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Molecular Interaction Studies of some Amino Acids with Aqueous K_2SO_4 solution at 308.15 K

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Abstract: ***Apparent molar compressibilities (φ_K) and apparent molar volumes (φ_V), of L-valine, L-asparagine and L-arginine in aqueous and aqueous potassium sulphate solutions (0, 0.5, and 1.0 mol.dm^{-3}) at 308.15 K have been determined from precise density and ultrasonic velocity measurements. Limiting apparent molar compressibilities (φ_K^0) and limiting apparent molar volumes (φ_V^0) and their constants (S_K, S_V) of these amino acids at infinite dilution is evaluated. Transfer adiabatic compressibilities ($\Delta\varphi_K^0$), transfer volumes ($\Delta\varphi_V^0$) at infinite dilution from water to aqueous potassium sulphate solutions and molar hydration number (n_H) have been calculated. Viscosity A and B coefficients of Jones-Dole equation have been determined from viscosity measurements. These parameters have been interpreted in terms of ion-solvent and ion-ion interactions in the studied solutions.***

Keywords: Viscosity coefficients, apparent molar compressibility, apparent molar volume, ultrasonic velocity, hydration number.

1. Introduction

In recent years, the studies of acoustical properties of amino acids in aqueous mixed electrolytic solutions have been found to be useful in understanding the specific ion-ion and ion-solvent interaction in solutions. The volumetric and compressibility studies of amino acids in aqueous salt solutions have been employed to understand the nature of interactions operative in solutions. K_2SO_4 influences the unfolding of protein [1]. Thus, the study of interactions in amino acid/aqueous K_2SO_4 systems is significant with a view to understanding the interactions in protein-aqueous K_2SO_4 systems. This study focuses on the measurements of density (ρ) viscosity (η) and ultrasonic velocity (U) values of L-valine, L-asparagine and L-arginine in aqueous and aqueous potassium sulphate solution at 308.15 K. The experimental values have been used to compute the various acoustical, volumetric and transfer parameters with the view to understanding the various types of interactions operative in the solutions.

2. Materials And Methods

Chemicals with analytical reagent (AR) and spectroscopic reagent (SR) grades are used as such without further purification. The density was determined using a specific gravity bottle by relative measurement method with an accuracy of ± 0.01kgm^{-3}. An ultrasonic interferometer having the frequency of 3 MHz (Mittal Enterprises, New Delhi, Model: F-81) with an overall accuracy of ± 0.01% has been used for velocity measurements. Solution viscosities were measured by Ostwald type capillary viscometer, which was placed in a water thermostat having temperature stability. The measured viscosity values have an uncertainty of ± 0.001m.Pa.s.

3. Theory and Calculations

Adiabatic compressibility

$$\beta = \frac{1}{U^2\rho} \quad (1)$$

Molar hydration number

$$n_H = \left(\frac{n_1}{n_2}\right)\left(1 - \frac{\beta}{\beta o}\right) \quad (2)$$

The apparent molar compressibility

$$\varphi_K = \frac{1000}{M\rho_0}(\rho_o\beta - \rho\beta o) + \left(\frac{\beta o M_w}{\rho_o}\right) \quad (3)$$

$$\varphi_K = \varphi_K^0 + S_k M^{1/2} \quad (4)$$

The apparent molar volume

$$\varphi_V = \left(\frac{M_w}{\rho}\right) - \left(\frac{1000(\rho - \rho_0}{M\rho\rho_0}\right) \quad (5)$$

$$\varphi_V = \varphi_V^0 + S_v M^{1/2} \quad (6)$$

The viscosity A and B coefficients

$$\left(\frac{\eta}{\eta_0}\right) = 1 + AM^{1/2} + BM \quad (7)$$

Transfer adiabatic compressibility ($\Delta\varphi_K^0$) and transfer volume ($\Delta\varphi_V^0$) of each amino acid from water to aqueous potassium sulphate solutions have been calculated as:

$\Delta\varphi_y^0 = \varphi_y^0$ (in aqueous potassium sulphate) - φ_y^0 (in water) (8)

Where φ_y^0 denotes, limiting apparent molar compressibility φ_K^0, limiting apparent molar volume φ_V^0.

