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Thermo Acoustical Study of 7-Hydroxy-4-Phenyl-2H-Chromen-2-One in Acetone-Water, DMF-Water and DMSO-Water at 308.15K

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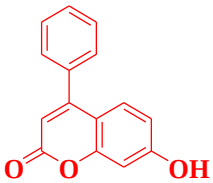
ABSTRACT

Due to the vast pharmacological activity of Coumarins derivatives the viscosity, ultrasonic velocity and density of 7-hydroxy-4-phenyl-2H-chromen-2-one has been measured in 70:30 (v/v) Acetone–water, 70:30 (v/v) DMF-water and 70:30 (v/v) DMSO-water with different concentration of 7-hydroxy-4-phenyl-2H-chromen-2-one at temperature 308.15K.To know the various interaction the various thermo acoustical parameter like free volume, isentropic compressibility, Relative association, acoustic impedance are calculated from experimental data of ultrasonic velocity, viscosity, and densities. The changes in values of this parameter with change concentration of solute represent the different types of interaction such as solute-solvent interaction, solvent-solvent and dipole-dipole interactions present in the solutions.

Keyword: 7-hydroxy-4-phenyl-2H-chromen-2-one, Acetone, DMF, DMSO, thermo acoustical parameter.

I. INTRODUCTION

Coumarins and chromones are ubiquitous and have relevant pharmacological activities such as anti-inflammatory, antioxidant, cardio protective, and antimicrobial properties[1,2]. The majority of the large numbers of drugs being introduced in pharmacopeias every year are heterocyclic compounds.



7-hydroxy-4-phenyl-2*H*-chromen-2-one

The knowledge of viscosities, densities, ultrasonic velocities, and various acoustical parameters are useful for the studies of thermo acoustical properties of a system. The study of molecular interaction in liquid gives valuable information about the internal structure, molecular association, complex formation, internal pressure.

The studies of the solution properties of a liquid solution of polar and non-polar components have great applications in industrial and technological process[3]. The literature survey[4, 5,6]. Reveals the many researchers give attention to the study of ultrasonic velocity measurement and the study of acoustical properties.

II. MATERIALS AND METHODS

The solvents i.e. Acetone, DMF, and DMSO used in this investigation were of AR grade and use without purification (Sigma-Aldrich 99% purity). The compound 7-hydroxy-4-phenyl-2H-chromen-2 one synthesize by known method[7]. The ultrasonic velocities of Coumarins derivative solutions of different concentrations were measured by ultrasonic interferometer (Mittal enterprises, model F-81s) at 2 MHz having accuracy ±1 m·s–1 in velocity. The densities and Viscosity of experimental solutions were measures by using digital density meter (Anton Paar DMA 35 of accuracy ± 0.001) and Ostwald's viscometer.

III. THEORY

Given acoustical parameters are calculated by using various equations.

Ultrasonic velocity $(u) = v\lambda$ ..... *(1)*

Where, U is the ultrasonic velocity, λ is the wavelength.

Isentropic compressibility $(\beta s) = 1/\rho u^2$ ..... *(2)*

Where, ρ is density, u is the speed of sound.

Intermolecular free length $(Lf) = K \beta s 1/2$ ..... *(3)*

Where, K-is the temperature-dependent constant called Jacobson constant[8]and is equal to 2.095×10^{-6}.

Acoustic impedance $(Z) = u\rho$ ..... *(4)*

Where, u-ultrasonic velocity, ρ- density.

Relative association $(R_A) = (\rho/\rho_o)\ (u_o/u)\ 1/3$ ..... *(5)*

Where, $\rho_\circ$ ρ are the densities and u_0 u are the ultrasonic velocities of the solvent and the solution.

