



## Study of enthalpy, entropy and free energy of activation of L-Alanine and L-Glutamine with distilled water at different temperatures

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### ABSTRACT

Enthalpy, entropy and free energy of activation have been calculated from the experimental values of density and viscosity of binary liquid mixtures of L-Alanine and L-Glutamine with water at different temperature. Densities and viscosities of liquid mixtures plays an important role in finding their heat content, mass transport, fluid flow and molecular structures etc. excess molar enthalpy of activation and free energy of activation are useful in understanding the nature of intermolecular interactions, dispersion forces and the extent of hydrogen bonding between two liquids. All the mixtures exhibited endothermic enthalpies, entropy of activation are negative over all composition range, its values suggesting weak molecular interaction, dispersive forces and extend of hydrogen bonding between constituent molecules.

**Keywords:** L- Alanine, L-Glutamine, Excess molar volume, Excess molar enthalpy.

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### INTRODUCTION

The physical properties of every substance depend directly on the nature of the molecule of the substance. The estimation of physical and thermodynamic properties would provide reliable information regarding mixing properties with varying intermolecular interactions may be generated, for pure substance and mixtures at any temperature and composition. The investigation is on the molecular association of binary mixtures of L-Alanine and L-Glutamine with water. In view of the importance mentioned, an attempt has been made to elucidate the molecular interaction in mixture of L-Alanine and L-Glutamine with water at 298.15 and 308.15K. Further excess properties are used to explain intermolecular interactions in these binary mixtures. Amino acids, which are the basic components of protein and are considered to be the model compounds of protein molecules, are suitable for better understanding of the interactions occurring between amino acid molecules and the entities present in the living cell. There are studies on volumetric and thermo chemical properties of amino acids in different salt-water mixed solvents, but very few in aqueous solvents. The transport and thermodynamic study on the binary mixtures containing aniline, acetonitrile, ethyl acetate, toluene and benzonitrile have been reported previously by Ali et al, [1]. Nikam et al [2-4] and Gill et al. [5]. Accurate knowledge of thermodynamic and excess properties used to design different industrial process.

### EXPERIMENTAL SECTION

L-Alanine and L-Glutamine (S.D. fine chem. Industries, Mumbai purity 99%) was kept in desiccators containing CaCl<sub>2</sub> for 24hrs after desiccators it is mixed in distilled water with different concentration. The mixtures of the desired composition were prepared by weighting on a HR-120 (A & D Japan) electronic balance with a precision of  $\pm 0.0001$  g. all mixed solvents were prepared by molality. The prepared solution was used within 12hrs.

The densities of pure liquids and binary mixtures were measured by using 15cm<sup>3</sup> double arm pycnometer as describe earlier [2-4]. The Pycnometer was calibrated by using conductivity water with 0.9970 g/cm<sup>3</sup> as its density [6] at 298.15 K. The pycnometer filled with air bubble free experimental liquid was kept in transparent walled water bath for 10-15 min. to attain thermal equilibrium. The position of liquid levels in the two arms was recorded.

The dynamic viscosities were measured using an Ubbelohde suspended level viscometer [3-7], calibrated with conductivity water. An electronic digital stopwatch with readability of  $\pm 0.01$  sec. was used for the flow time measurement, at least three repetitions of each data reproducible to  $\pm 0.05$  sec. were obtained and the result was averaged. Since all flow times were greater than 200 sec. and capillary radius (0.5 mm) was far less than its length (50 to 60mm.). The kinetic energy and corrections respectively were found to be negligible. The uncertainties in dynamic viscosities are of the order  $\pm 0.003$  m Pa s.

## RESULTS AND DISCUSSION

Experimental values of densities ( $\rho$ ) have been used to calculate excess and thermodynamic properties [8-10]. The free energy of activation of viscous flow  $\Delta G^\ddagger$  is calculated as-

$$\Delta G^\ddagger = \Delta H^\ddagger - T \Delta S^\ddagger \quad \dots\dots\dots (1)$$

The values of  $\Delta H^\ddagger$  for the binary mixtures are listed in table 1 and 2. The enthalpy of activation depends on geometrical effect as well as intermolecular interaction<sup>11-13</sup>. The values of  $\Delta H^\ddagger$  are positive for the binary mixtures of L-Alanine and L-Glutamine with water for entire composition range, suggesting the presence of specific interaction between constituent molecules. A close perusal of the table 1 and 2 show that, the mixture exhibited endothermic enthalpies which increased quasi-exponentially and then decreased with increasing concentration of L-Alanine and L-Glutamine. The negative values of  $\Delta S^\ddagger$  indicate that the formation of activated complex introduces molecular order probably due to interactions between the two components of mixtures. The values of  $\Delta G^\ddagger$  are positive for all the binary systems studied at all temperatures and the values of  $\Delta G^\ddagger$  depend on sign and magnitude of corresponding  $\Delta H^\ddagger$  and  $\Delta S^\ddagger$ . The values of  $\Delta G^\ddagger$  increases with temperature increases. [9-13]

**Tabel-1 Thermodynamic Activation Parameters for the L-Alanine + Water system**

$X_1$	$\Delta H^\ddagger \times 10^{-3}$ (J mol <sup>-1</sup> )	$\Delta S^\ddagger$ (JK <sup>-1</sup> mol <sup>-1</sup> )	$\Delta G^\ddagger \times 10^{-3}$ (J mol <sup>-1</sup> )	
			298.15K	308.15K
0.0003	13.4294	0.10489	13.39618	13.39713
0.0010	12.0557	-4.43971	13.37942	13.42384
0.0019	11.2583	-6.98162	13.33995	13.40976
0.0095	13.7096	1.55546	13.24586	13.26031

**Tabel-2 Thermodynamic Activation Parameters for the L-Glutamine + Water system**

$X_1$	$\Delta H^\ddagger \times 10^{-3}$ (J mol <sup>-1</sup> )	$\Delta S^\ddagger$ (JK <sup>-1</sup> mol <sup>-1</sup> )	$\Delta G^\ddagger \times 10^{-3}$ (J mol <sup>-1</sup> )	
			298.15K	308.15K
0.0002	14.18668	0.74655	13.36782	13.38033
0.0010	12.61943	-5.09914	13.13974	13.19073
0.0019	11.55888	-6.04742	13.15954	13.17906
0.0090	15.98074	2.12144	13.16119	13.26997

## CONCLUSION

This paper reports experimental data for density, and viscosity at 298.15 and 308.15 K for binary mixture of L-Alanine and L-Glutamine with water, from these data several thermodynamic excess functions have been calculated and studied to explain the intermolecular interactions between mixing components. Large negative deviations are observed for both the investigated binary systems. This reveals that the existence of molecular interactions in the binary mixtures. The present investigation shows that greater molecular interaction exists in L-Alanine and L-Glutamine with water, which may be due to hydrogen bond formation and weak molecular interaction that exists in the binary mixtures, which may be due to the interaction tends to be weaker with rise in temperature which may be due to weak intermolecular forces and thermal dispersion forces.

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