Acoustic Studies of Schiff Base N[1]-((5-Methylfuran–2-Yl) Methylene)-5- Nitrobenzene -1, 2–Diamine In 90% DMSO–Water Solvent at Different Temperatures

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***Abstract*—Ultrasonic studies provide valuable information into molecular interactions in solution. In the present work, density (ρ), ultrasonic velocity (U), and related acoustic parameters of a Schiff base compound N[1]-((5-methylfuran–2-yl) methylene)-5- nitrobenzene -1,2–diamine have been measured in 90% binary DMSO–water solvent at different concentrations (0.000625–0.01 mol·Kg⁻¹) and temperatures ranging from 298.15 K to 318.15 K. From the experimental data, adiabatic compressibility (βs), apparent molal volume (ΦV), apparent molal compressibility (ΦK), intermolecular free length (Lf), relative association (RA), and acoustic impedance (Z) were evaluated. The observed decrease in ultrasonic velocity and acoustic impedance with increasing temperature, along with the increase in adiabatic compressibility and intermolecular free length, indicates weakening of solute–solvent interactions at higher temperatures. Negative values of apparent molal compressibility and the concentration dependence of apparent molal volume suggest strong ion–dipole and hydrogen bonding interactions between Schiff base and the solvent mixture at lower temperatures. The results reveal that solute–solvent interactions dominate over solute–solute interactions, confirming the structure-making nature of Schiff base in 90% DMSO–water solvent.**

***Index Terms*—N[1]-((5-methylfuran–2-yl) methylene)-5-nitrobenzene -1,2–diamine; Ultrasonic velocity; Apparent molal volume; Adiabatic compressibility; 90% DMSO–water mixture; Solute–solvent interaction.**

I. INTRODUCTION

Schiff base name after Hugo Schiff, a German chemist who first prepared it in 1864 by reacting an aldehyde with an amine in the presence of an acid catalyst. Imines, known even as azomethines or Schiff bases are compounds that are represented by the general formula $R_3R_2C=NR_1$, involves the formation of an imine functional group (-C=N-) by the condensation of the carbonyl group of the aldehyde with the amino group of the amine[1].

Structural variation in Schiff base allows the researcher to explore its potential application. This is evident from the number of reviews published on the synthesis, structure and application of Schiff base [2-3].

The imine group (CH=N) of Schiff base is a key structural part which is found in various natural compounds of biological significance. Schiff bases show prominent biological activities such as anti-inflammatory[4], antimicrobial [5] and antiproliferative [6] properties.

Schiff bases are biologically useful compounds.[7-8] Enhanced antimicrobial,[9-11,] and antifungal [12-13] activities are shown by metal complexes as compared to their free ligands. Schiff base metal complexes are used as an antioxidant,[14-15] in dye-sensitized solar cells,[16] cancer diagnosis, and therapy,[17] anticancer,[18]and antiviral agents.[19]

Ultrasonic techniques are well-established tools for investigating intermolecular interactions in liquid mixtures. Measurements of ultrasonic velocity and density enable the evaluation of various acoustic and thermodynamic parameters such as adiabatic compressibility[20], apparent molal volume, intermolecular free length[21], and acoustic impedance. These parameters are highly sensitive to changes in molecular association, hydrogen bonding, and structural rearrangements in solution.

Dimethyl sulphoxide (DMSO) is a strongly polar aprotic solvent with high dielectric constant and excellent solvating ability. When mixed with water, it forms complex hydrogen-bonded networks. The presence of Schiff base molecules in DMSO–water mixtures can significantly alter these networks through solute–solvent interactions. However, systematic acoustic studies of Schiff bases in DMSO–water systems are limited.

The present study aims to evaluate the effect of concentration and temperature on the acoustic of Schiff base in 90% DMSO–water solvent, and to elucidate the nature of molecular interactions present in the system.

II. MATERIALS AND METHODS

The Schiff base compound N[1]-((5-methylfuran–2-yl) methylene)-5- nitrobenzene -1, 2–diamine was synthesized and purified by standard recrystallization techniques.[22] Analytical grade dimethyl sulphoxide (DMSO) and double-distilled water were used for preparing the solvent mixture (90% DMSO–water).

Solution Preparation:

Solutions of Schiff base were prepared at concentrations ranging from 0.000625 to 0.01 mol·kg^{-1} using the 90% DMSO–water solvent mixture. All solutions were freshly prepared prior to measurements.

Experimental Measurements:

Density of the solutions was measured using a calibrated specific gravity bottle. Ultrasonic velocity was measured using a single-frequency digital ultrasonic interferometer (f 05) operating at 2 MHz. Temperature was maintained at 298.15, 303.15, 308.15, 313.15, and 318.15 K using a thermostatically controlled water bath.

III. RESULT AND DISCUSSION

The density of the solution decreases slightly with increasing temperature at all concentrations, indicating thermal expansion of the solvent system. Ultrasonic velocity decreases both with decreasing concentration and increasing temperature.[23-24] This behaviour suggests reduced cohesive forces and weakening of intermolecular interactions at elevated temperatures.[25-26] Adiabatic compressibility increases with temperature and dilution, while intermolecular free length shows a corresponding increase. This inverse relationship between ultrasonic velocity and compressibility confirms that molecular packing becomes looser at higher temperatures. The increase in Lf indicates a reduction in solvent structure due to thermal agitation.

