Research Article

Acoustic Parameters of Amino Acids in Aqueous 1-propanol Solutions in Presence of Sodium Benzoate (a hydrotropic agent) at 298.15K.

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ABSTRACT

The acoustical parameters of amino acids have been measured in aqueous 1-propanol solutions, in presence of sodium benzoate at 298.15K. The molar sound velocity (R), molar compressibility (W), free length (L_f), free volume (V_f), internal pressure (π_i), relaxation time (τ), ultrasonic attenuation (α/f^2), and van der Waals constant (b) values have been calculated from the experimental data. These parameters are used to discuss the molecular interactions in the solutions.

Keywords: Acoustical parameters, 1-propanol, amino acids, sodium benzoate, Ultrasonic Velocity, Compressibility.

INTRODUCTION

The measurement of ultrasonic velocity provides qualitative information about the nature and strength of molecular interaction in solutions. The study of solution properties of the solutions consisting of polar and non- polar compounds finds applications in industrial and technical processes. In continuation of our work on determination of acoustic and thermodynamic parameters of the solutions of amino acids in aqueous solutions of hydrotropic agents,[1,2] in the present investigation, we have evaluated the acoustic parameters such as molar sound velocity (R), molar compressibility (W), free length (L_f), free volume (V_f), internal pressure (π_i), relaxation time (τ), ultrasonic attenuation (α/f^2) and van der Waals constant (b) at 298.15K for the solutions of amino acids in water + 1-propanol mixtures, in presence of 0.1M composition of sodium benzoate where the wt% percentage of 1-propanol was varied from 5 to15% with 5% increments. The results are discussed in the light of molecular interactions.

MATERIALS AND METHODS

All chemicals used were of AnalaR grades. Conductivity water (Sp and $\sim 10^{-6}$ Scm^{-1}) was used to prepare solutions of 1-propanol in different wt% and the solutions were used on the same day. The solution of amino acids were prepared on the molal basis and conversion of molality to molarity was done by using the standard expression[3] using the density values of the solutions determined at 298.15K. Solutions were kept for 2 hours in a water thermostat maintained at the required temperature accurate to within ± 0.1K before use for density measurements. Density measurements were done by using a specific gravity bottle (25ml capacity) as described elsewhere[4]. At least five observations were taken and differences in any two readings did not exceed ± 0.02%. An ultrasonic interferometer (model No.F-81, Mittal enterprises, New Delhi) operating at a frequency of 2MHz and overall accuracy of ± 0.5 m/s was used for the velocity measurement at 298.15K only. Viscosity measurements were made by using an Ostwald's Viscometer (25 ml capacity) in a water thermostat whose temperature was controlled to ± 0.05K. The values of viscosity so obtained were accurate to within ± 0.3 x 10^{-3} CP. Amino acids content in the solutions varied over a range of 0.006 to 0.08 mol dm^{-3} in all wt% of 1-propanol solutions in presence of 0.1M composition of sodium benzoate.

Theoretical Aspects

From the ultrasonic velocity (U), density (d), and viscosity (η) data, the following parameters have been calculated.

(1) Molar sound velocity[5] (R): $R = \bar{M} d^{-1} U^{1/3}$ where, $\bar{M}$ is the effective molecular weight ($\bar{M} = \sum m_i x_i$), in which m_i and x_i are the molecular weight and the mole fraction of individual constituents, respectively.

(2) Molar compresibility[6] (W): According to Wada, $W=\bar{M} d^{-1} K_S^{-1/7}$, where, W is a constant called Wada's constant or molecular compressibility which is independent of temperature and pressure.

(3) Intermolecular free length[7] (L_f): It is the distance between the surfaces of the molecules. It can be calculated using insentropic compressibility by Jacobson's empirical relation $L_f = K^I K_s^{1/2}$, where K^I is the Jacobson's constant which is temperature dependent and is obtained from the literature[7].

