CHAPTER IX

EXPLORATION OF MOLECULAR INTERACTIONS OF SOME STANDARD AMINO ACIDS IN H_2O + VITAMIN-B_3 MIXTURES

9.1 Introduction:

Amino acids are important in biochemistry, not only in biochemistry it also takes part a central role to life, and have many functions in metabolism. One particularly important function is to serve as the building blocks of proteins. Due to their central role in biochemistry; amino acids are important in nutrition and are commonly used in food technology and industry. Amino acids exist as zwitterions in aqueous solution. Thus, the study of low molecular model compounds such as amino acids, peptides and their derivatives which represents the building block of proteins in a variety of media is of immense importance.

On the other hand vitamins are essential precursors for various coenzymes. These coenzymes are therefore required in almost all metabolic pathways [1]. Nicotinic acid also known as Vitamin B3 is a water-soluble vitamin and an essential in micronutrient [2,3].

Studying the behavior of amino acids in aqueous nicotinic acid solutions will be useful in pharmaceutical industries and food technology as well as in every process of the reaction occurring in protein and peptides chain. Keeping in mind the great applicability of the studied systems, here, we have attempted to ascertain the molecular interaction of the cited amino acids in 0.01, 0.03, 0.05 mass fraction of aqueous nicotinic acid solutions at 298.15 K in terms of limiting apparent molar volume (ϕ_V^0), viscosity *B*-coefficients, limiting apparent molar adiabatic compressibility (ϕ_K^0) and molar refraction (*R*).

9.2 Experimental Section:

9.2.1 Materials

Glycine, L-Alanine, L-Valine and Nicotinic acid were procured from (Sigma Aldrich, purity > 99 %) and were used as such without further purification. Triply distilled water was used for the preparation of different aqueous nicotinic solutions, where the aqueous nicotinic solutions are treated as solvent in the present study. The experimentally observed physical properties of different aqueous nicotinic acid solutions are listed in Table 1.

9.2.2 Apparatus and Procedure

We have precisely checked the solubility of the chosen amino acids in aq. niconitic acid mixtures, and seen that the amino acids were freely soluble in all proportions of the nicotinic acid-water mixtures. 0.1 (M) stock solutions of amino acids in different mass fraction of aqueous nicotinic acid mixture were prepared by mass (Mettler Toledo AG-285 with uncertainty 0.0003g) and the working solutions were prepared by mass dilution. The uncertainties of concentration of different solutions were evaluated to ±0.0001 mol kg^{-1}.

The density, ρ, was measured with an Anton Paar density-meter (DMA 4500M). The uncertainty in the density measurements were within ± $5 \cdot 10^{-5} g \cdot cm^{-3}$. It was calibrated by double-distilled water and dry air [4].

The viscosity, η, was measured by means of a suspended Ubbelohde type viscometer, calibrated at the experimental temperatures with doubly distilled water and purified methanol. A thoroughly cleaned and perfectly dried viscometer filled with experimental solution was placed vertically in a glass-walled thermostat maintained to ± 0.01 K. After attainment of thermal equilibrium, efflux times of flow were recorded with a stop watch correct to ± 0.1 s. At least three repetition of each data reproducible to ± 0.1 s were taken to average the flow time. Viscosity of solution, η, was obtained using the following equation:

$$\eta = (Kt - L/t)\rho \qquad (1)$$

where K and L are the viscometer constants and t and ρ are the efflux time of flow in seconds and the density of the experimental liquid, respectively. The uncertainty in viscosity measurements is within ± 0.003 mPa·s [4].

Refractive index was measured with the help of a Digital Refractometer Mettler Toledo. The light source was LED, λ=589.3nm. The refractometer was calibrated twice using distilled water, and calibration was checked after every few measurements. The uncertainty of refractive index measurement was ±0.0002 units.

The ultrasonic velocities, u (m s^{-1}), were measured using an ultrasonic interferometer (Model M-83) from Mittal enterprises, India. The interferometer working at 2 MHz is based on the same principle as was used by Freyer et al. [5] and Kiyoharo et al.[6, 7] The obtained velocities were corrected for diffraction errors as given by Subrahmayan et al.[8] The maximum uncertainty in the velocity is ±0.5 m s^{-1}. The temperature was controlled within ±0.01 K using a Lauda thermostat for velocity measurements.