4. Results and Discussion

The values of density, viscosity, ultrasonic velocity, adiabatic compressibility , molar hydration number, apparent molar compressibility, apparent molar volume, limiting apparent molar compressibility, limiting apparent molar volume, and their constants (S_K, S_V), transfer adiabatic compressibility, transfer volume and viscosity A and B

coefficient of Jones-Dole equation of each of the three amino acids viz., L-valine, L-asparagine and L-arginine in aqueous and aqueous potassium sulphate solutions are shown in Tables I-III. In all the three amino acids system (Table I) the values of density and ultrasonic velocity increases with increase in molar concentration of amino acids as well as potassium sulphate (K_2SO_4) content. This increasing trend suggests a moderate strong electrolytic nature in which the solutes (amino acids) tend to attract the solvent (aqueous potassium sulphate) molecules.

In all the three systems the value of adiabatic compressibility (Table II) decreases with increase in concentration of solute (amino acids) as well as increase in concentration of aqueous K_2SO_4. The increasing electrostrictive compression of water around the molecules results in a large decrease in the compressibility of the solutions. The decreasing behaviour of n_H shows the strength of interaction gets weakened between the ion-solvent molecules, but however it increases the ion-ion interaction in the mixtures [2]. Appreciable negative values of φ_K^0, and its behaviour for all systems reinforce our earlier view regarding existence of ion-solvent interaction in the mixtures. The decrease in φ_V^0 may be attributed to the increased hydrophobicity / non-polar character of the side chain of the amino acids. The magnitude of φ_V^0 is in the order: L-arginine < L-asparagine < L-valine. It is evident from the Table III that S_K and S_V are positive in all the three systems suggesting the presence of strong ion-ion interactions.

The magnitude of $\Delta\varphi_V^0$ (Table III) is in order: L-arginine < L-asparagine < L-valine. Generally, the interactions between amino acids and potassium sulphate can be classified as [3]:

1) ion-ion interactions among the K^+,SO_4^{2-}, and (NH_3^+ and COO^-) zwitterionic end groups.
2) Ion-hydrophilic interactions between ions and hydrophilic groups ($-CONH_2$, $-CONH$) of amino acids.
3) Ion-nonpolar group interactions occurring between ions and the nonpolar groups ($-CH_2/-CH_3$) of amino acids.

According to co-sphere overlap model [4], ion-ion group interactions and ion-hydrophilic interactions contribute positively, whereas ion–non-polar group interactions contribute negatively to the $\Delta\varphi_V^0$ values. Therefore, from Figs. 1-2, the negative $\Delta\varphi_K^0$ and $\Delta\varphi_V^0$ values observed in all the three amino acids suggest that the interaction contribution of type (iii) is stronger than that of type (i) and (ii).

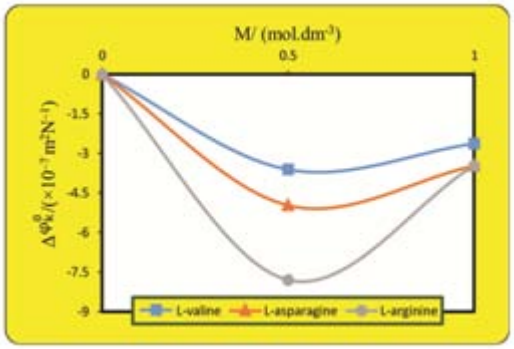

Figure 1: Variation of transfer adiabatic compressibility ($\Delta\varphi_k^0$) of some amino acids with molarity of aqueous potassium sulphate solutions at 308.15 K

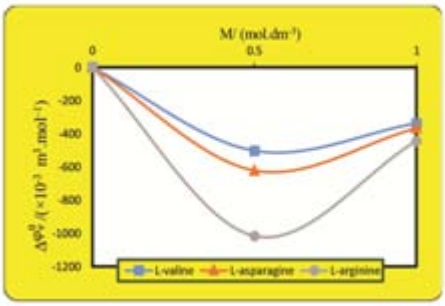

Figure 2: Variation of transfer volume ($\Delta\varphi_v^0$) of some amino acids with molarity of aqueous potassium sulphate solutions at 308.15 K

Table 1: Values of density (ρ), viscosity (η), and ultrasonic velocity (U) of amino acids in aqueous potassium sulphate solutions at 308.15K