(4) Free Volume (V_f): Suryanarayan[8] obtained a formula for free volume in terms of the ultrasonic velocity (U) and the viscosity of the liquid (η) as $V_f = (\bar{M}U/K\eta)^{3/2}$ where $\bar{M}$ is the effective molecular weight ($\bar{M}=\sum m_i x_i$), in which m_i and x_i are molecular weight and the mole fraction of the individual constituents, respectively, K is temperature independent constant which is equal to 4.28 x 10^9 for all liquids.

Table 1: (Values of parameters U(ms^{-1}), R($m^{-8/3}$ $S^{-1/3}$), W (N^{-1} m^{-1}), L_f (m), V_f (m^3/mol), π_i (Nm^{-2}), ϒ (s), α/f^2 and b for amino acids in aqueous solutions of 1-propanol in presence of sodium benzoate at 298.15 K.)

c	U	R	W	L_f(m)	$V_f x10^{-8}$	π_i	ϒ (s)	α / f^2	b
mol dm^{-3}	ms^{-1}	$m^{-8/3}$ $s^{-1/3}$	$m^{-1}N^{-1}$	x 10^{-10}	m^3/mol	Nm^{-2}	x 10^{-13}	x 10^{-15}	m^3mol^{-1}
Glycine + 5wt% 1-propanol+.0.1MSB									
0.006	1546.8	0.2116	0.4118	5.2 38	56178	863284.4	7.72	9.1 33	0.19608
0.008	1549.2	0.2118	0.4122	5.2 32	56146	863964.6	7.70	9.032	0.19616
0.02	1554.0	0.2125	0.4128	5.2 30	56118	864862.4	7.68	9.0 06	0.19626
0.04	1558.2	0.2132	0.4139	5.2 26	55399	865143.4	7.64	8.198	0.19698
0.06	1562.0	0.2134	0.4146	5.2 22	55373	866532.2	7.82	8.108	0.19602
0.08	1566.8	0.2142	0.4162	5.2 18	55351	871236.4	7.61	8.098	0.19612
Glycine + 10wt%1-propanol +0.1MSB									
0.006	1570.8	0.2206	0.43 64	6.852	57164	872246.4	8.26	9.224	0.20 424
0.008	1576.0	0.2222	0.43 66	6.846	57122	873126.2	8.24	9.122	0.20 426
0.02	1578.0	0.2226	0.43 68	6.832	57098	874262.4	8.22	9.106	0.20 431
0.04	1584.8	0.2229	0.43 72	6.828	57062	875016.2	8.20	9.087	0.20 436
0.06	1586.0	0.2232	0.43 81	6.822	57032	875112.4	8.18	9.064	0.20 439
0.08	1590.8	0.2238	0.43 93	6.816	57021	875422.4	8.16	9.022	0.20 442
Glycine + 15wt% 1-propanol+0.1MSB									
0.006	1628.8	0.2374	0.4614	7.124	59624	893462.2	8.86	10.126	0.22382
0.008	1632.2	0.2382	0.4616	7.122	59612	893844.6	8.84	10.120	0.22384
0.02	1636.0	0.2386	0.4620	7.118	59596	893896.4	8.82	10.073	0.22396
0.04	1638.8	0.2392	0.4628	7.112	59587	893912.4	8.79	10.062	0.22398
0.06	1642.0	0.2394	0.4634	7.106	59573	893946.4	8.73	10.048	0.22406
0.08	1646.0	0.2398	0.4642	7.102	59564	893984.2	8.70	10.019	0.22421
α -alanine+ 5wt% 1-propanol+0.1MSB									
0.006	1562.8	0.2248	0.4067	5.124	55142	871064.2	7.08	8.639	0.20426
0.008	1568.2	0.2296	0.4069	5.122	55126	871362.4	7.06	8.331	0.20463
0.02	1574.0	0.2332	0.4072	5.118	55104	881112.4	7.02	8.224	0.20468
0.04	1582.0	0.2346	0.4086	5.116	54996	882321.2	6.98	8.168	0.20472
0.06	1586.0	0.2348	0.4163	5.108	54963	883216.4	6.96	8.122	0.20476
0.08	1590.0	0.2353	0.4132	5.106	54952	891012.2	6.89	8.073	0.20482