9.3 Results and Discussion:

The apparent molar volume (ϕ_V) was determined from the solution densities using the following equation: [9]

$$\phi_V = \frac{M}{\rho} - \frac{1000(\rho - \rho_0)}{m\rho\rho_0} \qquad (2)$$

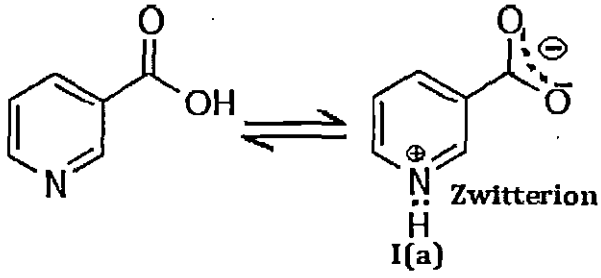
where the symbols are usual meaning. The plots of ϕ_V values against square root of molality ($\sqrt{m}$), the trends is approximate linear; thus the ϕ_V values were fitted to the Masson equation: [10]

$$\phi_V = \phi_V^0 + S_V^* \sqrt{m} \qquad (3)$$

From where, ϕ_V^0, the limiting apparent molar volume at infinite dilution and S_V^* is the experimental slope have been determined and listed in Table 2. Graphical representation (in Figure 1) of limiting apparent molar volume, ϕ_V^0, of the Glycine, L-alanine, and L-valine in different concentrations of aqueous nicotinic acid solutions at 298.15K, shows that the ϕ_V^0 values are positive, which indicates the presence of strong solute-solvent interaction. The increasing ϕ_V^0 values with increase in the

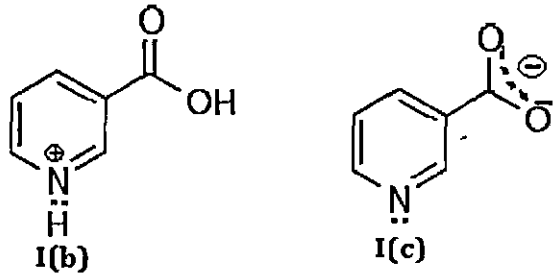
concentration of the nicotinic acid in solution, also shows the positive trend of solute-solvent interaction with increasing amount of nicotinic acid in solution.

In solid state the nicotinic acid exists as neutral molecule instead of zwitterion; on the other hand in aqueous solution it exists as zwitterionic form according to the equilibrium of neutral aqueous solutions is shown in bellow;



I(a)

and as acidic and basic form in acidic and basic medium shown in I(a) and I(b), i.e.:



I(b) I(c)

The zwitterionic I(a), acidic I(b), and basic I(c) form of the nicotinic acid exists in aqueous, are open the phase of interacting centre to interact with the incoming solute or studies α-amino acids molecules in the present chosen solution systems; as a result, strong interactions are present between amino acids and nicotinic acid in solution media.

As evident from the ϕ_V^0 values, the solute-solvent interaction is high in case of L-valine as compared to the other two amino acids. The trend in the solute-solvent interaction of the amino acid is given below:

glycine < L-alanine < L-valine

The trend also supports the same shape, i.e., the interaction arises positively with growing number of -CH_2 groups in the chain length of the chosen amino acids. The positive strength of solute-solvent interactions taking placed in solutions have been explained by plausible interaction between

(i) The positive centre of N atom of the ring of nicotinic acid I(a) and nucleophile (-COO^-) of the zwiterionic form of the amino acid

(ii) The nucleophile (-COO^-) of the nicotinic acid and -CH_2 groups of the hydrophobic part of the chain of amino acids.

(iii) When nicotinic acid exists as zwiterionic form, than both the electrophile (positive centre of N atom of the ring) and nucleophile (-COO^-) group is interacting with the incoming -NH_2 and –COO^- group of the zwiterionic form of the amino acid.

(iv) Hydrophobic- hydrophobic interaction of the amino acids itself.

Since the hydrophobic-hydrophobic interaction (iv) is gives the negative change in ϕ_V^0, so it is neglected. The assumptions of type the interactions (i) to (iii) are give the positive change in ϕ_V^0. Therefore, we may say that the interaction must be occurred through the nucleophilic groups, ion-ion or ion-dipole interactions. A schematic representation of the plausible interaction is represented in **Scheme I**.

The parameter, S_V^*, is the volumetric virial coefficient that characterizes the pair-wise interaction of solvated species in solution [11-14]. The sign of S_V^* is determined by the interaction between the solute species. In the present study S_V^* values were found to be negative and decrease with the increase in the concentration of the nicotinic acid solution. This trend in S_V^* values indicates weak solute-solute interactions in the mixtures. A quantitative comparison of the magnitude of values shows that ϕ_V^0 values are much greater in magnitude than those of S_V^* for all the solutions. These suggest that solute-solvent interactions dominate over solute-solute interactions in all the solutions. Again, the S_V^* values decrease with the increase in the concentration of the nicotinic acid solution which may be attributed due to the increase in the solute-solvent interaction.

