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Study of Solvation Behavior of Some Biologically Active Compounds in Aqueous Barium Chloride Solution

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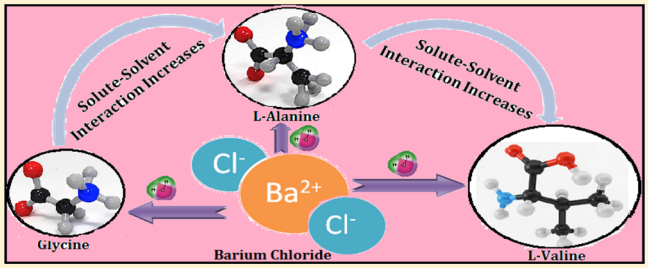
ABSTRACT: The density (ρ), viscosity (η), refractive index (n_D), and speed of sound (u) of glycine, L-alanine, and L-valine have been determined in different mass fractions (w_1 = 0.01, 0.03, 0.05) aqueous barium chloride solutions at 298.15 K. The limiting apparent molar volumes (ϕ_V^0), experimental slopes (S_V^*) have been found out from the Masson equation. A and B coefficients have been obtained from the Jones−Dole equation. The Lorentz−Lorenz equation has been employed to measure molar refractions (R). Limiting apparent molar adiabatic compressibilities (ϕ_K^0) of the studied amino acids at infinite dilution have also been measured. These derived parameters have been used to explore solute−solute and solute−solvent interactions in the solutions.



1. INTRODUCTION

Amino acids are bioactive compounds containing amine ($-NH_2$) and carboxylic acid ($-COOH$) groups with a specific side-chain. They serve as the formation units of proteins. Amino acids play a key role in nutrition and are commonly used in fertilizers, food technology and industry.

Various interactions namely ion−ion, ion−solvent, and solvent−solvent interactions[1−5] were obtained from the extensive studies on the effect of concentration (molality), the apparent molar volumes of solutes. A methodical investigation on the density, viscosity, refractive index, and ultrasonic speed of three amino acids have been performed in aqueous barium chloride solutions at 298.15 K to evaluate the limiting apparent molar volume (ϕ_V^0), experimental slopes (S_V^*), and viscosity B coefficients, molar refraction (R), and limiting apparent molar adiabatic compressibility (ϕ_K^0) for these amino acids.

2. EXPERIMENTAL METHODS

2.1. Source and Purity of Samples. The mass fraction of purity of barium chloride of puriss grade (Sigma-Aldrich, Germany) was ≥ 0.99. The recrystallization of barium chloride was done from aqueous ethanol solution followed by drying under vacuum at T = 348 K, and it was stored over P_2O_5 in a desiccator.[6] The three amino acids namely glycine, L-alanine and L-valine (SD. Fine Chemicals, > 99 %) were taken without any further purification. Freshly distilled conductivity water was used for the preparation of the barium chloride solution. The physical properties of different mass fractions of aqueous barium chloride solution are shown in Table 1.

2.2. Apparatus and Procedure. A vibrating-tube Anton Paar density meter (DMA 4500M) with a precision of 0.00005 g·cm^{-3} was used to measure density (ρ) after being calibrated by double-distilled water and dry air.[7] The temperature was fixed within ± 0.01 K.

The viscosity (η) was measured by using a Ubbelohde type viscometer, calibrated at 298.15 K with distilled water and pure methanol. Experimental solution was taken in a thoroughly cleaned and dried viscometer which is placed vertically in a glass-walled thermostat (Bose Panda Instruments Pvt. Ltd.). The flow times were accurate to ± 0.1 s. Airtight-stopper bottles were used for the preparation of the mixtures. A triplicate measurement was taken into account with sufficient precautions to minimize the evaporation loss. A Mettler AG-285 electronic balance with a precision of ± 0.01 mg was used to measure the mass. The precision of the density measurements was ± 3·10^{-4} g·cm^{-3}.