α-alanine+ 10wt%1-propanol+0.1MSB									
0.006	1592.6	0.2346	0.43 92	6.1 48	56898	893246.2	8.22	9.329	0. 21894
0.008	1596.0	0.2348	0.43 96	6.1 42	56872	894134.4	8.20	9.312	0.21 898
0.02	1600.0	0.2356	0.44 10	6.1 38	56822	895264.2	8.18	9.264	0.21 932
0.04	1604.8	0.2369	0.44 12	6.1 32	56724	896012.4	8.16	9.124	0.21 936
0.06	1612.0	0.2376	0.44 26	6.1 28	56638	896214.6	8.14	9.097	0.21 936
0.08	1622.0	0.2388	0.44 28	6.1 24	56631	896312.2	8.1 2	9.093	0.21 948
α-alanine+ 15wt% 1-propanol+0.1MSB									
0.006	1636.6	0.2492	0.4654	6.998	58824	915464.4	8.96	10.228	0.23228
0.008	1642.0	0.2494	0.4656	6.996	58818	915612.2	8.92	10.222	0.23229
0.02	1646.4	0.2412	0.4663	6.986	58812	915.616.6	8.90	10.218	0.23232
0.04	1652.8	0.2436	0.4674	6.982	58806	915713.2	8.88	10.212	0.23236
0.06	1658.0	0.2444	0.4682	6.980	58796	915814.6	8.86	10.208	0.23238
0.08	1664.8	0.2452	0.4694	6.976	58716	915818.2	8.82	10.202	0.23243
β-alanine+ 5wt% 1-propanol+0.1MSB									
0.006	1604.8	0.23126	0.4208	5.098	54716	897362.1	7.78	9.098	0.21128
0.008	1610.0	0.23169	0.4214	5.096	54711	898460.2	7.76	8.986	0.21144
0.02	1616.8	0.23182	0.4216	5.092	54682	907463.4	7.74	8.972	0.21146
0.04	1624.0	0.23312	0.4220	5.091	54612	917164.2	7.72	8.964	0.21152
0.06	1630.0	0.23420	0.4296	5.088	54606	918264.2	7.70	8.872	0.21156
0.08	1581.0	0.23624	0.4312	5.082	53828	919964.4	7.68	8.864	0.21162
β-alanine+ 10wt% 1-propanol+0.1MSB									
0.006	1622.8	0.2416	0.44 86	5.224	56264	902463.1	8.92	9.826	0.22 402
0.008	1627.0	0.2419	0.44 94	5.220	56262	903216.2	8.90	9.822	0.22 412
0.02	1631.8	0.2432	0.44 98	5.196	56258	904012.4	8.88	9.816	0.22 432
0.04	1636.8	0.2434	0.45 04	5.194	56246	915126.2	8.86	9.801	0.22 448
0.06	1638.0	0.2436	0.4506	5.188	56242	915232.2	8.82	9.796	0.22 462
0.08	1644.2	0.2438	0.45 12	5.182	56238	926124.4	8.80	9.788	0.22 472
β-alanine+ 15wt% 1-propanol+0.1MSB									
0.006	1658.4	0.2532	0.4698	6.824	57928	931234.6	9.64	10.624	0.24342
0.008	1661.6	0.2534	0.4699	6.826	57929	932236.4	9.62	10.622	0.24344
0.02	1664.8	0.2542	0.4712	6.798	57924	932296.4	9.60	10.618	0.24348
0.04	1670.0	0.2556	0.4717	6.786	57922	933216.2	9.56	10.612	0.24352
0.06	1672.8	0.2562	0.4726	6.782	57898	933418.2	9.52	10.608	0.24364
0.08	1676.0	0.2576	0.4728	6.684	57892	934216.4	9.48	10.601	0.24368

(5) Internal Pressure (π_i): According to Suryanarayan[8], internal pressure is given by, $\pi_i = b^I RT (K\eta/U)^{1/2} (d^{2/3}/\bar{M}^{1/6})$, where b^I is the packing factor, which is equal to 1.78 for close packed hexagonal structure and 2 for cubic packing. For many liquids b^I is equal to 2. K^I is a dimensionless constant having a value of 4.28 x 10^9, independent of temperature and nature of liquid.