The viscosity data of the experimental solutions have been analyzed using the Jones–Dole equation [15]

$$(\eta/\eta_0 - 1)/\sqrt{m} = (\eta_r - 1)/\sqrt{m} = A + B\sqrt{m} \qquad (4)$$

where $\eta_r = \eta/\eta_0$, and η are the viscosities of the solvent and solution respectively, and m is the molality of a solution. A and B are the Jones-Dole [15] constants indicating the solute-solute and solute-solvent interaction respectively, estimated by

a least-squares method and reported in Table 3. The values of the *A*-coefficient are found to decrease with the increase in the concentration of the nicotinic acid solution for each amino acid and with increase in alkyl chain in amino acids. These results are in excellent agreement with those obtained from S_v^* values which indicate that the solute-solute interaction decreases with the increase in the concentration of the nicotinic acid solutions. Also the solute-solute interaction is more in case of glycine compared to the other two amino acids in all the concentration of nicotine acid solutions. The viscosity *B*-coefficient [16, 17] is a valuable tool to provide information concerning the solvation of solutes and their effects on the structure of the solvent in the local vicinity of the solute molecules. The viscosity *B*-coefficient reflects the solute-solvent interactions on the solutions. From the Figure 2 it is evident that the *B*-coefficients of amino acids in the aqueous nicotinic acid solution suggests the presence of strong solute-solvent interactions, and these type of interactions are strengthened with the increase in the concentration of the nicotinic acid solution and with increase in alkyl chain in amino acids. Thus the trend in viscosity *B*-coefficient is

L-valine > L-alanine > glycine

The solute-solvent interaction is more in case of L-valine compared to the other two amino acids in all the concentration of nicotine acid solutions. These conclusions are in excellent agreement with the results drawn from the limiting apparent molar volume, ϕ_v^0, discussed earlier.

The molar refraction *R* can be evaluated from the Lorentz-Lorenz relation [18]

$$R = \{(n_D^2-1)/(n_D^2+2)\}\ (M/\rho) \qquad (5)$$

where *R*, n_D, M and ρ are the molar refraction, refractive index, molar mass and density of solution respectively. The refractive index of a substance is defined as the ratio c_0/c, where c is the speed of light in the medium and c_0 the speed of light in vacuum. Stated more simply, the refractive index of a compound describes its ability to refract light as it moves from one medium to another and thus, the higher the refractive index of a compound, the more the light is refracted [18]. As stated by Deetlefs et al. [19] the refractive index of a substance is higher when its molecules are more tightly packed or in general when the compound is denser. Hence a perusal of Table 4 we found that the refractive index and molar refraction are higher for L-

Valine in nicotinic acid solution indicating the fact that the valine are more interact with the nicotinic acid in solution or tightly packed in the solution. As R is directly proportional to molecular polarisability, it is evident from the Table 4 that the overall polarisability of the studied amino acids increases with the increase in the concentration of the nicotinic acid in solution, leading to more solute-solvent interaction. The molecular polarisability is higher for L-Valine compared to the other two amino acids in all the concentration of nicotine acid solutions. This shows that L-Valine is more solvated by the aqueous solution of nicotinic acid rendering to high solute-solvent interaction.

The Limiting apparent molar adiabatic compressibility (ϕ_K^0) is another tool, which also deals the ion-solvent interaction in solution. For this reason, the adiabatic compressibility (β_S) was evaluated from the following equation:

$$\beta_S = 1/u^2\rho \tag{6}$$

where ρ is the density of solution and u is the speed of sound in the solution. Using β_S values, the apparent molar adiabatic compressibility (ϕ_K) of the solutions was determined from the relation,

$$\phi_K = M\beta_S/\rho + 1000(\beta_S\rho_o - \beta_o\rho)\ /m\rho\rho_o \tag{7}$$

where β_0, β_S are the adiabatic compressibility of the solvent and solution respectively and m is the molality of the solution. After that the limiting apparent molar adiabatic compressibilities (ϕ_K^0) and experimental slopes (S_K^*) were obtained by fitting ϕ_K against the square root of molarity ($\sqrt{m}$) of the amino acids using the method of least squares.

$$\phi_K = \phi_K^0 + S_K^* \cdot \sqrt{m} \tag{8}$$

The values of β_S and ϕ_K are reported in Table 5. Since the values of ϕ_K^0 and S_K^* are measures of solute-solvent and solute-solute interactions respectively, a perusal of Table 5 and Figure 3 the values of ϕ_K^0 increases from glycine to L-valine; which shows that the solute-solvent interaction is highest in case of L-valine in comparison to glycine and L-alanine in all the concentration of nicotine acid solutions and the solute-solvent interaction increases with the increase in the concentration of the

nicotinic acid solutions. From the S_K^* values it was seen that the solute-solute interaction is highest in case of glycine and the values decrease with the increase in the nicotinic acid solution. The values are in agreement with results drawn from the values of ϕ_V^0 and S_V^* discussed earlier.