Table 1. The Values of Density (ρ), Viscosity (η), Refractive Index (n_D), and Speed of Sound (u) in Different Mass Fractions of Barium Chloride at Temperature (T[a]) of 298.15 K and Experimental Pressure of 0.1 MPa

mass fraction of barium chloride	ρ·10^{-3}/(kg m^{-3})[b]	η/(mPa s)[c]	n_D[d]	u/ms^{-1} [e]
w_1 = 0.01	0.99756	0.909	1.3330	1516.7
w_1 = 0.03	0.99866	0.915	1.3337	1521.4
w_1 = 0.05	0.99974	0.921	1.3345	1525.3

[a]Uncertainty in the temperature values: ± 0.01 K. [b]Uncertainty in the density values: ± 0.01 kg m^{-3}. [c]Uncertainty in the viscosity values: ± 0.003 mPas. [d]Uncertainty in the refractive index values: ± 0.0002 units. [e]Uncertainty in the speed of sound: ± 0.2 m·s^{-1}.

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Table 2. Experimental Values of Molality (m), Density (ρ), Viscosity (η), Refractive Index (n_D), and Ultrasonic Speed (u) of Glycine, L-Alanine and L-Valine in Different Mass Fractions of Barium Chloride in the Solvent Mixture ($BaCl_2$ + Water) at Temperature (T[a]) of 298.15 K and Experimental Pressure of 0.1 MPa

w_1 = 0.01					w_1 = 0.03					w_1 = 0.05				
m / (mol kg^{-1})[b]	$\rho\cdot10^{-3}$ / (kg m^{-3})[c]	η / (mPa s)[d]	n_D[e]	u / ms^{-1}[f]	m / (mol kg^{-1})[b]	$\rho\cdot10^{-3}$ / (kg m^{-3})[c]	η / (mPa s)[d]	n_D[e]	u / ms^{-1}[f]	m / (mol kg^{-1})[b]	$\rho\cdot10^{-3}$ / (kg m^{-3})[c]	η / (mPa s)[d]	n_D[e]	u / ms^{-1}[f]
Glycine														
0.1001	0.99781	0.913	1.3331	1521.3	0.1001	0.99886	0.919	1.3342	1526.8	0.1000	0.99992	0.926	1.3353	1531.2
0.1584	0.99823	0.916	1.3335	1535.8	0.1583	0.99921	0.923	1.3346	1542.8	0.1582	1.00025	0.929	1.3357	1548.9
0.2004	0.99868	0.918	1.3338	1555.9	0.2003	0.9996	0.926	1.3349	1565.9	0.2002	1.00063	0.933	1.336	1574.9
0.2351	0.99915	0.921	1.3341	1582.6	0.2350	1.00002	0.929	1.3352	1594.9	0.2349	1.00104	0.937	1.3363	1607.3
0.2653	0.99964	0.923	1.3344	1613.4	0.2652	1.00046	0.932	1.3355	1630.1	0.2651	1.00148	0.940	1.3366	1648.0
0.2925	1.00015	0.926	1.3347	1651.6	0.2923	1.00094	0.935	1.3358	1673.1	0.2922	1.00194	0.944	1.3369	1696.2
L-Alanine														
0.1002	0.99777	0.915	1.3333	1520.5	0.1001	0.9988	0.924	1.3343	1525.7	0.1001	0.99985	0.930	1.3354	1530.3
0.1584	0.99815	0.922	1.3337	1533.8	0.1584	0.99911	0.931	1.3347	1540.4	0.1583	1.00012	0.938	1.3358	1546.7
0.2005	0.99857	0.929	1.334	1553.1	0.2004	0.99949	0.939	1.335	1561.4	0.2003	1.0005	0.946	1.3361	1571.1
0.2352	0.99902	0.936	1.3343	1577.9	0.2351	0.99991	0.946	1.3353	1588.9	0.2350	1.00092	0.954	1.3365	1602.3
0.2655	0.99951	0.942	1.3346	1608.6	0.2654	1.00038	0.954	1.3356	1621.9	0.2652	1.0014	0.962	1.3368	1640.9
0.2927	1.00003	0.949	1.3349	1645.3	0.2925	1.00089	0.961	1.3359	1663.2	0.2924	1.00191	0.970	1.3371	1689.2
L-Valine														
0.1002	0.99769	0.919	1.3335	1519.5	0.1001	0.99873	0.930	1.3344	1524.8	0.1001	0.99978	0.937	1.3355	1529.5
0.1585	0.99798	0.931	1.334	1532.0	0.1584	0.99897	0.944	1.335	1538.3	0.1583	1.00001	0.953	1.3361	1545.5
0.2006	0.99833	0.944	1.3344	1550.3	0.2005	0.99930	0.958	1.3355	1558.1	0.2004	1.00038	0.968	1.3366	1569.1
0.2354	0.99872	0.956	1.3346	1574.2	0.2353	0.99968	0.973	1.3359	1583.9	0.2352	1.00082	0.984	1.3371	1600.2
0.2658	0.99917	0.969	1.3352	1602.9	0.2656	1.00014	0.987	1.3363	1617.6	0.2655	1.00134	1.000	1.3375	1640.1
0.2931	0.99967	0.981	1.3356	1637.6	0.2929	1.00065	1.001	1.3367	1655.2	0.2927	1.00189	1.015	1.3379	1686.3

