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Volumetric behaviour of amino acids and their group contributions in aqueous lactose solutions at different temperatures

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ABSTRACT

Densities, ρ, for glycine, L-alanine, L-valine, and L-leucine [(0.05 to 0.30) m] in aqueous lactose solutions ranging from pure water to 6 mass% lactose were determined at T = (293.15, 298.15, 303.15, and 308.15) K. The density was used to compute apparent molar volume, V_φ, partial molar volume at infinite dilution, V^0_ϕ, and experimental slope, S_V were obtained and interpreted in terms of solute–solvent and solute–solute interactions. These data were used to calculate the $(\partial V^0_\phi/\partial T)_P$ values. The partial molar volume of transfer, ΔV^0_ϕ from water to aqueous lactose solutions at infinite dilution has also been calculated. In addition to this, the linear correlation of V^0_ϕ with number of carbon atoms in the alkyl chain of amino acids was utilized to determine the respective contributions of $NH_3^+COO^-$, and CH_2 groups to V^0_ϕ.

1. Introduction

Polyhydroxy compounds play a very important role in stabilizing the native conformations of proteins/enzymes [1–3]. From literature survey, it has been found that stabilizing potential of polyols and saccharides are related to the number of the hydroxyl groups. Due to the complex nature of these biological macromolecules, the stabilization mechanism of proteins and their unfolding behaviour in solution is not well understood yet [4].

In living systems, interactions of carbohydrates with proteins play a key role in a wide range of biochemical processes. In particular, carbohydrates located at cell surfaces, are very important as receptors with regard to the bioactive structures of hormones, enzymes, viruses, antibodies etc. [5]. Amino acids, which are the building blocks of protein, are suitable to this kind of research work. Therefore, the study of volumetric properties of these model compounds with saccharides in aqueous medium is very useful to obtain information about various types of interactions in solutions. Most of these interactions are hydrophobic and electrostatic. Moreover, the study of these interactions can give valuable information about various biochemical processes such as protein hydration, aggregation, and denaturation. In recent years, a number of workers have determined the various thermodynamic properties of these model compounds in aqueous solutions containing simple electrolytes having smaller cations of hydrophilic nature [6–19] but very few studies have been done in aqueous saccharide solutions [3,20–22].

In the present study, densities are reported for glycine, L-alanine, L-valine, and L-leucine [(0.05 to 0.30) m] in water and in aqueous lactose solutions at T = (293.15, 298.15, 303.15, and 308.15) K. The parameters like apparent molar volume, V_φ, partial molar volume at infinite dilution, V^0_ϕ, and partial molar volume of transfer at infinite dilution, ΔV^0_ϕ, are evaluated from measured density data. Such data are expected to help to understand the role of amino acids in presence of aqueous lactose solution and the temperature effect on hydration. The contributions of zwitterionic end groups $NH_3^+COO^-$ and $-CH_2$ groups to V^0_ϕ are also evaluated. The results have been discussed in terms of the solute–solute and solute–solvent interactions occurring in the ternary system of the present study.

2. Experimental

Glycine (AR Grade) from (S.D. Fine-chemicals, Mumbai), L-alanine (minimum assay 0.99), L-valine (minimum assay 0.99), L-leucine (minimum assay 0.99), and lactose monohydrate (minimum assay 0.98) from (Hi Media, Mumbai) were used as such without further purifications. Before use these were dried under vacuum at T = 323 K. Thereafter, they were stored over P_2O_5 in desiccators before use. Doubly distilled water (specific conductance < 10^{-6} s · cm^{-1}) which has been freshly degassed was used for the preparation of the aqueous solutions. Solutions of saccharides were prepared by mass in the range 2% to 6%. Solutions of glycine,

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TABLE 1
Values of densities, ρ, and apparent molar volumes, V_φ of amino acids in aqueous lactose solutions at $T = (293.15, 298.15, 303.15, \text{and } 308.15)$ K.

