Probing Solute-Solute and Solute-Solvent Interactions of Amino Acid + Carbohydrate/Drug + Water Systems Using Physicochemical Methods

Abstract Submitted to the University of Delhi for the Award of the Degree of

DOCTOR OF PHILOSOPHY

By

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2013
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The work compiled in this thesis entitled, “Probing solute-solute and solute-solvent interactions of amino acid + carbohydrate/drug + water systems using physicochemical methods” includes the studies of intermolecular interactions occurring between the solute-solute and solute-solvent molecules in solutions of amino acids in aqueous carbohydrate solvents and aqueous drug solvents. The thesis has been divided into eight chapters. A brief account of the work included in each chapter is given below.

Keywords: Density, Viscosity, Ultrasonic Speed, Volumetric properties, Compressibility, Molecular Interactions

Abstract of the Ph.D. Thesis

Chapter 1
This is an introductory chapter. It consists of the scope and objective of the proposed work. Various aspects of the work have been explained. An up to date literature survey has been presented to illustrate the work being carried out in this field.

Chapter 2
Experimental techniques, which have been used in the present investigations, are presented in this chapter. Density, ultrasonic velocity and viscosity have been measured at different temperatures for aqueous-carbohydrate/drug solvents and the solutions of amino acids in aqueous-carbohydrate/drug solvents. The standard procedures for all the apparatus and instruments used have been explained in detail.

Chapter 3
The densities, $\rho$, ultrasonic velocities, $u$, and viscosities, $\eta$ for $l$-histidine + aqueous-glucose solutions have been measured over whole composition range at different temperatures (293.15, 298.15, 303.15, 308.15, 313.15 and 318.15 K). From the experimental data, the values of apparent molar volume, $V_\phi$, limiting apparent molar
volume, $V_\phi^o$ and the slope, $S_v$, transfer volume, $V_{\phi,ir}^o$, apparent molar compressibility, $K_{s,\phi}$, limiting apparent molar compressibility $K_{s,\phi}^o$ and the slope, $S_k$, transfer compressibility, $K_{s,\phi,ir}^o$, viscosity $A$–and $B$ – coefficients and $dB/dT$ have been calculated. The results are interpreted in terms of solute-solvent and solute-solute interactions in these systems.

Chapter 4

The densities, $\rho$, ultrasonic velocities, $u$ and viscosities, $\eta$ for $l$-histidine + aqueous-sucrose solutions have been measured over whole composition range at different temperatures. From the experimental data, the values of $V_\phi$, $V_\phi^o$ and $S_v$, $V_{\phi,ir}^o$, $K_{s,\phi}$, $K_{s,\phi}^o$ and $S_k$, $V_{\phi,ir}^o$, $K_{s,\phi,ir}$, $A$, $B$ and $dB/dT$ have been calculated. The results indicate the presence of strong solute-solvent interactions between $l$-histidine and aqueous-sucrose.

Chapter 5

The densities, $\rho$ and viscosities, $\eta$ had been measured for the mixtures of $l$-threonine with glucose and water and the values of $V_\phi$, $V_\phi^o$ and $S_v$, $V_{\phi,ir}^o$, $A$, $B$ and $dB/dT$, $\Delta \mu_1^{\#}$, $\Delta \mu_2^{\#}$ and $H_n$ have been calculated. It has been observed that there exist strong solute-solvent interactions in these systems, which increase with increase in glucose concentration. The thermodynamics of viscous flow has also been discussed.

Chapter 6

The densities, $\rho$, ultrasonic velocities, $u$ and viscosities, $\eta$ for $l$-threonine + sucrose + water solutions had been measured over the entire composition range and at six different temperatures. The values of $V_\phi$, $V_\phi^o$ and $S_v$, $V_{\phi,ir}^o$, $K_{s,\phi}$, $K_{s,\phi}^o$ and $S_k$, $K_{s,\phi,ir}$, $E_\phi^o$, $(\partial^2 V_\phi^o / dT^2)$, $A$, $B$ and $n_{11}$ have been calculated from the measured data. $\Delta \mu_1^{\#}$ and $\Delta \mu_2^{\#}$ were also calculated and discussed in terms of transition state theory. It has been observed that there exist strong solute-solvent interactions in these systems.
and these interactions increase with increase in sucrose concentration in these solutions.