IV. RESULTS AND DISCUSSION

The experimentally determined values of density(ρ) and ultrasonic velocities (u) and viscosity (η) for 7-hydroxy-4-phenyl-2H-chromen-2-one- 70% Acetone, 7-hydroxy-4-phenyl-2H-chromen-2-one-70% DMF and 7-hydroxy-4-phenyl-2H-chromen-2-one-70% DMSO solutions measured at 318.5K are given in Table 1.From fig 1 it is observed that ultrasonic velocity (u) increases with an increase in the concentration of 7-hydroxy-4-phenyl-2H-chromen-2-one at a constant temperature, also fig 2 and 3 indicates an increase of density (ρ) and viscosity (η) with an increase in the concentration of solute at a constant temperature. An increase in concentration allows for a closer approach of solvent and solute molecules and a stronger association between solute and solvent molecules. This leads to a decrease in the volume and an increase in the density of the solution[9]. The increased values of viscosity (η) and ultrasonic velocity (u) indicates molecular association in the experimental systems, which is possible due to the presence of hydroxyl group solute structure, it is notable that molecular interactions are less at lower values of velocities[10]. It may be due to breaking of molecular clusters, presence of dipole-dipole interaction, solute-solvent interactions, solvent- solvent interactions, and presence of hydrogen bonding between the solute molecule and water molecule solvents.

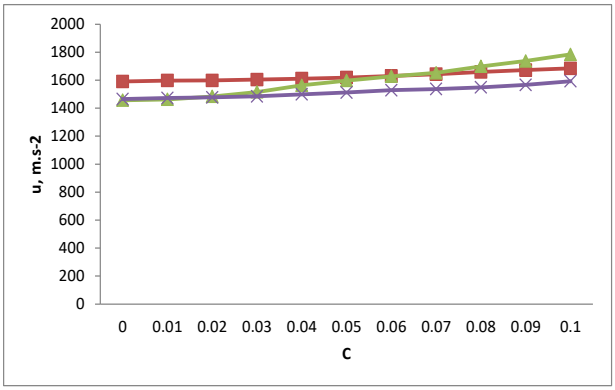


Figure1. Ultrasonic velocity (u) plotted against concentration of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone (■),7-hydroxy-4-phenyl-2H-chromen-2one – 70% DMF (▲) and 7-hydroxy-4-phenyl-2H-chromen-2one – DMSO (×), at 308.15K

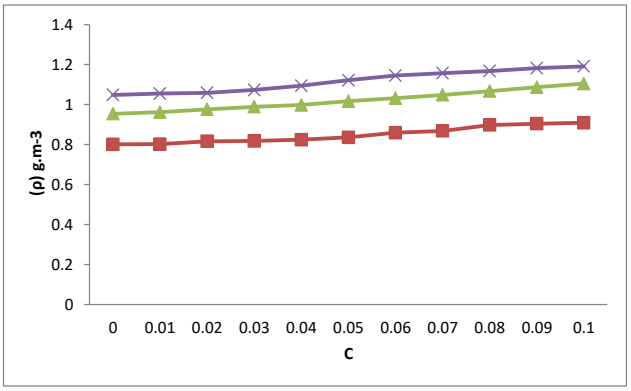


Figure2. Density (ρ) plotted against concentration of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone (■),7-hydroxy-4-phenyl-2H-chromen-2one– 70% DMF (▲) and 7-hydroxy-4-phenyl-2H-chromen-2one –DMSO (×), at 308.15K.

Table 1. Experimental values of ultrasonic velocity, density and viscosity of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone, 7-hydroxy-4-phenyl-2H-chromen-2one – 70% m DMF and 7-hydroxy-4-phenyl-2H-chromen-2one – DMSO solutions at temperatures 308.15K.

C	u, $m.s^{-2}$			(ρ) $kg.m^{-3}$			(η) 10^{-3} $N.s.m^{-2}$		
	7O% Ac+L	70% DMF+L	70% DMSO+ L	7O% Ac+L	70% DMF+L	70% DMSO+L	7O% Ac+L	70% DMF+L	70% DMSO +L
0	1590.1	1456.2	1464.5	0.801	0.954	1.048	1.185	1.643	1.822
0.01	1596.9	1462.3	1472.2	0.802	0.962	1.055	1.311	1.658	1.841
0.02	1598.3	1483.7	1476.9	0.816	0.976	1.059	1.352	1.678	1.852
0.03	1604.4	1515.6	1484.3	0.818	0.989	1.073	1.417	1.695	1.867
0.04	1610.5	1563.1	1498.6	0.824	0.998	1.094	1.483	1.724	1.876
0.05	1618.6	1596.9	1512.1	0.836	1.017	1.122	1.523	1.738	1.882
0.06	1630.1	1627.2	1528.5	0.859	1.032	1.145	1.585	1.756	1.896
0.07	1642.7	1652.8	1536.7	0.868	1.048	1.157	1.603	1.764	1.907
0.08	1658.3	1698.4	1548.6	0.898	1.067	1.168	1.762	1.789	1.923
0.09	1672.1	1736.8	1566.4	0.904	1.087	1.182	1.819	1.802	1.945
0.1	1684.6	1784.3	1592.8	0.909	1.105	1.191	1.898	1.835	1.961