9.4 Conclusion:

In summary, ϕ_V^0 and viscosity *B*-coefficient values for amino acids indicate the presence of strong solute-solvent interactions and these interactions are further strengthened at higher concentration of aqueous nicotinic acid solution. The solute-solvent interaction is dominant over the solute-solute interaction for all the amino acids in all the aqueous solution of nicotinic acid. The molecular polarisability is higher for L-valine leading to more solute-solvent interaction compared to the other two amino acids. ϕ_K^0 and *R* also supports the same fact.

Tables:

Table 1. The values of density (ρ), viscosity (η), refractive index (n_D), and speed of sound (u) in different mass fractions (m_1) of aqueous nicotinic acid (NA) solutions at 298.15K.

Mass fraction of NA	ρ x 10^{-3} (kg m^{-3})	η (mPa s)	n_D	u (ms^{-1})
$m_1 = 0.01$	0.99757	0.817	1.3320	1492.8
$m_1 = 0.03$	0.99841	0.823	1.3326	1495.7
$m_1 = 0.05$	0.99922	0.828	1.3332	1498.4

Table 2. Values of concentration, density (ρ), apparent molar volume, limiting apparent molar volume and experimental slope (obtained from eq. 3) of glycine, L-alanine and L-valine in different mass fractions (m_1) of aqueous nicotinic acid solutions at 298.15K.

molality (mol kg^{-1})	ρx 10^{-3} (kg m^{-3})	ϕ_V x 10^6 (m^3 mol^{-1})	$^a\phi_V^0$ x 10^6 (m^3 mol^{-1})	S_V^* x 10^6 (m^3 mol$^{-3/2}$ kg$^{1/2}$)
		m_1 = 0.01		
		Glycine		
0.0100	0.99782	50.19		
0.0251	0.99823	48.79		
0.0402	0.99866	47.94	52.38	−22.22
0.0553	0.99911	47.18		
0.0704	0.99958	46.47		
0.0855	1.00006	45.89		
		L-Alanine		
0.0100	0.99778	68.26		
0.0251	0.99814	66.45		
0.0402	0.99853	65.25	71.10	−28.97
0.0553	0.99894	64.33		
0.0705	0.99938	63.38		
0.0857	0.99983	62.65		
		L-Valine		
0.0100	0.99771	103.40		
0.0251	0.99798	100.99		
0.0403	0.99829	99.39	107.10	−38.05
0.0554	0.99863	98.11		
0.0707	0.99899	97.10		
0.0859	0.99939	95.97		
		m_1 = 0.03		
		Glycine		
0.0100	0.99860	56.15		
0.0251	0.99892	54.75		
0.0401	0.99927	53.65	58.68	−25.03
0.0552	0.99964	52.79		
0.0704	1.00003	52.00		
0.0855	1.00043	51.38		

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		L-Alanine		
0.0100	0.99855	75.20		
0.0251	0.99881	73.20		
0.0402	0.99911	71.70	78.87	−35.97
0.0553	0.99944	70.47		
0.0705	0.9998	69.34		
0.0856	1.00019	68.25		
		L-Valine		
0.0100	0.99847	111.32		
0.0251	0.99864	108.12		
0.0402	0.99887	105.81	116.70	−54.74
0.0554	0.99915	103.86		
0.0706	0.99947	102.16		
0.0859	0.99981	100.83		
		$m_1 = 0.05$		
		Glycine		
0.0100	0.99936	61.11	64.21	−31.67
0.0251	0.99962	59.11		
0.0401	0.99991	57.86		
0.0552	1.00023	56.75		
0.0703	1.00057	55.82		
0.0855	1.00093	54.99		
		L-Alanine		
0.0100	0.99926	85.15		
0.0251	0.99939	82.35		
0.0402	0.99957	80.40	89.85	−47.14
0.0553	0.99979	78.78		
0.0704	1.00005	77.29		
0.0856	1.00033	76.09		
		L-Valine		
0.0100	0.99920	119.24		
0.0251	0.99928	114.83		
0.0402	0.99944	111.73	126.3	−72.13
0.0554	0.99965	109.41		
0.0706	0.99993	107.09		
0.0858	1.00023	105.34		

[a] The values have been tally with the Ref. [20].

