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Partial molar adiabatic compressibilities of transfer of some amino acids from water to aqueous lactose solutions at different temperatures

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Apparent molar adiabatic compressibilities ($K_{\phi,\ s}$) of glycine, L-alanine, L-valine, and L-leucine have been determined in aqueous and mixed aqueous solutions of lactose (2 to 6 mass%) at T = (293.15, 298.15, 303.15, and 308.15) K. From these data partial molar adiabatic compressibilities at infinite dilution ($K^0_{\phi,\ s}$) have been evaluated to calculate corresponding transfer function. The transfer partial molar adiabatic compressibilities at infinite dilution ($\Delta K^0_{\phi,\ s}$) are found to be positive. The decrease in the magnitude of transfer partial molar adiabatic compressibilities from glycine to L-leucine indicates the dominance of hydrophobic–hydrophobic interactions between the increasing side chains of amino acids. Also, the contributions of $NH_3^+COO^-$, and CH_2 groups have been calculated by the linear correlation of $K^0_{\phi,\ s}$ with number of carbon atoms in the alkyl chain of amino acids.

1. Introduction

In nearly all chemical and biological processes proteins play a vital role. The detailed three-dimensional structure of proteins and nucleic acids provides information about the molecules but they provide no information about the stability of a molecule or the energetic of its interactions [1]. The interactions of water with the various functional groups of proteins are important factors in determining the conformational stability of proteins [2–4]. Direct study of solute/solvent interactions is difficult due to complex conformation of biological macromolecules [5]. Therefore, the convenient approach is to study simpler model compounds i.e. amino acids and peptides, which are the basic components of proteins [5,6]. When dissolved in water amino acids convert into zwitterionic forms due to the ionization of their carboxyl ($-COOH$) and amino groups (NH_2). In physiological media, this dipolar character of amino acids has an important bearing on biological functions. Amino acids differ from each other in size, charge, hydrogen-bonding capacity, hydrophobicity and chemical reactivity. Hence, these side chains contribute to the structure and function of proteins, individually and collectively [7].

Interactions of carbohydrates and proteins play a key role in a wide range of biochemical process. Therefore, the studies of carbohydrate–protein interactions are very important for biosynthesis, pharmacology and medicine. Analysis of literature data shows that thermodynamic studies of the interactions between the carbohydrates and amino acids are rare in solutions.

In our previous work [8–12], we have studied the thermodynamic and transport properties of amino acid and peptides in amino acid/peptides + saccharides + water ternary systems using DSA 5000 (density and speed of sound analyzer) and Ubbelhode's type viscometer. In this paper, we will report the speeds of sound measurement of amino acids in aqueous saccharide solutions at T = (293.15, 298.15, 303.15 and 308.15) K. From these data, apparent molar adiabatic compressibilities ($K_{\phi,\ s}$), partial molar adiabatic compressibilities at infinite dilution ($K^0_{\phi,\ s}$) and their corresponding transfer function ($\Delta K^0_{\phi,\ s}$), side chain contributions of amino acids, hydration numbers and interaction coefficients have been calculated. These parameters have been discussed in terms of various interactions.

2. Experimental

2.1. Materials

Materials used in the present study are of same origin and purity as used in earlier studies [8,12]. Prior to the preparation of solutions, all the materials were dried under vacuum at T = 323 K and, thereafter, stored over P_2O_5 in vacuum desiccators. Water used (specific conductance $< 10^{-6}\ s \cdot cm^{-1}$) for these investigations was deionized, doubly glass distilled and degassed with vacuum pump. Solutions of lactose were prepared by mass in the range 2% to 6% and used on the day they were prepared. Solutions of glycine, L-alanine, and L-valine in the concentration range 0.05–0.30 $mol \cdot kg^{-1}$ and of L-leucine in the concentration range 0.03–0.14 $mol \cdot kg^{-1}$ were prepared by mass on the molality concentration scale with an accuracy of $\pm 1 \times 10^{-5}$ on an A & D Company, Limited electronic balance (Japan, Model GR-202) with a precision of ±0.01 mg. Uncertainties in solution molalities were estimated at $\pm 2 \times 10^{-5}\ mol \cdot kg^{-1}$ in calculations.

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Table 1
Speeds of sound u, and apparent molar adiabatic compressibilities $K_{\phi,s}$ of amino acids in aqueous lactose solutions at T = (293.15, 298.15, 303.15, and 308.15) K.