Table 2. Isentropic compressibility, linear free length, acoustic impedance, relative free length, sound velocity number, free volume, relaxation time and available volume of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone, 7-hydroxy-4-phenyl-2H-chromen-2one-70% DMF and 7-hydroxy-4-phenyl-2H-chromen-2one-DMSO solutions at different concentration and at temperature 308.15K.

C	βs	Lf,	Z	R_A

	10^{-10}, $m^2.N^{-1}$	A^0	10^{-3} $kg.m^2s^1$	
70%Acetone+7-hydroxy-4-phenyl-2H-chromen 2one				
0	3.955	4.1425	1273.67	-
0.01	3.9214	4.1248	1280.873	1.014149
0.02	3.9145	4.1212	1304.373	1.034568
0.03	3.8848	4.1055	1313.041	1.049024
0.04	3.8554	4.09	1328.179	1.068818
0.05	3.8169	4.0695	1353.473	1.100827
0.06	3.7633	4.0408	1400.582	1.155394
0.07	3.7058	4.0098	1427.013	1.194782
0.08	3.6364	3.9721	1490.148	1.271627
0.09	3.5766	3.9393	1506.395	1.312349
0.1	3.5237	3.9101	1532.649	1.349424
70% NNDMF+7-hydroxy-4-phenyl-2Hchromen2one				
0	4.9432	4.6312	1389.215	
0.01	4.8612	4.5926	1406.733	1.021111
0.02	4.6543	4.4938	1448.091	1.082123
0.03	4.4018	4.3702	1498.928	1.168796
0.04	4.101	4.2182	1559.974	1.293836
0.05	3.8558	4.0902	1624.047	1.405862
0.06	3.6596	3.9848	1679.27	1.509354
0.07	3.493	3.893	1732.134	1.606241
0.08	3.249	3.7546	1812.193	1.774487
0.09	3.0498	3.6376	1887.902	1.933159
0.1	2.8425	3.5118	1971.652	2.130858

70% DMSO+7-hydroxy-4-phenyl-2H-chromen-2one				
0	4.4489	4.3935	1534.796	
0.01	4.3733	4.356	1553.171	1.022642
0.02	4.3291	4.3339	1564.037	1.036382
0.03	4.2301	4.2841	1592.654	1.065946
0.04	4.0701	4.2023	1639.468	1.118523
0.05	3.898	4.1125	1696.576	1.178433
0.06	3.7382	4.0273	1750.133	1.242145
0.07	3.66	3.985	1777.962	1.275473
0.08	3.57	3.9357	1808.765	1.317744
0.09	3.448	3.8678	1851.485	1.380054

Uncertainties in isentropic compressibility (βs) 0.01×10^{-10}, $m^2.N^{-1}$, Linear free length (L_F) $0.001A_0$, Acoustic impedance (z) velocity 1×10^{-3}, $kg.m^2$,Relative association (R_A) 0.010.

From fig 4 and table 2 it is found that isentropic compressibility (βs) decreases with an increase in the concentration of solution it is since surrounded molecules experience electrostatic field[11]. These decrease values of compressibility indicate that there is an increase in molecular association with an increase in solute concentration, as new species form due to the molecular association become compact and less compressible. These also suggest that the compressibility of the solvent is greater than that of the solution. The increase in isentropic compressibility also indicates a change in the conformation orientation of the solute molecules in solution, leading to weaker inter-molecular interaction. This is attributed to the steric requirement of arranging an increasing number of large molecules. In this situation, the steric factor takes predominance over intermolecular interactions. An increase in isentropic compressibility indicates a change in the orientation of the solvent molecules.