Table 3. Values of concentration, viscosity (η), $(\eta/\eta_0-1)/m^{1/2}$, Viscosity *A*, *B* coefficients of L -glycine, L-alanine, and L-valine in different mass fractions (m_1) of aqueous nicotinic acid solutions at 298.15K.

molality (mol kg^{-1})	η (mPas)	$(\eta/\eta_0-1)/m^{1/2}$ (kg$^{1/2}$ mol$^{-1/2}$)	*A* (kg mol^{-1})	^{a}B (kg$^{1/2}$ mol$^{-1/2}$)
		m_1 = 0.01		
		Glycine		
0.0100	0.825	0.098		
0.0251	0.832	0.116		
0.0402	0.838	0.128	0.068	0.299
0.0553	0.844	0.141		
0.0704	0.849	0.148		
0.0855	0.854	0.155		
		L-Alanine		
0.0100	0.825	0.098		
0.0251	0.833	0.124		
0.0402	0.840	0.140	0.054	0.430
0.0553	0.847	0.156		
0.0705	0.854	0.171		
0.0857	0.860	0.180		
		L-Valine		
0.0100	0.827	0.1222		
0.0251	0.839	0.1699		
0.0403	0.850	0.2013	0.049	0.752
0.0554	0.861	0.2287		
0.0707	0.871	0.2487		
0.0859	0.881	0.2673		
		m_1 = 0.03		
		Glycine		
0.0100	0.830	0.085		
0.0251	0.837	0.107		
0.0401	0.843	0.121	0.052	0.337
0.0552	0.849	0.134		
0.0704	0.854	0.142		
0.0855	0.859	0.150		

		L-Alanine		
0.0100	0.832	0.109		
0.0251	0.842	0.146		
0.0402	0.852	0.176	0.043	0.657
0.0553	0.862	0.202		
0.0705	0.871	0.220		
0.0856	0.879	0.233		
		L-Valine		
0.0100	0.832	0.109		
0.0251	0.844	0.161		
0.0402	0.855	0.194	0.030	0.810
0.0554	0.866	0.222		
0.0706	0.877	0.247		
0.0859	0.887	0.265		
		$m_1 = 0.05$		
		Glycine		
0.0100	0.831	0.036		
0.0251	0.836	0.061		
0.0401	0.841	0.078	−0.004	0.412
0.0552	0.846	0.093		
0.0703	0.851	0.105		
0.0855	0.856	0.116		
		L-Alanine		
0.0100	0.831	0.036		
0.0251	0.838	0.076		
0.0402	0.846	0.108	−0.039	0.741
0.0553	0.854	0.134		
0.0704	0.863	0.159		
0.0856	0.871	0.177		
		L-Valine		
0.0100	0.832	0.048		
0.0251	0.843	0.114		
0.0402	0.854	0.157	−0.062	1.099
0.0554	0.866	0.195		
0.0706	0.878	0.227		
0.0858	0.892	0.264		

[a] The values have been tally with the Ref. [20].

Table 4. Values of concentration, refractive indices (n_D) and molar refraction (R) of of Glycine, L-alanine and L-valine in different mass fractions (m_1) of aqueous nicotinic acid solutions at 298.15K

molality (mol kg^{-1})	n_D	R (cm^3 mol^{-1})	molality (mol kg^{-1})	n_D	R (cm^3 mol^{-1})	molality (mol kg^{-1})	n_D	R (cm^3 mol^{-1})
				m_1 = 0.01				
	Glycine			L-Alanine			L-Valine	
0.0100	1.3323	15.45	0.0100	1.3323	18.33	0.0100	1.3324	24.11
0.0251	1.3327	15.46	0.0251	1.3328	18.35	0.0251	1.3328	24.13
0.0402	1.333	15.46	0.0402	1.3332	18.36	0.0403	1.3332	24.15
0.0553	1.3333	15.47	0.0553	1.3336	18.37	0.0554	1.3335	24.16
0.0704	1.3336	15.47	0.0705	1.334	18.39	0.0707	1.3338	24.17
0.0855	1.3339	15.48	0.0857	1.3343	18.39	0.0859	1.3341	24.18
				m_1 = 0.03				
	Glycine			L-Alanine			L-Valine	
0.0100	1.3332	15.47	0.0100	1.333	18.35	0.0100	1.3331	24.14
0.0251	1.3338	15.49	0.0251	1.3337	18.38	0.0251	1.3337	24.18
0.0401	1.3343	15.51	0.0402	1.3343	18.41	0.0402	1.3341	24.20
0.0552	1.3348	15.52	0.0553	1.3348	18.43	0.0554	1.3345	24.22
0.0704	1.3352	15.53	0.0705	1.3352	18.44	0.0706	1.3349	24.23
0.0855	1.3356	15.54	0.0856	1.3356	18.45	0.0859	1.3353	24.25
				m_1 = 0.05				
	Glycine			L-Alanine			L-Valine	
0.0100	1.3338	15.49	0.0100	1.3338	18.38	0.0100	1.3342	24.20
0.0251	1.3345	15.51	0.0251	1.3346	18.42	0.0251	1.3351	24.25
0.0401	1.3351	15.53	0.0402	1.3352	18.44	0.0402	1.3359	24.30
0.0552	1.3355	15.54	0.0553	1.3358	18.47	0.0554	1.3365	24.34
0.0703	1.336	15.56	0.0704	1.3363	18.49	0.0706	1.3371	24.37
0.0855	1.3364	15.57	0.0856	1.3368	18.51	0.0858	1.3376	24.39