m/mol kg^{-1}	T/K = 293.15		T/K = 298.15		T/K = 303.15		T/K = 308.15	
	u/m·s^{-1}	$K_{\phi,s}$·10^6/m^3·mol^{-1}·GPa^{-1}	u/m·s^{-1}	$K_{\phi,s}$·10^6/m^3·mol^{-1}·GPa^{-1}	u/m·s^{-1}	$K_{\phi,s}$·10^6/m^3·mol^{-1}·GPa^{-1}	u/m·s^{-1}	$K_{\phi,s}$·10^6/m^3·mol^{-1}·GPa^{-1}
Glycine + water								
0.00000	1482.98		1497.20		1509.46		1519.91	
0.05482	1485.93	−28.13	1500.06	−26.12	1512.26	−24.59	1522.66	−23.48
0.11064	1488.95	−28.05	1502.98	−26.01	1515.12	−24.52	1525.45	−23.31
0.17921	1492.66	−27.91	1506.61	−25.98	1518.66	−24.49	1528.92	−23.30
0.20435	1494.00	−27.72	1507.86	−25.71	1519.89	−24.27	1530.13	−23.11
0.27545	1497.79	−27.48	1511.59	−25.58	1523.47	−24.03	1533.68	−22.98
0.29661	1498.83	−27.30	1512.64	−25.40	1524.50	−23.90	1534.69	−22.83
Glycine + 2.00 mass% lactose								
0.00000	1489.33		1503.29		1515.35		1525.61	
0.04519	1491.78	−27.50	1507.68	−25.64	1517.67	−23.96	1527.89	−22.80
0.11020	1495.34	−27.41	1509.14	−25.52	1521.01	−23.73	1531.18	−22.69
0.16151	1498.18	−27.39	1511.89	−25.47	1523.67	−23.71	1533.77	−22.54
0.20538	1500.61	−27.28	1514.23	−25.31	1525.96	−23.63	1535.92	−22.25
0.24287	1502.63	−27.06	1516.18	−25.11	1527.86	−23.46	1537.76	−22.06
0.29858	1505.59	−26.68	1519.09	−24.85	1530.70	−23.25	1540.57	−21.96
Glycine + 3.97 mass% lactose								
0.00000	1495.96		1509.65		1521.44		1531.47	
0.05031	1498.76	−27.02	1512.38	−25.20	1524.08	−23.40	1533.99	−21.53
0.11135	1502.18	−26.87	1515.73	−25.19	1527.28	−23.22	1537.06	−21.43
0.15179	1504.43	−26.68	1517.89	−24.87	1529.38	−23.02	1539.06	−21.21
0.20020	1507.20	−26.65	1520.55	−24.74	1531.93	−22.94	1541.49	−21.12
0.24643	1509.82	−26.54	1523.12	−24.73	1534.30	−22.71	1543.76	−20.92
0.29921	1512.80	−26.42	1526.05	−24.61	1537.12	−22.70	1546.32	−20.67
Glycine + 5.84 mass% lactose								
0.00000	1502.25		1515.56		1527.37		1536.78	
0.05181	1505.19	−26.51	1518.45	−25.07	1530.10	−22.62	1539.45	−21.44
0.10076	1507.98	−26.50	1521.18	−24.97	1532.68	−22.57	1541.96	−21.32
0.15902	1511.30	−26.35	1524.47	−24.94	1535.75	−22.42	1544.98	−21.26
0.20044	1513.68	−26.29	1526.80	−24.87	1537.94	−22.35	1547.10	−21.15
0.25603	1516.82	−26.07	1529.90	−24.69	1540.80	−22.10	1549.89	−20.90
0.28892	1518.66	−25.94	1531.70	−24.53	1542.71	−22.38	1551.69	−21.05
L-alanine + 2.12 mass% lactose								
0.00000	1492.24		1505.95		1517.37		1526.42	
0.05319	1496.01	−27.64	1509.38	−23.08	1520.75	−21.75	1529.60	−19.15
0.09804	1499.20	−27.59	1512.25	−22.83	1523.60	−21.66	1532.26	−18.95
0.15416	1503.20	−27.53	1515.86	−22.69	1527.16	−21.52	1535.60	−18.84
0.19488	1506.10	−27.45	1518.43	−22.45	1529.72	−21.39	1537.99	−18.67
0.24413	1509.60	−27.30	1521.58	−22.33	1532.82	−21.23	1540.95	−18.66
0.32455	1515.34	−27.14	1526.75	−22.17	1537.86	−21.04	1545.72	−18.51
L-alanine + 3.94 mass% lactose								
0.00000	1496.55		1510.14		1521.74		1531.48	
0.05829	1500.44	−24.13	1513.92	−22.20	1525.41	−20.50	1535.07	−19.22
0.10803	1503.77	−24.10	1517.14	−22.08	1528.54	−20.39	1538.14	−19.17
0.15002	1506.51	−23.78	1519.86	−22.04	1531.16	−20.24	1540.75	−19.17
0.19743	1509.60	−23.50	1522.88	−21.78	1534.09	−20.02	1543.58	−18.83
0.25318	1513.36	−23.56	1526.49	−21.73	1537.63	−20.05	1547.05	−18.85
0.31114	1517.24	−23.52	1530.15	−21.47	1541.18	−19.81	1550.60	−18.74
L-alanine + 5.92 mass% lactose								
0.00000	1502.52		1515.88		1527.37		1537.14	
0.05906	1506.56	−23.94	1519.80	−21.94	1531.18	−20.25	1540.83	−18.58
0.10210	1509.50	−23.81	1522.67	−21.90	1533.97	−20.24	1543.51	−18.48
0.14760	1512.64	−23.80	1525.70	−21.82	1536.90	−20.12	1546.29	−18.21
0.21007	1516.90	−23.59	1529.84	−21.65	1540.90	−19.92	1550.23	−18.30
0.24103	1519.05	−23.58	1531.86	−21.48	1542.84	−19.75	1552.09	−18.12
0.28869	1522.25	−23.34	1534.97	−21.33	1545.87	−19.62	1555.05	−18.06
L-valine + 2.06 mass% lactose								
0.00000	1489.53		1503.44		1515.45		1525.69	
0.05162	1495.04	−34.86	1508.77	−31.41	1520.40	−26.26	1530.50	−23.91
0.10621	1500.87	−34.66	1514.41	−31.27	1525.62	−26.03	1535.43	−22.98
0.14958	1505.45	−34.32	1518.49	−29.61	1529.76	−25.88	1539.17	−22.01
0.19905	1510.68	−34.04	1523.42	−29.37	1534.46	−25.67	1543.61	−21.89
0.24951	1515.37	−32.30	1527.98	−28.09	1538.81	−24.51	1547.84	−21.12
0.30083	1520.19	−31.21	1532.64	−27.25	1543.29	−23.81	1552.20	−20.68

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