[a]Uncertainty in the temperature values: ± 0.01 K. [b]Uncertainty in the molality: ± 0.0001 mol kg^{-1}. [c]Uncertainty in the density values: ± 0.01 kg m^{-3}. [d]Uncertainty in the viscosity values: ± 0.003 mPas. [e]Uncertainty in the refractive index values: ± 0.0002 units. [f]Uncertainty in the speed of sound: ± 0.2 m·s^{-1}.

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Table 3. Molality (m), Apparent Molar Volume (φ_V), $(\eta/\eta_0 - 1)/m^{1/2}$, Molar Refraction ($R$), Adiabatic Compressibility (β) and Apparent Molal Adiabatic Compressibility (φ_K) of Glycine, L-Alanine and L-Valine in Barium Chloride at Temperature (T^b) of 298.15 K and Experimental Pressure of 0.1 MPa

m^a	$\varphi_V \cdot 10^6$	$(\eta/\eta_0 - 1)/m^{1/2}$	R	$\beta \cdot 10^{10}$	$\varphi_K \cdot 10^{10}$
mol kg^{-1}	m^3 mol^{-1}	kg$^{1/2}$ mol$^{-1/2}$	m^3 mol^{-1}	Pa^{-1}	m^3 mol^{-1} Pa^{-1}
		w_1 = 0.01			
		Glycine			
0.1001	50.1925	0.036	15.4797	4.3303	−2.6967
0.1584	48.3881	0.043	15.4900	4.2471	−4.2830
0.2004	47.1851	0.049	15.4957	4.1362	−5.3760
0.2351	46.2738	0.054	15.5010	3.9960	−6.4086
0.2653	45.4667	0.059	15.5060	3.8430	−7.1816
0.2925	44.7085	0.063	15.5107	3.6654	−7.9721
		L-Alanine			
0.1002	68.2565	0.061	18.3814	4.3350	−2.1447
0.1584	65.6502	0.088	18.3944	4.2585	−3.7506
0.2005	63.9962	0.107	18.4017	4.1516	−4.9179
0.2352	62.6975	0.123	18.4084	4.0203	−5.8936
0.2655	61.3826	0.137	18.4143	3.8664	−6.7764
0.2927	60.1780	0.148	18.4197	3.6939	−7.5676
		L-Valine			
0.1002	104.4047	0.102	24.1859	4.3411	−1.3813
0.1585	100.5955	0.152	24.2118	4.2693	−3.1686
0.2006	98.1395	0.190	24.2296	4.1676	−4.3686
0.2354	96.2940	0.219	24.2333	4.0405	−5.3810
0.2658	94.3803	0.245	24.2618	3.8953	−6.2198
0.2931	92.5523	0.270	24.2759	3.7301	−7.0005
		w_1 = 0.03			
		Glycine			
0.1001	55.1439	0.035	15.5097	4.2946	−2.9000
0.1583	53.1412	0.044	15.5211	4.2045	−4.6315
0.2003	51.6392	0.051	15.5277	4.0798	−5.9350