(6) Relaxation time[8] (τ): $\tau = 4\eta/3dU^2$ where the symbols have their usual meanings.

(7) Ultrasonic Attenuation[9] (α/f^2):

$\alpha/f^2=4\pi^2 \tau /2U$.

(8) van der Waals constant: van der Waals constant (b) also called co-volume in van der Waals equation is given by the formula

$b=\bar{M}/d[1-(RT/\bar{M}U^2)\{1+\bar{M}U^2/3RT)\}^{1/2}-1]$

where R is the gas constant and $\bar{M}$ is the effective molecular weight.

RESULTS AND DISCUSSION

From the measured values of the ultrasonic velocity and density of the solutions of amino acids in aqueous 1-propanol solutions, in presence of 0.1M composition of sodium benzoate the values of the molar sound velocity (R) evaluated by means of eqn.(1) are given in Table 1.

As observed, the molar sound velocity increases with increase in concentration of the solutions of amino acids in all wt% of 1-propanol solutions in presence of sodium benzoate studied. This type of behavior is similar to that observed earlier. It is of interest to note that the acoustic parameters including the sound velocity decrease in the solutions of amino acids in presence of sodium benzoate as follows:

β-Alanine>α-alanine>glycine. It follows that the β-alanine has a greater contribution towards the molecular interactions followed by α-alanine and in turn glycine.

It is known that when a solute dissolves in a solvent some of the solvent molecules are attached to the ions (generated from the solute) because of ion-solvent interactions. Since the solvent molecules are oriented in the ionic field (i.e., electrostatic fields of ions) the solvent molecules are more compactly packed in the primary solvation shell as compared to the packing in the absence of the ions. This is the reason, why the solvent is compressed by the introduction of ions. Thus the electrostatic field of the ions causes compression of the medium giving rise to a phenomenon called electrostriction. Since the solvent molecules are compressed, they do not respond to any further application of pressure. So the solution becomes harder to compress; i.e., the compressibility decreases and internal pressure increases. Hence isentropic compressibility as well as internal pressure describes the molecular arrangement in the liquid medium. The increase in internal pressure π_i due to electronic field of ion is given by eqn(5).

Suryanarayan showed that the free energy of activation, ΔG is almost equal to the cohesive energy, $\pi_i V_m$. Positive values of π_i indicate the presence of some specific interactions between unlike molecules in the components.

Free volume, V_f is the effective volume accessible to the centre of a molecule in a liquid. The structure of a liquid is determined by strong repulsive forces in the liquid with the relatively weak attractive forces providing the internal pressure which held the liquid molecules together.

The free volume seems to be conditional by repulsive forces, whereas the internal pressure is more sensitive to attractive forces. These two factors together uniquely determine the entropy of the system. Thus, the internal pressure, free volume and temperature seem to be thermodynamic variables that describe the liquid system of fixed composition.

It is seen that free volume decreases with increase in concentration of the solutions in case of all amino acids. As observed, the internal pressure changes in a manner opposite to that of free volume. The decrease of V_f (or increase of π_i) indicates the formation of hard and/or tight solvation layer around the ion.

The fractional free volume (V_f/V) is a measure of disorderliness due to increased mobility of the molecules in a liquid. It is observed that mobility decreases with concentration. This implies that the frictional force exerted by different layers of liquid increases with concentration and the wt% of 1-propanol in water. As the frictional force increases, ultrasonic absorption increases. In the present case, ultrasonic absorption or attenuation increases with concentrations of the amino acids contents.

CONCLUSION

From the ultrasonic velocity and density values of the solutions of amino acids in aqueous solutions of 1-propanol; in presence of sodium benzoate the acoustic parameters like molar sound velocity, molar compressibility, free volume, free length, internal pressure, and ultrasonic attenuation. The results show that the specific ion-ion, ion-solvent and solvent-solvent interactions play an important role for explaining the acoustic parameters. However, any deviation from the usual behavior is probably due to characteristic structural changes in the systems concerned.

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