Chapter 7

The densities, \( \rho \), ultrasonic velocities, \( u \) and viscosities, \( \eta \) for \( l \)-phenylalanine + arabinose/glucose/sucrose + water have been measured and the values of \( V_\phi \), \( V_\phi^o \) and \( S_v \), \( V_{\phi,tr} \), \( K_{s,\phi} \) and \( S_k \), \( K_{s,\phi,tr} \), \( E_\phi \), \( (\partial^2 V_\phi^o / \partial T^2) \), \( A \), \( B \) and \( n_{H1} \) were calculated. The values of \( \Delta \mu_1^o \), \( \Delta \mu_2^o \), \( \Delta S^o \) and \( \Delta H^o \) were also found for all the solutions. The structure-making/breaking ability of the amino acid has also been discussed in terms of \( (\partial^2 V_\phi^o / \partial T^2) \) and \( dB/dT \). The results have been interpreted in terms of solute-solvent and solute-solute interactions in these systems.

Chapter 8

The densities, \( \rho \), ultrasonic velocities, \( u \) and viscosities, \( \eta \) for glycine/ \( l \)-alanine/ \( l \)-valine/ \( l \)-isoleucine with aqueous-streptomycin (1%, 2% w/w) have been measured and the values of \( V_\phi \), \( V_\phi^o \) and \( S_v \), \( V_{\phi,tr} \), \( K_{s,\phi} \) and \( S_k \), \( K_{s,\phi,tr} \), \( E_\phi \), \( (\partial^2 V_\phi^o / \partial T^2) \), \( A \), \( B \) and \( n_{H1} \), \( dB/dT \) were calculated. The structure-making or –breaking ability of the amino acid has also been discussed in terms of the sign of \( (\partial^2 V_\phi^o / \partial T^2) \). In addition to this, \( V_\phi^o \), \( K_{s,\phi} \), \( B \) and \( \Delta \mu_2^o \), have been split into group contributions of the amino acids using linear correlation with number of carbon atoms in the alkyl chain of the amino acids.
List of Publications

1. A. K. Nain, Renu Pal and R. K. Sharma, Volumetric, ultrasonic and viscometric behaviour of l-histidine in aqueous-glucose solutions at different temperatures

2. A. K. Nain, Renu Pal and R. K. Sharma, Physicochemical study of solute-solute and solute-solvent interactions of l-histidine in water + sucrose solutions at different temperatures

3. A. K. Nain and Renu Pal, Study of solute-solute and solute-solvent interactions of l-threonine in aqueous-glucose solutions at different temperatures by using volumetric and viscometric methods,
   *Journal of Chemical Thermodynamics*, 60, 98-104 (2013).

4. A. K. Nain, Renu Pal and Neetu, Volumetric, ultrasonic and viscometric studies of solute-solute and solute-solvent interactions of l-threonine in aqueous-sucrose solutions at different temperatures,
   *Journal of Chemical Thermodynamics*, 64, 172-181 (2013).

5. A. K. Nain, Renu Pal and Neetu, Physicochemical study of solute-solute and solute-solvent interactions of l-phenylalanine in water + arabinose/glucose/sucrose solutions at different temperatures,
   *Journal of Chemical Thermodynamics* (2013) in press.

6. A. K. Nain and Renu Pal, Probing solute-solute and solute-solvent interactions of glycine, l-alanine, l-valine and l-isoleucine in aqueous-streptomycin solutions at different temperatures using physicochemical methods,
   *Journal of Chemical Thermodynamics*, communicated.