0.2350	50.4103	0.057	15.5338	3.9311	−6.9652
0.2652	49.4219	0.063	15.5395	3.7615	−7.8541
0.2923	48.3112	0.067	15.5447	3.5690	−8.7012
		L-Alanine			
0.1001	75.1908	0.071	18.4124	4.3011	−2.1675
0.1584	71.1854	0.096	18.4267	4.2181	−4.0116
0.2004	68.4317	0.114	18.4346	4.1038	−5.2616
0.2351	66.4518	0.131	18.4419	3.9613	−6.3460
0.2654	64.6051	0.145	18.4482	3.8000	−7.2378
0.2925	62.9390	0.159	18.4537	3.6118	−8.1325
		L-Valine			
0.1001	110.2978	0.126	24.2199	4.3065	−1.4772
0.1584	104.8906	0.174	24.2535	4.2302	−3.3807
0.2005	101.2857	0.211	24.2783	4.1220	−4.6644
0.2353	98.7369	0.243	24.2953	3.9873	−5.7337
0.2656	96.1360	0.273	24.3103	3.8211	−6.7986
0.2929	93.8640	0.295	24.3241	3.6476	−7.5756
		w_1 = 0.05			
		Glycine			
0.1000	57.0848	0.034	15.5395	4.2655	−3.0083
0.1582	54.6842	0.046	15.5512	4.1672	−5.0022
0.2002	52.8337	0.054	15.5579	4.0292	−6.4984
0.2349	51.4470	0.061	15.5641	3.8668	−7.6244
0.2651	50.2259	0.068	15.5699	3.6765	−8.6673
0.2922	49.2004	0.073	15.5753	3.4689	−9.5466
		L-Alanine			
0.1001	78.1103	0.071	18.4480	4.2708	−2.3855
0.1583	73.9092	0.096	18.4629	4.1796	−4.4223
0.2003	70.1082	0.116	18.4709	4.0492	−5.9213
0.2350	67.6530	0.134	18.4830	3.8914	−7.1040

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Table 3. continued

m^a	$\varphi_V \cdot 10^6$	$(\eta/\eta_0 - 1)/m^{1/2}$	R	$\beta \cdot 10^{10}$	$\varphi_K \cdot 10^{10}$
mol kg^{-1}	m^3 mol^{-1}	kg$^{1/2}$ mol$^{-1/2}$	m^3 mol^{-1}	Pa^{-1}	m^3 mol^{-1} Pa^{-1}
		L-Alanine			
0.2652	65.3927	0.148	18.4891	3.7087	−8.1384
0.2924	63.5771	0.162	18.4946	3.4979	−9.1391
		L-Valine			
0.1001	113.1794	0.130	24.2666	4.2755	−1.7575
0.1583	106.3777	0.182	24.3004	4.1865	−4.0044
0.2004	101.1763	0.219	24.3242	4.0600	−5.5172
0.2352	97.5390	0.255	24.3462	3.9020	−6.7822
0.2655	94.3174	0.286	24.3597	3.7125	−7.9586
0.2927	91.8798	0.310	24.3725	3.5100	−8.8742

[a]Uncertainty in the molality: ± 0.0001 mol·kg^{-1}. [b]Uncertainty in the temperature values: ± 0.01 K.