Table 5. Values of concentration, ultrasonic speed (u), adiabatic compressibility (β), apparent molar adiabatic compressibility (ϕ_K), limiting apparent molar adiabatic compressibility (ϕ_K^0), and experimental slope (S_K^*) (obtained from eq. 8) of Glycine, L-alanine, and L-valine in different mass fractions (m_1) of aqueous nicotinic acid solutions at 298.15K

molality (mol kg^{-1})	u (m s^{-1})	β x 10^{10} (Pa^{-1})	ϕ_K x 10^{10} (m^3 mol^{-1} Pa^{-1})	ϕ_K^0 x 10^{10} (m^3 mol^{-1} Pa^{-1})	S_K^* x 10^4 (m^3 mol$^{-3/2}$ Pa^{-1} kg$^{1/2}$)
			m_1 = 0.01		
			Glycine		
0.0100	1495.8	4.4792	-2.3674		
0.0251	1504.4	4.4263	-3.7936		
0.0402	1516.7	4.3529	-4.7626	0.107	−17.65
0.0553	1531.8	4.2656	-5.6308		
0.0704	1550.4	4.1619	-6.3018		
0.0855	1571.3	4.0500	-6.9824		
			L-Alanine		
0.0100	1494.6	4.4865	-1.7987		
0.0251	1502.3	4.4391	-3.2169		
0.0402	1514.2	4.3678	-4.2272	1.145	−20.32
0.0553	1529.1	4.2818	-5.0864		
0.0705	1546.6	4.1832	-5.9037		
0.0857	1568.2	4.0669	-6.6275		
			L-Valine		
0.0100	1493.7	4.4923	-1.0809		
0.0251	1500.8	4.4486	-2.5738		
0.0403	1512.1	4.3810	-3.6863	2.062	−22.48
0.0554	1527.1	4.2939	-4.5725		
0.0707	1544.7	4.1951	-5.3977		
0.0859	1565.9	4.0807	-6.1489		
			m_1 = 0.03		
			Glycine		
0.0100	1499.3	4.4548	-2.5846		
0.0251	1510.4	4.3881	-4.1839		
0.0401	1526.2	4.2962	-5.2589	0.194	−22.15
0.0552	1546.0	4.1854	-6.1701		
0.0704	1568.3	4.0656	-7.0559		

0.0855	1595.2	3.9281	-7.7790		
			L-Alanine		
0.0100	1498.4	4.4604	-2.0036		
0.0251	1508.1	4.4020	-3.6683		
0.0402	1522.5	4.3178	-4.8442	1.631	−25.83
0.0553	1541.2	4.2123	-5.8090		
0.0705	1565.1	4.0832	-6.6564		
0.0856	1591.5	3.9473	-7.4649		
			L-Valine		
0.0100	1497.5	4.4661	-1.2925		
0.0251	1506.3	4.4133	-3.0819		
0.0402	1520.5	4.3303	-4.3159	2.538	−27.82
0.0554	1539.2	4.2245	-5.3670		
0.0706	1562.1	4.1002	-6.2677		
0.0859	1588.1	3.9657	-7.0826		
			$m_1 = 0.05$		
			Glycine		
0.0100	1503.7	4.4254	-2.8085		
0.0251	1516.8	4.3481	-4.5722		
0.0401	1535.6	4.2411	-5.8505	0.390	−26.72
0.0552	1559.2	4.1124	-6.9133		
0.0703	1588.0	3.9632	-7.7756		
0.0855	1620.3	3.8054	-8.6352		
			L-Alanine		
0.0100	1501.8	4.4370	-2.1905		
0.0251	1513.5	4.3681	-4.0256		
0.0402	1532.1	4.2619	-5.2728	2.168	−32.21
0.0553	1556.2	4.1300	-6.3868		
0.0704	1585.1	3.9798	-7.3201		
0.0856	1618.4	3.8166	-8.2226		
			L-Valine		
0.0100	1500.9	4.4426	-1.4384		
0.0251	1511.4	4.3808	-3.3035		
0.0402	1529.1	4.2792	-4.6369	3.136	−34.33
0.0554	1552.5	4.1503	-5.7678		
0.0706	1581.4	3.9989	-6.7293		
0.0858	1615.9	3.8288	-7.6119		