M/(mol.dm^{-3})	ρ / (kgm^{-3})			η / (x 10^{-3} Nsm^{-2})			U / (m.s^{-1})		
water + potassium sulphate (K_2SO_4)									
	0.0 M	0.5M	1.0 M	0.0M	0.5M	1.0M	0.0M	0.5M	1.0M
System - I : water + potassium sulphate + L-valine									
0.00	994.0	1008.2	1040.3	0.7190	0.7775	0.8309	1528.6	1584.9	1614.9
0.02	995.6	1016.5	1046.9	0.7235	0.7845	0.8399	1529.2	1585.0	1615.9
0.04	997.2	1017.9	1047.1	0.7257	0.7930	0.8439	1531.8	1587.6	1616.5
0.06	999.8	1019.7	1048.3	0.7325	0.7961	0.8461	1532.5	1590.8	1617.5
0.08	1001.2	1021.8	1051.2	0.7394	0.7997	0.8503	1534.2	1593.3	1618.9
0.10	1003.5	1022.5	1052.4	0.7486	0.8069	0.8541	1535.6	1594.2	1619.4
System – II : water + potassium sulphate + L-asparagine									
0.00	994.0	1008.2	1040.3	0.7190	0.7775	0.8309	1528.6	1584.9	1614.9
0.02	996.2	1020.2	1049.3	0.7242	0.7952	0.8404	1530.3	1587.1	1618.9
0.04	998.6	1023.1	1052.6	0.7294	0.8019	0.8452	1532.5	1589.5	1620.4
0.06	1001.1	1028.6	1058.4	0.7370	0.8102	0.8717	1534.2	1591.4	1621.9
0.08	1003.2	1034.1	1063.2	0.7416	0.8190	0.8808	1535.7	1594.3	1623.2
0.10	1004.6	1038.9	1069.6	0.7594	0.8267	0.8900	1538.2	1596.2	1624.1
System - III : water + potassium sulphate + L-arginine									
0.00	994.0	1008.2	1040.3	0.7190	0.7775	0.8309	1528.6	1584.9	1614.9
0.02	998.4	1025.2	1050.6	0.7337	0.7961	0.8452	1532.2	1588.2	1619.5

0.04	1002.6	1028.6	1056.5	0.7452	0.8023	0.8487	1534.4	1590.5	1621.4
0.06	1009.8	1032.4	1062.3	0.7549	0.8140	0.8795	1536.6	1593.7	1623.3
0.08	1019.4	1036.5	1069.8	0.7695	0.8208	0.8884	1539.2	1595.9	1625.2
0.10	1024.8	1040.9	1074.8	0.7781	0.8303	0.8988	1541.4	1598.5	1627.9

Table 2: Values of adiabatic compressibility (β), apparent molar compressibility ( ), hydration number (nH) and apparent molar volume ( ) of amino acids in aqueous potassium sulphate solutions at 308.15 K

M/ (mol.dm^{-3})	**β / (x 10^{-10} m^2 N^{-1})**			**n_H**			**-φ_K/ (x 10^{-7} m^2 N^{-1})**			**-φ_V/(x 10^{-3} m^3 mol^{-1})**		
water + potassium sulphate (K_2SO_4)												
	0.0M	0.5M	1.0M	0.0M	0.5M	1.0M	0.0M	0.5M	1.0M	0.0M	0.5M	1.0M
System - I : water + potassium sulphate + L-valine												
0.00	4.3055	3.9487	3.6860	--	--	--	--	--	--	--	--	--
0.02	4.2952	3.9159	3.6582	6.65	21.27	17.68	0.8615	3.2654	2.5593	80.68	404.83	302.89
0.04	4.2738	3.8977	3.6548	10.23	16.54	9.92	1.1390	2.2248	1.3823	80.58	236.18	155.95
0.06	4.2588	3.8752	3.6461	10.04	15.89	8.46	1.1971	1.9757	1.1374	97.15	186.32	122.15
0.08	4.2434	3.8551	3.6297	10.02	15.18	8.95	1.1661	1.8358	1.1865	90.32	164.91	124.48
0.10	4.2260	3.8481	3.6234	10.26	13.05	7.96	1.2065	1.5661	1.0547	95.12	138.60	110.41
System – II : water + potassium sulphate + L-asparagine												
0.00	4.3055	3.9487	3.6860	--	--	--	--	--	--	--	--	--
0.02	4.2865	3.8914	3.6363	12.26	37.16	31.60	1.4265	5.2147	4.0795	110.94	583.19	412.11
0.04	4.2639	3.8687	3.6182	13.42	25.94	21.55	1.5381	3.4589	2.7845	115.71	360.98	280.67
0.06	4.2438	3.8388	3.5917	13.27	23.75	19.99	1.5401	3.1632	2.6405	118.77	327.71	273.84
0.08	4.2267	3.8045	3.5698	12.71	23.38	18.47	1.4831	3.0705	2.4668	115.18	310.38	258.66
0.10	4.2071	3.7779	3.5445	12.70	22.15	17.99	1.4431	2.9104	2.4532	106.00	292.96	263.18
System - III : water + potassium sulphate + L-arginine												
0.00	4.3055	3.9487	3.6860	--	--	--	--	--	--	--	--	--
0.02	4.2664	3.8671	3.6291	25.23	52.94	36.19	2.9079	7.4092	4.6698	221.51	822.19	471.04
0.04	4.2364	3.8431	3.6004	22.29	34.24	27.21	2.6588	4.6375	3.5750	215.56	491.62	368.33
0.06	4.1941	3.8136	3.5724	23.96	29.21	24.08	2.9973	3.8245	3.1925	262.18	387.33	331.63
0.08	4.1406	3.7881	3.5390	26.60	26.04	23.37	3.4365	3.3930	3.1441	313.17	338.35	331.18
0.10	4.1071	3.7598	3.5109	25.60	24.50	22.27	3.3181	3.1697	2.9734	302.19	311.60	308.39