Table 4. Limiting Apparent Molar Volumes (ϕ_V^0), Experimental Slopes (S_V^*), A, B Coefficients, Limiting Partial Adiabatic Compressibility (ϕ_K^0), and Experimental Slope (S_K^*) of Glycine, L-Alanine, and L-Valine in Aqueous Barium Chloride at Temperature (T^a) of 298.15 K and Experimental Pressure of 0.1 MPa

salt	$\phi_V^0 \cdot 10^6$	$S_V^* \cdot 10^6$	A	B	$\phi_K^0 \cdot 10^{10}$	$S_K^* \cdot 10^4$
	m^3 mol^{-1}	m^3 mol$^{-3/2}$ kg$^{1/2}$	kg mol^{-1}	kg$^{1/2}$ mol$^{-1/2}$	m^3 mol^{-1} Pa^{-1}	m^3 mol$^{-3/2}$ Pa^{-1} kg$^{1/2}$
			w_1 = 0.01			
glycine	52.939	−28.292	0.0217	0.1393	0.0604	−27.387
L-alanine	72.330	−41.376	0.0164	0.4529	0.6993	−28.145
L-valine	110.350	−60.425	0.0147	0.8616	1.4782	−29.030
			w_1 = 0.03			
glycine	58.707	−35.300	0.0135	0.1701	0.1233	−30.158
L-alanine	81.332	−63.255	0.0103	0.4688	0.8997	−30.805
L-valine	118.490	−84.382	0.0089	0.9096	1.6759	−31.679
			w_1 = 0.005			
glycine	61.181	−41.267	0.0078	0.2001	0.3820	−34.105
L-alanine	85.771	−76.625	0.0073	0.4706	1.1105	−34.991
L-valine	124.030	−111.560	0.0058	0.9279	1.8971	−36.961

[a]Uncertainty in the temperature values: ± 0.01 K.

Viscosity of the solution is evaluated using the appropriate equation as reported earlier.[8] The uncertainty in viscosity measurements was within ± 0.003 mPa·s.

Refractive index was calculated by means of Mettler Toledo digital refractometer. The light source was LED, λ = 589.3 nm. The calibration of refractometer was done twice using distilled water and being checked after every few measurements. The uncertainty of refractive index measurement was ± 0.0002 units.

An ultrasonic interferometer (model M-83 from Mittal enterprises) was utilized to measure the ultrasonic velocities, u (ms^{-1}). The interferometer (2 MHz) is based on the principle used by Freyer et al.[9] and Kiyoharo et al.[10,11] The obtained velocities were corrected for diffraction errors as given by Subrahmayan et al.[12] The maximum uncertainty in the velocity was ± 0.5 m s^{-1}. The temperature control was carried out within ± 0.01 K using a Lauda thermostat for velocity measurements.

The solutions under investigation were prepared by mass, and the conversion of molarity into molality was accomplished[4] from the studied density values. The experimental values of densities (ρ), viscosities (η), refractive indices (n_D), and ultrasonic speeds (u) of solutions are reported in Table 2, and the derived parameters are listed in Table 3 and Table 4.

3. RESULTS AND DISCUSSIONS

3.1. Density Calculation. The determination of apparent molar volumes (φ_V) were calculated from the solution densities using the following equation.[13]

$$\phi_V = M/\rho - 1000(\rho - \rho_o)/m\rho\rho_o \quad (1)$$

where M is the molar mass of the solute, m is the molality of the solution, ρ_o and ρ are the densities of the solution and the mixture, respectively. The limiting apparent molar volume ϕ_V^0 was obtained using a least-squares treatment to the plot of φ_V versus $\sqrt{m}$ with the help of Masson equation.[14]

$$\phi_V = \phi_V^0 + S_V^*\sqrt{m} \quad (2)$$

where ϕ_V^0 is the limiting apparent molar volume at infinite dilution and S_V^* is the experimental slope. The plots of φ_V against square root of molal concentration ($\sqrt{m}$) were found to be linear. Values of ϕ_V^0 and S_V^* are reported in Table 4.