The apparent molal volume values are positive at higher concentrations and tend to become negative at very low concentrations. This behaviour suggests strong solute–solvent interactions at lower concentrations, where solvent molecules surround the solute more effectively, leading to electrostriction and volume contraction.

Table -1. Acoustic parameters of N[1]-((5-methylfuran–2-yl) methylene)-5- nitrobenzene -1,2–diamine.

Temperature (ºK)	Concentration (M) Mole Fraction	Density of Solution (ds) Kgm^{-3}	Ultrasonic Velocity of Solution (Us)M Sec^{-1}	Adiabatic Compressibility (βs x 10^{-10}) N/m2 or Pa-1	Apparent Molal Volume (ΦV) m^3 mol^{-1}	Apparent Molal Compressibility (ΦK X 10^{-10}) m3 mol-1 Pa-1	Intermolecular Free Length (Lf x 10^{-11}) M	Relative Association	Acoustic impedance (Z x 104) Kg m-2 S-1
298.15	0.01	1096.72	1570.975	2.5793	0.000194	-1.0369	3.3033	0.99946	172.2919
	0.005	1096.7	1569.949	2.5844	0.000168	-2.0645	3.3065	0.99966	172.1763
	0.0025	1096.68	1568.924	2.5894	0.000118	-4.1102	3.3098	0.99986	172.0607
	0.00125	1096.66	1568	2.594	0.000025	-8.1867	3.3127	1.00004	171.9563
	0.000625	1096.64	1567.077	2.5986	-0.000149	-16.3057	3.3156	1.00022	171.852

303.15	0.01	1091.88	1552.206	2.674	0.000193	-1.058	3.3941	0.99925	169.4822
	0.005	1091.86	1551.18	2.6793	0.000165	-2.1062	3.3974	0.99945	169.3671
	0.0025	1091.84	1550.154	2.6846	0.000111	-4.1928	3.4008	0.99965	169.252
	0.00125	1091.82	1549.231	2.6894	0.00001	-8.3499	3.4038	0.99983	169.1482
	0.000625	1091.8	1548.206	2.6948	-0.000179	-16.6207	3.4072	1.00004	169.0331
308.15	0.01	1086.88	1538.118	2.7481	0.000192	-1.0755	3.4719	0.9993	167.175
	0.005	1086.86	1537.059	2.7538	0.000162	-2.1404	3.4755	0.99951	167.0568
	0.0025	1086.84	1536.236	2.7583	0.000104	-4.2643	3.4783	0.99967	166.9642
	0.00125	1086.82	1535.177	2.764	-0.000005	-8.4862	3.4819	0.99988	166.8461
	0.000625	1086.8	1534	2.7703	-0.000208	-16.878	3.4859	1.00012	166.7152
313.15	0.01	1082.06	1527.18	2.8076	0.000191	-1.094	3.5407	0.99932	165.25
	0.005	1082.04	1526.154	2.8133	0.000159	-2.0726	3.5442	1.00191	165.136
	0.0025	1082.02	1525.231	2.8184	0.000097	-4.1261	3.5474	1.00209	165.0331
	0.00125	1082	1524.103	2.8247	-0.00002	-8.2055	3.5514	1.00232	164.9079
	0.000625	1081.98	1523.18	2.8298	-0.000239	-16.3342	3.5546	1.0025	164.805
318.15	0.01	1076.98	1520.513	2.8447	0.00019	-1.1136	3.5956	0.9994	163.7562
	0.005	1076.96	1519.488	2.8505	0.000156	-2.2164	3.5992	0.99961	163.6427
	0.0025	1076.94	1518.565	2.8557	0.00009	-4.4133	3.6025	0.99979	163.5403
	0.00125	1076.92	1517.436	2.862	-0.000035	-8.7788	3.6065	1.00002	163.4158
	0.000625	1076.9	1516.513	2.8673	-0.00027	-17.479	3.6098	1.0002	163.3133

The negative values of ΦK across all temperatures indicate the dominance of solute–solvent interactions over solute–solute interactions. The magnitude of negativity decreases with increasing temperature, implying weakening of these interactions due to thermal disruption of hydrogen bonds.

Relative association values remain close to unity, indicating moderate association between solute and solvent molecules. Acoustic impedance decreases with increasing temperature[24], consistent with the observed decrease in density and ultrasonic velocity, further supporting reduced intermolecular cohesion.

Overall, the acoustic parameters clearly indicate that Schiff base behaves as a structure-making solute in 90% DMSO–water at lower temperatures and higher concentrations.

IV. CONCLUSION

The ultrasonic studies of Schiff base in 90% DMSO–water solvent reveal significant solute–solvent interactions influenced by both concentration and temperature. Decreasing ultrasonic velocity and acoustic impedance with increasing temperature indicate weakening molecular interactions. Negative apparent molal compressibility values confirm strong solvation effects and hydrogen bonding between Schiff base and the solvent mixture. The study demonstrates that acoustic methods are effective in probing molecular interactions in Schiff base systems and provides valuable insight into the solution behaviour of Schiff base in mixed solvents.

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