m/ (mol · kg^{-1})	T = 293.15 K		T = 298.15 K		T = 303.15 K		T = 308.15 K	
	$\rho \cdot 10^{-3}$/ (kg · m^{-3})	$V_\varphi \cdot 10^{6}$/ (m^3 · mol^{-1})	$\rho \cdot 10^{-3}$/ (kg · m^{-3})	$V_\varphi \cdot 10^{6}$/ (m^3 · mol^{-1})	$\rho \cdot 10^{-3}$/ (kg · m^{-3})	$V_\varphi \cdot 10^{6}$/ (m^3 · mol^{-1})	$\rho \cdot 10^{-3}$/ (kg · m^{-3})	$V_\varphi \cdot 10^{6}$/ (m^3 · mol^{-1})
				(Glycine + water)				
0.00000	0.998219		0.997050		0.995645		0.994020	
0.05482	0.999976	42.96	0.998789	43.30	0.997364	43.69	0.995728	43.91
0.11064	1.001749	43.03	1.000545	43.36	0.999102	43.72	0.997455	43.94
0.17921	1.003911	43.08	1.002680	43.44	1.001223	43.75	0.999562	43.97
0.20435	1.004694	43.12	1.003457	43.47	1.001996	43.76	1.000332	43.98
0.27545	1.006902	43.19	1.005644	43.53	1.004172	43.79	1.002496	44.01
0.29661	1.007578	43.22	1.006284	43.57	1.004814	43.81	1.003131	44.03
				(Glycine + 2.00 mass% lactose)				
0.00000	1.005719		1.004512		1.003074		1.001423	
0.04519	1.007174	42.75	1.005947	43.20	1.004495	43.52	1.002830	43.85
0.11020	1.009241	42.89	1.007988	43.32	1.006518	43.63	1.004835	43.94
0.16151	1.010849	43.02	1.009582	43.40	1.008095	43.72	1.006401	44.01
0.20538	1.012207	43.13	1.010923	43.52	1.009425	43.82	1.007728	44.07
0.24287	1.013362	43.20	1.012071	43.56	1.010562	43.87	1.008855	44.12
0.29858	1.015057	43.32	1.013754	43.65	1.012232	43.95	1.010513	44.20
				(Glycine + 3.97 mass% lactose)				
0.00000	1.013245		1.011996		1.010523		1.008841	
0.05031	1.014846	43.02	1.013576	43.44	1.012085	43.81	1.010391	44.07
0.11135	1.016759	43.20	1.015470	43.56	1.013961	43.90	1.012252	44.16
0.15179	1.018011	43.30	1.016709	43.66	1.015190	43.97	1.013471	44.23
0.20020	1.019486	43.45	1.018167	43.81	1.016651	44.04	1.014922	44.30
0.24643	1.020887	43.55	1.019560	43.88	1.018034	44.11	1.016296	44.36
0.29921	1.022453	43.71	1.021116	44.02	1.019598	44.19	1.017849	44.43
				(Glycine + 5.84 mass% lactose)				
0.00000	1.020434		1.019145		1.017634		1.015930	
0.05181	1.022070	43.17	1.020764	43.50	1.019236	43.84	1.017517	44.14
0.10076	1.023606	43.20	1.022281	43.56	1.020740	43.87	1.019007	44.17
0.15902	1.025420	43.24	1.024074	43.60	1.022517	43.90	1.020767	44.21
0.20044	1.026697	43.29	1.025339	43.64	1.023771	43.93	1.022011	44.23
0.25603	1.028395	43.36	1.027022	43.70	1.025445	43.97	1.023669	44.27
0.28892	1.029399	43.38	1.028011	43.73	1.026430	43.99	1.024644	44.29
				(L-Alanine + water)				
0.00000	0.998219		[27]		0.995645		[27]	
0.05513	0.999806	59.96			0.997215	60.66		
0.09996	1.001121	59.94			0.998487	60.63		
0.15466	1.002698	59.92			1.000030	60.61		
0.20028	1.004007	59.90			1.001298	60.58		
0.24424	1.005268	59.87			1.002572	60.55		
0.30387	1.006962	59.85			1.004211	60.53		
				(L-Alanine + 2.12 mass% lactose)				
0.00000	1.006173		1.004957		1.003515		1.001861	
0.05319	1.007684	60.40	1.006462	60.55	1.005003	60.91	1.003340	61.13
0.09804	1.008947	60.43	1.007718	60.60	1.006247	60.94	1.004577	61.16
0.15416	1.010518	60.45	1.009272	60.68	1.007790	60.98	1.006110	61.21
0.19488	1.011649	60.46	1.010389	60.73	1.008905	60.99	1.007213	61.24
0.24413	1.013001	60.51	1.011728	60.78	1.010234	61.04	1.008537	61.27
0.32455	1.015189	60.56	1.013884	60.88	1.012404	61.04	1.010677	61.33
				(L-Alanine + 3.94 mass% lactose)				
0.00000	1.013315		1.012059		1.010580		1.008897	
0.05829	1.014952	60.47	1.013691	60.60	1.012194	60.95	1.010500	61.19
0.10803	1.016338	60.49	1.015070	60.64	1.013558	60.99	1.011856	61.22
0.15002	1.017499	60.51	1.016224	60.68	1.014702	61.01	1.012991	61.25
0.19743	1.018802	60.53	1.017516	60.72	1.015983	61.04	1.014264	61.27
0.25318	1.020322	60.55	1.019020	60.77	1.017478	61.07	1.015749	61.30
0.31114	1.021890	60.57	1.020568	60.82	1.019029	61.11	1.017279	61.33
				(L-Alanine + 5.92 mass% lactose)				
0.00000	1.020737		1.019447		1.017935		1.016225	
0.05906	1.022376	60.55	1.021070	60.85	1.019545	61.12	1.017819	61.44
0.10210	1.023559	60.59	1.022240	60.90	1.020707	61.16	1.018972	61.45
0.14760	1.024796	60.65	1.023467	60.95	1.021928	61.18	1.020184	61.46
0.21007	1.026478	60.71	1.025135	61.00	1.023587	61.22	1.021835	61.47
0.24103	1.027302	60.75	1.025950	61.04	1.024401	61.24	1.022648	61.48
0.28869	1.028565	60.79	1.027202	61.08	1.025650	61.27	1.023891	61.49
				(L-Valine + water)				
0.00000	0.998219		0.997050		0.995645		0.994020	
0.04524	0.999424	90.52	0.998244	90.84	0.996827	91.19	0.995195	91.46
0.09973	1.000872	90.48	0.999672	90.81	0.998242	91.15	0.996600	91.43

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