A perusal of Table 4 reveals that ϕ_V^0 values for amino acids are positive and increase with an increase in concentrations of aqueous barium chloride mixture, indicating the presence of strong solute−solvent interactions, and these interactions are further strengthened with the increase of the mass fraction of $BaCl_2$ in the solvent mixture. The trend in the solute−solvent interaction is

glycine < L-alanine < L-valine

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This indicates that the solute−solvent interaction increases with the increase in the number of carbon atoms in the three amino acids.

The S_V^* values of the amino acid solution (Table 4) follow a decreasing order with the increase in the number of carbon atoms of the above-mentioned amino acids and also the mass fraction of barium chloride in its aqueous mixture. Thus solute−solute interaction is minimized in the higher analogues.

The predominance of solute−solvent interactions over solute−solute interactions was cemented from the higher values of ϕ_V^0 than S_V^* obtained from Figure 1. The same result was obtained for each of the studied amino acids as well as mass fraction of barium chloride in the mixture.

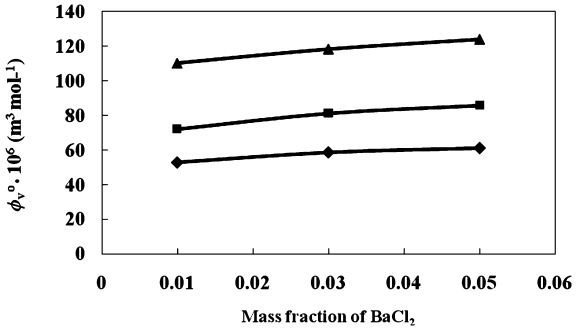

Figure 1. The plots of limiting apparent molar volumes (ϕ_V^0) for ♦, glycine; ■, L-alanine; ▲, L-valine in different mass fractions (w_1) of $BaCl_2$ in aqueous mixture at 298.15 K.

3.2. Viscosity Calculation. The viscosity data has been analyzed using the Jones−Dole equation.[15]

$$(\eta/\eta_0 - 1)/m^{1/2} = A + Bm^{1/2} \quad (3)$$

where η_0 and η are the viscosities of the solvent and solution, respectively. A and B are the viscosity coefficient estimated by a least-squares method and are reported in Table 4. The values of the A coefficient are found to decrease with the increase in the number of carbon atoms of amino acids (starting from glycine to L-valine) and with the increase in mass fraction of barium chloride in the solvent mixture. The results reveal the presence of very weak solute−solute interactions. These results are in excellent agreement with those obtained from S_V^* values discussed earlier.

The effects of solute−solvent interactions on the solution viscosity can be inferred from the B coefficient.[16,17] The viscosity B coefficient is an important tool to provide information concerning the solvation of the solutes and their effects on the structure of the solvent. From Table 4 and Figure 2 it is evident that the values of the B coefficient are positive, thereby suggesting the presence of strong solute−solvent interactions, and strengthened with an increase in the number of carbon atoms of amino acids and with the increase of mass fraction of $BaCl_2$ in the solvent mixture. This observation is in a fine agreement with the results obtained from ϕ_V^0 values discussed earlier.

3.3. Refractive Index Calculation. The molar refraction R has been evaluated from the Lorentz−Lorenz relation.[18]

$$R = \{(n_D^2\text{-}1)/(n_D^2 + 2)\}(M/\rho) \quad (4)$$

where R, n_D, ρ, and M are the molar refraction, the refractive index, density, and the molar mass of the solution, respectively.

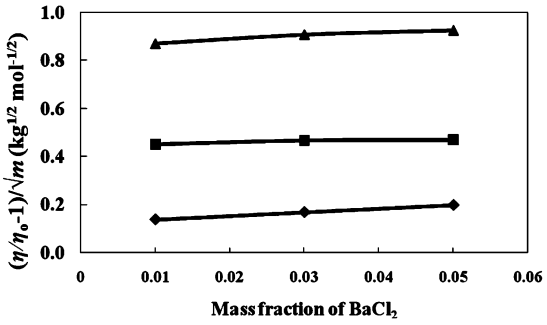

Figure 2. The plots of viscosity B coefficient for ♦, glycine; ■, L-alanine; ▲, L-valine in different mass fractions (w_1) of $BaCl_2$ in aqueous mixture at 298.15 K.