Table 3: Values of limiting apparent molar compressibility (φ_K^0), limiting apparent molar volume (φ_V^0) and their constants S_K and S_V, transfer adiabatic compressibility ($\Delta\varphi_K^0$), transfer volumes ($\Delta\varphi_V^0$) and A and B co-efficients of Jones – Dole equation of each amino acids in aqueous potassium sulphate solution at 308.15 K

Amino acids	*K_2SO_4 M/ (mol.dm^{-3})*	*-φ_k^0/(×10^{-7} m^{2}N^{-1})*	*-φ_v^0/(×10^{-3} m^3.mol^{-1})*	*S_k/(×10^{-7}N^{-1} m^{-1}.mol^{-1})*	*S_v/(×10^{-3} m^3 L^{½}.mol$^{-3/2}$)*	*$\Delta\varphi_k^0$/(×10^{-7} m^{2}N^{-1})*	*$\Delta\varphi_v^0$/(×10^{-3} m^3.mol^{-1})*	*A /(dm$^{3/2}$. mol$^{-1/2}$)*	*B /(dm$^{3/2}$ mol^{-1})*
L-valine	0.0	0.69	67.31	1.77	90.51	--	--	0.0417	0.5116
	0.5	4.31	569.01	9.00	1446.23	-3.62	-501.7	0.0339	0.2634
	1.0	3.33	404.60	7.85	1018.40	-2.64	-337.29	0.0666	0.0569
L-asparagine	0.0	1.48	117.16	0.03	16.21	--	--	0.0509	0.6489
	0.5	6.45	739.24	12.17	1536.32	-4.97	-622.08	0.8270	0.2747
	1.0	4.95	484.90	8.72	789.70	-3.47	-367.74	0.0646	0.9515
L-arginine	0.0	2.23	124.29	3.50	584.80	--	--	0.0461	0.6822
	0.5	10.03	1139.64	23.38	2823.86	-7.80	-1015.35	0.1436	0.2807
	1.0	5.69	568.54	9.21	870.82	-3.46	-444.25	0.0289	0.9607

From the Table III, it is observed that the values of A and B coefficients are positive for all the system indicating the presence of ion-ion interactions [5] and strong ion-solvent interaction. The magnitude of B values is in the order L-arginine > L-asparagine > L-valine. This conclusion is in excellent agreement with that drawn from φ_V^0 and $\Delta\varphi_V^0$.

5. Conclusion

In the present work, volumetric, compressibility and transport parameters of L-valine, L-asparagine and L-arginine in aqueous and aqueous potassium sulphate solutions (0, 0.5 and 1.0 mol.dm^{-3}) at 308.15 K were obtained using density, viscosity and ultrasonic velocity data and the results have been used to study the existence of ion-solvent interactions. From the magnitude of φ_V^0, $\Delta\varphi_V^0$ and the values of B-coefficient it can be concluded that L-arginine possesses strong ion-solvent interaction than the other two amino acids. The transfer adiabatic compressibility $\Delta\varphi_K^0$ and transfer volume $\Delta\varphi_V^0$ data suggest that ion-non polar group interactions are dominating over the ion-ion and ion-hydrophilic group interactions.

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