentration. For both the compounds, $S_n$ values increases with concentration in both the solvents and the values are positive. The positive value of solvation number suggests structure forming tendency of these compounds in both the solvents. Further, as concentration increases, structure forming tendency is found to increase.
Thus, it is concluded that solute solvent interactions exist for both the studies compounds in both the solvents.

REFERENCES


Figure 1: Structure of pyrazole derivatives

![Structure of pyrazole derivatives](image)

SF-1

SF-2

Table 1: Physical constants of pyrazole derivatives.

<table>
<thead>
<tr>
<th>Compound code</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
<th>M.P. °C</th>
<th>% yield</th>
<th>Rf value</th>
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<tr>
<td>SF-1</td>
<td>C_{22}H_{17}N_{4}SCl</td>
<td>404.5</td>
<td>142</td>
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<td>SF-2</td>
<td>C_{22}H_{17}N_{4}SF</td>
<td>388</td>
<td>148</td>
<td>65</td>
<td>0.76</td>
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Table 2: The density and ultrasonic velocity of SF-1 and SF-2 in both the solvents at 298.15 K.

<table>
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<tr>
<th>Conc. M</th>
<th>Density gm/cm$^3$</th>
<th>Ultrasonic velocity m/sec</th>
<th>Density gm/cm$^3$</th>
<th>Ultrasonic velocity m/sec</th>
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<tr>
<td></td>
<td>SF-1</td>
<td></td>
<td>SF-2</td>
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<tr>
<td></td>
<td>DMF</td>
<td></td>
<td>DMSO</td>
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<tr>
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Figure 2: The variation of ultrasonic velocity with concentration for [A] SF-I and [B] SF-II in DMF and DMSO at 298.15 K.
Figure 3: The variation of intermolecular free path length (L_f) with concentration for [A] SF-I and [B] SF-II in DMF and DMSO at 298.15K.
Figure 4: The variation of isentropic compressibility ($\kappa_s$) with concentration for [A] SF-I and [B] SF-II in DMF and DMSO at 298.15.
Figure 5: The plot of salvation number ($S_n$) with concentration for [A] SF-I and [B] SF-2 in DMF and DMSO at 298.15K.
Solvation number vs Concentration (M)