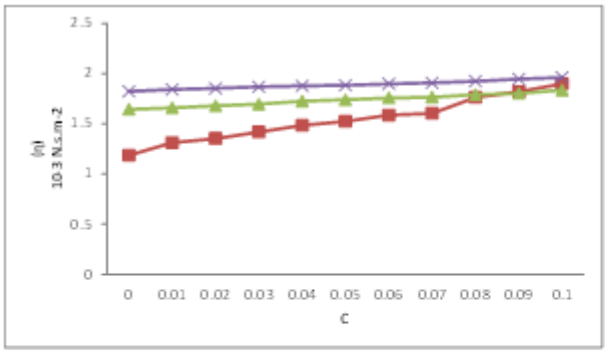


Figure 3. Viscosity (η) plotted against concentration of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone (■),7-hydroxy-4-phenyl-2H-chromen-2one – 70% DMF (▲) and 7-hydroxy-4-phenyl-2H-chromen-2one –DMSO (×),at 308.15K.

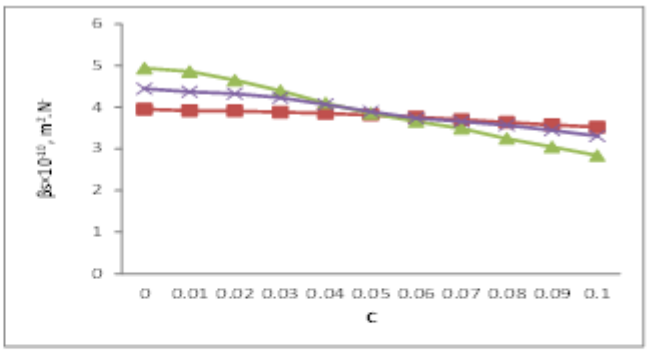


Figure 4. Isentropic compressibility (βs) plotted against concentration of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone (■),7-hydroxy-4-phenyl-2H-chromen-2one – 70% DMF (▲) and 7-hydroxy-4-phenyl-2H-chromen-2one –DMSO (×), at 308.15K.

The decreasing value of intermolecular free length (Lf) indicates closer packing[12] which is evident from fig 5. The intermolecular free length on the mixing of solute to the solvent is responsible for the variation of the ultrasonic velocity of the same solution. Based on a model for sound propagation given by Trying and Kincaid[13] free length decreases with an increase of ultrasonic velocity. Variation in free length indicates variation in the molecular forces in the mixture, which depends on the experimental density as well as the temperature of the mixture. Intermolecular free length (Lf) is the distance between the surfaces of the neighboring molecules and indicates a significant interaction between solute–solvent as well as dipole-dipole interaction[14] in 7-hydroxy-4-phenyl-2H-chromen-2-one-70%Acetone,7-hydroxy-4-phenyl-2H-chromen-2-one-70%NNDMF and 7-hydroxy-4-phenyl-2H-chromen-2-one-70% DMSO solutions[15].

When the ultrasonic wave propagates through a solution, some parts of it moves through the medium, and the remaining part of the ultrasonic wave gets reflected by the solute[16] it indicates that solutes will restrict the free flow of an ultrasonic wave. The property that decreases this shortening or astern movement of ultrasonic waves is known as acoustic impedance (Z). The specific acoustic impedance is dependent on both the concentration and temperature of the solution. As the internal pressure and cohesive energy[17] increases with solute concentration, strong dipole-dipole and solute-solvent interaction occur between 7-hydroxy-4-phenyl-2H-chromen-2-one which is solute Acetone, DMF, and DMSO which are solvents which is evident from fig 6. Hence, an increase in specific acoustic impedance is due to a rise in instantaneous pressure occurs on any

molecule in the given experimental system with traveling of a sound wave. The linear variation in acoustic impedance with concentration confirms the presence of a molecular association between the solute-solvent molecules, also increasing trends of impedance further support the possibility of molecular interaction between the solute-solvent.