Figures:

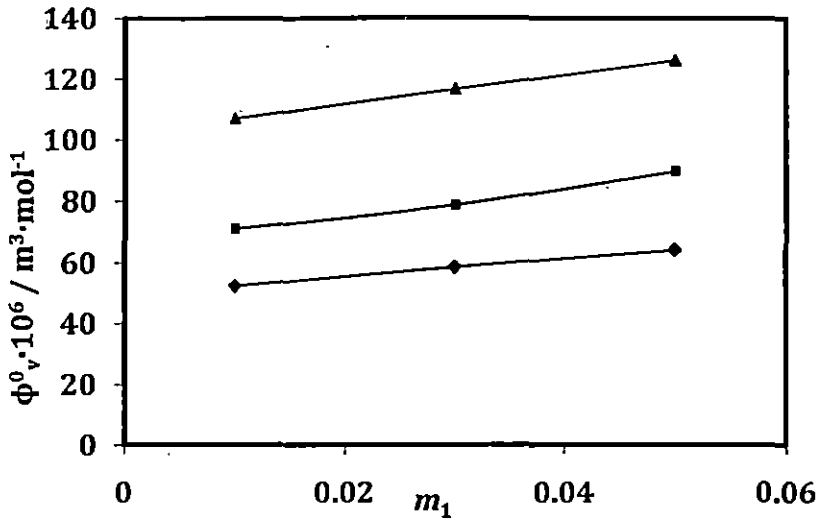


Figure 1: Plot of $\phi_v^\circ \cdot 10^6/m^3 \cdot mol^{-1}$ of Glycine (—▯—), L-Alanine (—■—) and L-Valine (—▲—) in different mass fractions (m_1)of aqueous nicotinic acid solutions at 298.15K.

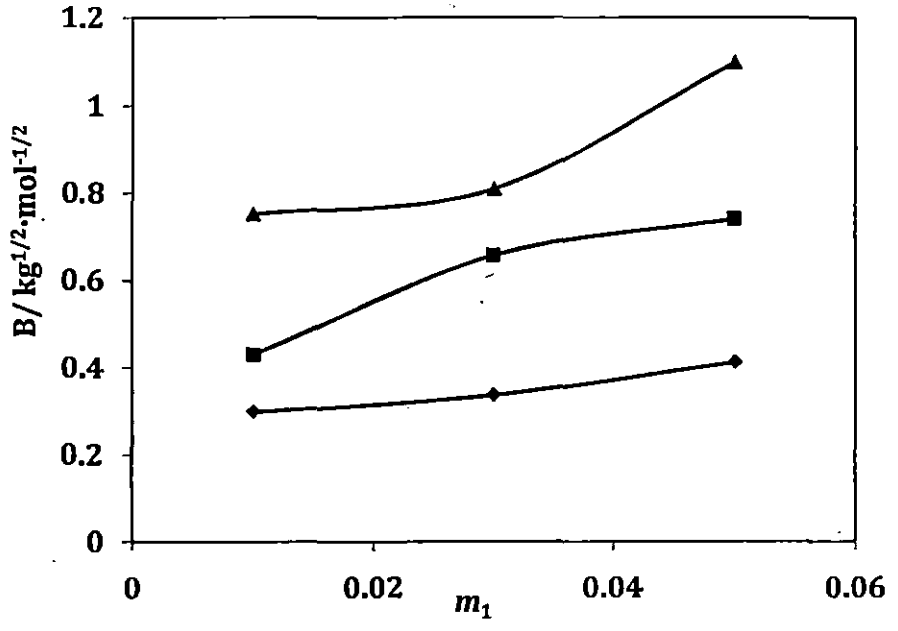


Figure 2: Plot of $B/kg^{1/2}$ $mol^{-1/2}$ of Glycine (—♦—), L-Alanine (—■—) and L-Valine (—▲—) in different mass fractions (m_1)of aqueous nicotinic acid solutions at 298.15K.