The ratio c_0/c is refractive index of a substance, where c and c_0 are the speed of light in that particular medium and the speed of light in vacuum, respectively. The refractive index of a compound denotes its capability to refract light as it goes from one medium to another. According to Deetlefs et al.[19] the greater the refractive index of a substance is, the more the light is refracted[20]

A more tightly packed substance, that is, a more denser solution has a higher refractive index. So refractive index values rise with the increase of mass fraction of $BaCl_2$ in the solvent mixture. Hence from Table 2 and Table 3 it is clear that for L-valine the refractive index and the molar refraction values are higher than that of the other two amino acids. Thus solute−solvent interaction predominates over solute−solute interaction. This fact also supports the results obtained from density and viscosity parameters discussed above. The studied amino acids in aqueous barium chloride solution obey the same trend of solute solvent interaction, that is,

glycine < L-alanine < L-valine

3.4. Ultrasonic Speed Calculation. The adiabatic compressibility (β) was evaluated with the help of the following equation:

$$\beta = 1/u^2\rho \quad (5)$$

where u is the sound speed in the solution and ρ is the solution density. The apparent molal adiabatic compressibility (φ_K) of the solutions was analyzed from the relation

$$\phi_K = M\beta/\rho + 1000(\beta\rho_o - \beta_o\rho)/m\rho\rho_o \quad (6)$$

where β and β_0 are the adiabatic compressibility of the solution and solvent, respectively, and m is the molality of the solution. Limiting partial molal adiabatic compressibilities (ϕ_K^0) and experimental slopes (S_K^*) were achieved by fitting φ_K against the square root of molality of the electrolyte ($\sqrt{m}$) using the least-squares method.

$$\phi_K = \phi_K^0 + S_K^*\sqrt{m} \quad (7)$$

The values of β and φ_K are enlisted in Table 3 and the values of ϕ_K^0 and S_K^* are presented in Table 4. The values of ϕ_K^0 and S_K^* also represent the extent of solute−solvent and solute−solute interactions respectively. An inspection of Table 4 and Figure 3 confirms that the ϕ_K^0 values are in an excellent agreement with those drawn from the values of ϕ_V^0 discussed earlier.

Owing to the greater +I effect of alkyl chain in L-valine in comparison with that of the other two studied amino acids negative charge density becomes maximum on the oxygen atom

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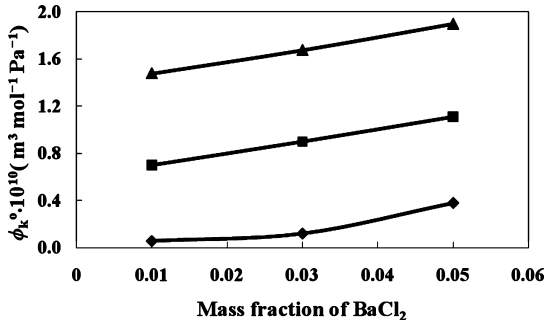

Figure 3. The plots of limiting partial adiabatic compressibility (ϕ_K^0) for ♦, glycine; ■, L-alanine; ▲, L-valine in different mass fractions (w_1) of $BaCl_2$ in aqueous mixture at 298.15 K.

of the carboxylic part. So the solute−solvent interaction of L-valine with the Ba^{2+} ion is highest among the three and thereby supporting the order of interactions mentioned above.

4. CONCLUSION

The values of the limiting apparent molar volume (ϕ_V^0), viscosity *B* coefficients and limiting partial isentropic compressibility (ϕ_K^0) point toward the presence of strong solute−solvent interactions which increase with the increase in the number of carbon atoms of the amino acids and also with the increase of mass fraction of barium chloride in the aqueous mixture. The refractive index and the molar refraction values indicate that molecules of L-valine are more tightly packed in the solution resulting in higher solute−solvent interactions than that of the other two amino acids.

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Notes

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