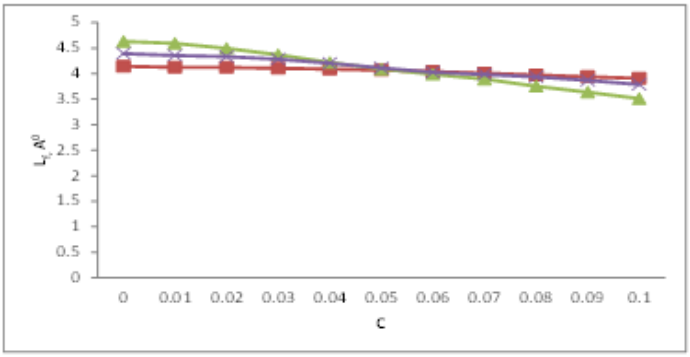


Figure 5. Linear free length (Lf) plotted against concentration of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone (■),7-hydroxy-4-phenyl-2H-chromen-2one – 70% DMF (▲) and 7-hydroxy-4-phenyl-2H-chromen-2one –DMSO (×),at 308.15K.

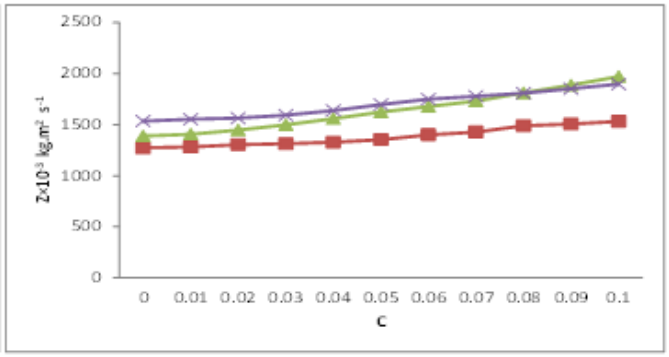


Figure 6. Acoustic impedance (z) plotted against concentration of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone (■),7-hydroxy-4-phenyl-2H-chromen-2one – 70% DMF (▲)and 7-hydroxy-4-phenyl-2H-chromen-2one –DMSO (×), at 308.15.

An increase in relative association (RA) with an increase in the concentration of 7-hydroxy-4-phenyl 2H-chromen-2-one indicates the presence of solute-solvent interaction, solvent-solvent interaction, and hydrogen bonding which is evident from fig 7.

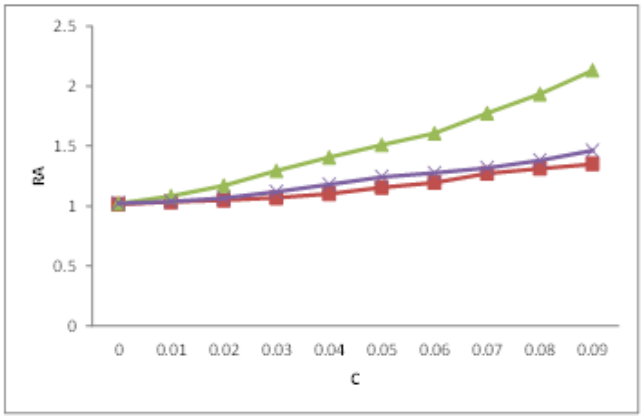


Figure 7. Relative association (RA) plotted against concentration of 7-hydroxy-4-phenyl-2H-chromen-2one -70% Acetone (■),7-hydroxy-4-phenyl-2H-chromen-2one – 70% DMF (▲) and 7-hydroxy-4-phenyl-2H-chromen-2one –DMSO (×), at 308.15K.

V. CONCLUSION

In the present article, the densities, ultrasonic velocities, viscosity, and thermo dynamical parameters at temperatures, 308.15K over the entire range of composition of 7-hydroxy-4-phenyl-2H-chromen-2one in 70% Acetone, 70% DMF and 70% DMSO have been measured. From these measured physical property data, isentropic compressibility, linear free length, acoustic impedance are calculated and used to found the solute-solvent, solvent-solvent interaction, and hydrogen bonding. From the above investigation it is found that 7-hydroxy-4-phenyl-2H-chromen-2one shows interesting interactive behavior with solvents like Acetone, DMF and DMSO.

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