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Volumetric Properties of Diglycine from Water to Aqueous Amino Acids solutions at 298.15 K and 310.15 K

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Abstract Densities of diglycine in aqueous solutions of L-alanine and L-serine were measured at 298.15 K and 310.15 K. The standard partial molar volume (V_ϕ^0), standard partial molar volumes of transfer ($\Delta_{tr}V_\phi^0$) have been determined. The results show that, the $\Delta_{tr}V_\phi^0$ values of diglycine are positive and vary in the sequence L-serine>L-alanine. And the $\Delta_{tr}V_\phi^0$ increase with the increasing concentration of amino acids, but decrease with the increasing temperature. The results have been interpreted in terms of structure interaction model.

1. Introduction

Weak interactions such as hydrogen bonding, electrostatic, hydrophobic interactions etc. play an important role in the stabilization of proteins. Because the structure of protein is very complicate, direct research on the nature of proteins is difficult. Dipeptides and amino acids have been used as models by researchers for understanding the thermodynamic behavior of proteins. Volumetric methods have been widely used to provided the interaction information between model moleculars and different solvents[1-3]. For further understanding the interaction between amino acid residues and peptide backbone, and as a continuation of volumetric investigations on model moleculars systems in our laboratory[4,5], the interactions between diglycine and amino acids have been studied in this paper.

2. Experimental

Diglycine (>99%, Aldrich), L-alanine and L-serine (>99%, Shanghai Chem. Co.) were used without further purification. The water was deionized and distilled twice. All solutions were prepared freshly by mass on a METTLER AE200 balance with a sensitivity of ± 0.0001g.

The densities of the solutions were measured by DMA 5000M digital densimeter(Anton Paar, Austria) at 298.15 K and 310.15 K respectively. The uncertainty of densitiy is within 5×10^{-6} g·cm^{-3}. The densimeter was calibrated with twice distilled water and dried air. All the measurements were carried out under atmosphere pressure.

3. Result and Discussion

The density of diglycine in aqueous L-alanine and L-serine solutions at 298.15 K and 310.15 K are given in table 1-2. Apparent molar volumes (V_ϕ) of diglycine were calculated by using the equation

$$V_\phi = M/\rho - 1000(\rho-\rho_0)/m\rho\rho_0 \quad (1)$$

where M is the molar mass of diglycine, ρ and ρ_0 is the density of solution and solvent respectively, m is the molality of diglycine in the solvent. The calculated apparent molar volumes for diglycine are also listed in table 1-2.

Table 1 Densities and apparent molar volume of glycylglycine in aqueous solutions of L-alanine at 298.15 K and 310.15 K

m[mol·kg^{-1}]	ρ[g·cm^{-3}]	V_ϕ[cm^3·mol^{-1}]	m[mol·kg^{-1}]	ρ[g·cm^{-3}]	V_ϕ[cm^3·mol^{-1}]
	298.15 K			310.15 K	
	m=0.0503 mol·kg^{-1}			m=0.0501 mol·kg^{-1}	
0.0000	0.998498	--	0.0000	0.994786	--
0.1027	1.004144	76.73	0.1003	1.000243	77.42
0.2006	1.009429	76.81	0.2019	1.005644	77.62
0.2527	1.012191	76.92	0.2525	1.008292	77.71
0.3023	1.014774	77.05	0.3034	1.010928	77.79
0.3557	1.017549	77.12	0.3575	1.013661	77.98
	m=0.1002 mol·kg^{-1}			m=0.1001 mol·kg^{-1}	
0.0000	0.999903	--	0.0000	0.996086	--
0.1051	1.005669	76.80	0.1010	1.001567	77.52
0.2033	1.010940	76.99	0.2004	1.006857	77.64
0.2575	1.013775	77.18	0.2518	1.009521	77.81
0.3053	1.016277	77.22	0.3015	1.012065	77.97
0.3557	1.018882	77.30	0.3551	1.014800	78.06
	m=0.1492 mol·kg^{-1}			m=0.1500 mol·kg^{-1}	
0.0000	1.001292	--	0.0000	0.997515	--
0.1001	1.006808	77.01	0.2029	1.008359	77.90
0.1996	1.012226	77.10	0.2539	1.010980	78.09
0.2502	1.014863	77.24	0.3034	1.013511	78.22
0.3010	1.017517	77.38	0.3497	1.015845	78.33
0.3500	1.020113	77.44	0.4047	1.018684	78.35
	m=0.2002 mol·kg^{-1}			m=0.2000 mol·kg^{-1}	
0.0000	1.002702	--	0.0000	0.998871	--
0.1001	1.008223	76.99	0.1026	1.004411	77.72
0.2001	1.013417	77.24	0.2041	1.009720	78.15
0.3002	1.018896	77.43	0.3046	1.014877	78.34
0.3502	1.021218	77.51	0.3529	1.017344	78.38
	m=0.2483 mol·kg^{-1}			m=0.2502 mol·kg^{-1}	
0.0000	1.004033	--	0.0000	1.000264	--
0.1015	1.009564	77.11	0.1039	1.005840	78.01
0.2539	1.017620	77.47	0.2554	1.013736	78.32
0.3056	1.020298	77.54	0.3052	1.016281	78.37
0.3534	1.022753	77.59	0.3535	1.018707	78.50