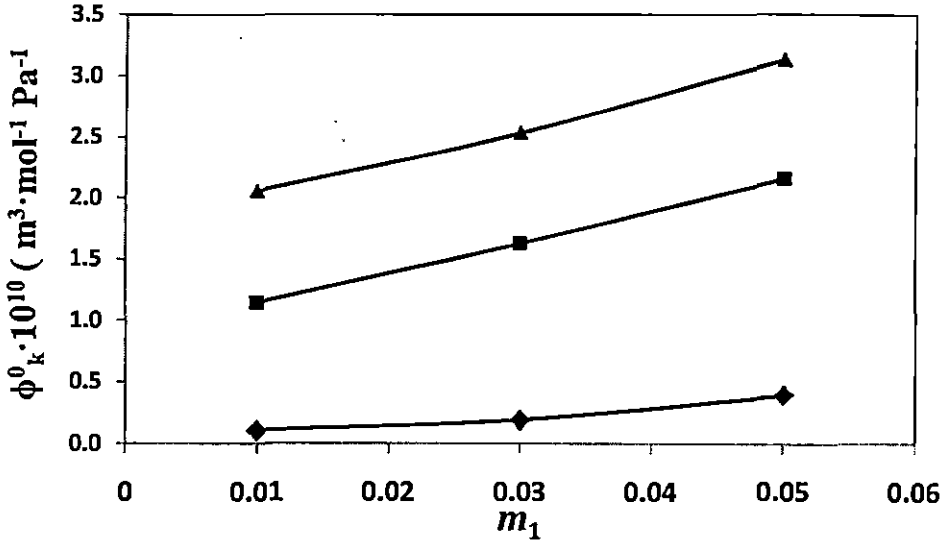
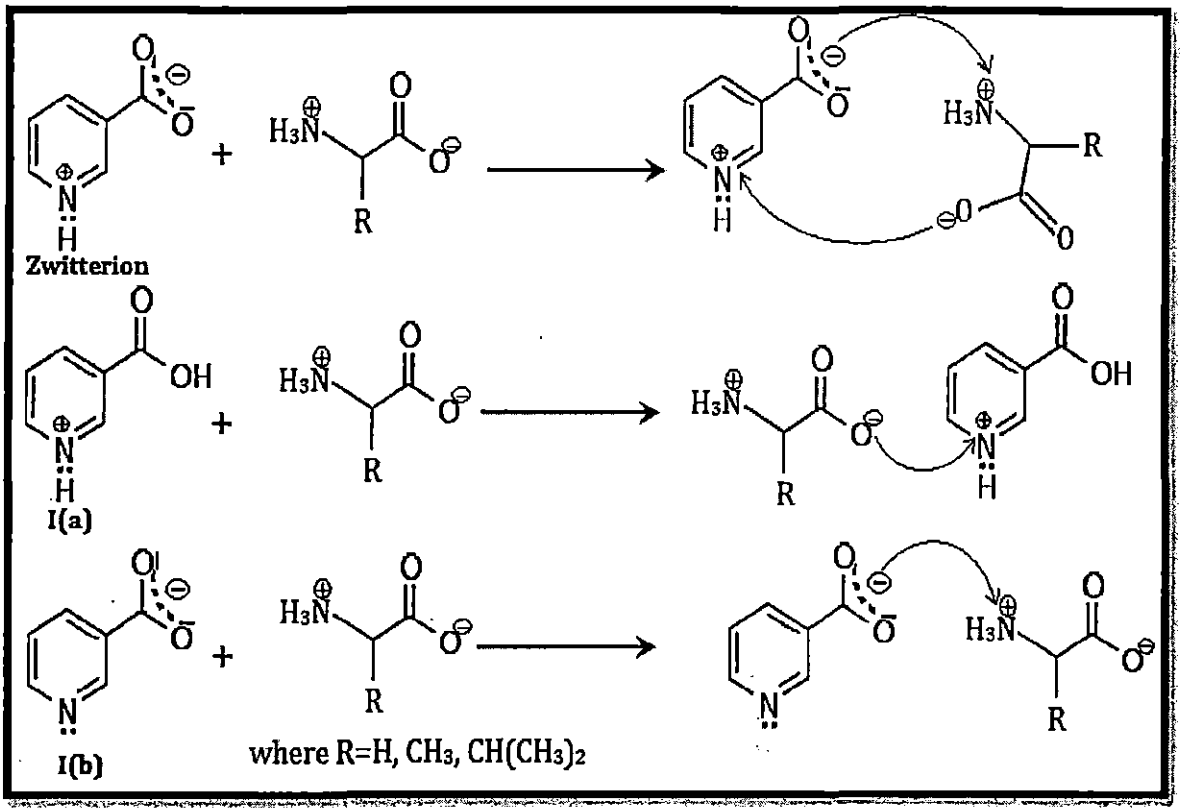


Figure 3: Plot of ϕ_K x 10^{10} (m^3 mol^{-1} Pa^{-1}) of Glycine (—▫—), L-Alanine (—■—) and L- Valine (—▲—) in different mass fractions (m_1) of aqueous nicotinic acid solutions at 298.15K

Scheme:



Scheme I: A schematic representation of the plausible interaction amino acids with nicotinic acids in aqueous solution