Table 2 Densities and apparent molar volume of glycylglycine in aqueous solutions of L-serine at 298.15 K and 310.15 K

m[mol·kg^{-1}]	ρ[g·cm^{-3}]	V_ϕ[cm^3·mol^{-1}]	m[mol·kg^{-1}]	ρ[g·cm^{-3}]	V_ϕ[cm^3·mol^{-1}]
	298.15 K			310.15 K	
	m=0.0503 mol·kg^{-1}			m=0.0501 mol·kg^{-1}	
0.0000	0.999273	--	0.0000	0.994711	--
0.1002	1.004774	76.81	0.1135	1.000887	78.16
0.2038	1.010339	76.99	0.2122	1.006228	78.59
0.2533	1.012963	77.05	0.2613	1.008833	78.96
0.3043	1.015628	77.12	0.3049	1.011148	79.22
0.3543	1.018193	77.27	0.3579	1.014060	79.70
	m=0.1004 mol·kg^{-1}			m=0.1003 mol·kg^{-1}	
0.0000	1.001469	--	0.0000	0.997628	--
0.1007	1.006991	76.85	0.1951	1.008072	77.82
0.2033	1.012484	77.06	0.2532	1.011106	77.89
0.2546	1.015168	77.23	0.3016	1.013602	77.97

0.3028	1.017691	77.26	0.3531	1.016220	78.07
0.3538	1.021319	77.35	0.4069	1.018901	78.23
	m=0.1461 mol·kg^{-1}			m=0.1499 mol·kg^{-1}	
0.0000	1.003464	--	0.0000	0.999773	--
0.1015	1.009009	77.01	0.1004	1.005197	77.68
0.2045	1.014505	77.19	0.2528	1.013153	78.15
0.2438	1.016570	77.26	0.3017	1.015662	78.22
0.3544	1.022294	77.44	0.4051	1.020864	78.40
	m=0.2001 mol·kg^{-1}			m=0.1994 mol·kg^{-1}	
0.0000	1.005804	--	0.0000	1.001929	--
0.1013	1.011342	77.09	0.1012	1.007371	77.87
0.2001	1.016628	77.40	0.2012	1.012604	78.17
0.3005	1.021899	77.58	0.3042	1.017865	78.44
0.3506	1.024494	77.67	0.3542	1.020358	78.60
	m=0.2492 mol·kg^{-1}			m=0.2501 mol·kg^{-1}	
0.0000	1.007888	--	0.0000	1.004040	--
0.1023	1.013432	77.33	0.1005	1.009412	78.14
0.2064	1.018925	77.59	0.2027	1.014754	78.31
0.2533	1.021358	77.70	0.3036	1.019926	78.45
0.3036	1.023954	77.75	0.3500	1.022237	78.60
0.3556	1.026620	77.78	0.4025	1.024812	78.77

The apparent molar volumes can be fit by the equation

$$V_\phi = V_\phi^0 + B_v m \tag{2}$$

where V_ϕ^0 is the standard partial molar volume and B_v is an experimentally determined parameter. Values of V_ϕ^0 are listed in table 3.

Table 3 Standard partial molar volume(V_ϕ^0) and transfer partial molar volume ($\Delta_{tr}V_\phi^0$) of glycylglycine in aqueous amino acid solutions

$m[\mathrm{mol\cdot kg^{-1}}]$	$V_\phi^0[\mathrm{cm^3\cdot mol^{-1}}]$	$\Delta_{trs}V_\phi^0[\mathrm{cm^3\cdot mol^{-1}}]$	$m[\mathrm{mol\cdot kg^{-1}}]$	$V_\phi^0[\mathrm{cm^3\cdot mol^{-1}}]$	$\Delta_{trs}V_\phi^0[\mathrm{cm^3\cdot mol^{-1}}]$
	298.15 K			310.15 K	
		L-alanine			
0.0000	76.16[a]	--	0.0000	77.20	--
0.0510	76.53	0.37	0.0502	77.21	0.01
0.1002	76.60	0.44	0.1001	77.26	0.05
0.1492	76.80	0.64	0.1500	77.49	0.29
0.2002	76.81	0.65	0.2000	77.53	0.33
0.2483	76.95	0.80	0.2502	77.80	0.60
		L-serine			
0.0503	76.63	0.47	0.0501	77.37	0.17
0.1004	76.66	0.50	0.1003	77.42	0.22
0.1461	76.83	0.67	0.1499	77.49	0.29
0.2001	76.91	0.75	0.1994	77.59	0.39
0.2492	77.18	1.02	0.2501	77.91	0.71

[a] Literature values:76.23[6], 76.29[7]

The transfer partial molar volumes ($\Delta_{tr}V_\phi^0$) of diglycine from water to aqueous L-alanine and L-serine solutions were calculated by the equation (3), and the results are listed in table 3.

$$\Delta_{tr}V_\phi^0 = V_\phi^0(\text{in aqueous amino acid solutions}) - V_\phi^0(\text{in water}) \tag{3}$$

The V_ϕ^0 of diglycine can be viewed as [8]

$$V_\phi^0 = V_{VW} + V_{void} - V_{shrinkage} \tag{4}$$

Where V_{VW} is the van der Waals volume, V_{void} is the contribution associated with the voids and empty volume, $V_{shrinkage}$ is the shrinkage in volume due to solute-solvent interaction. It is generally

assumed that V_{VW} and V_{void} remains approximately the same in water and in aqueous solutions[8], so the $\Delta_{tr}V_{\phi}^{0}$ reflect solely the interactions between diglycine and amino acids.

It can be seen from table 3, the $\Delta_{tr}V_{\phi}^{0}$ values are positive and increase with the increasing concentration of amino acids. The positive $\Delta_{tr}V_{\phi}^{0}$ values indicating that the interaction between diglycine and amino acid make water molecules relaxed to bulk water, and the volume of the solution increases.

The relative order of $\Delta_{tr}V_{\phi}^{0}$ at the same temperature is L-serine> L-alanine. The two amino acids have similar structures but different side groups. So the difference in $\Delta_{tr}V_{\phi}^{0}$ primarily comes from the influence of side group.The result can be well explained by structure interaction model[9]. Diglycine and amino acids in aqueous solutions are major in the form of zwitterions. The structure interaction can be separated into: (a) Hydrophilic-hydrophilic interaction between diglycine and zwitterionic head group of amino acid, and between diglycine and side $–CH_2OH$ group of L-serine, which lead a positive contribution to $\Delta_{tr}V_{\phi}^{0}$ [9]. (b) Hydrophilic-hydrophobic interaction between diglycine and the side $–CH_3$ group of L-alanine, which gives a negative contribution to $\Delta_{tr}V_{\phi}^{0}$ [9].The positive $\Delta_{tr}V_{\phi}^{0}$ values reflect that the interaction of type (a) is predominent. For L-serine, the side $-CH_2OH$ group lead additional hydrophilic-hydrophilic interaction and for L-alanine the $–CH_3$ group of provides a tendency of hydrophobic-hydrophilic.

For the same amino acid, the decrease $\Delta_{tr}V_{\phi}^{0}$ values as can be seen in table 3 with the increasing temperature which shows that the increase in temperature strengthens water molecules around diglycine molecular rather than banding them to amino acids.

4. Conclusions

Density of diglycine in aqueous solutions of L-alanine and L-serine were measured at 298.15 K and 310.15 K. The influence of different interactions between diglycine and amino acids on $\Delta_{tr}V_{\phi}^{0}$ is discussed. The results show that hydrophilic-hydrophilic interaction has great contributions to $\Delta_{tr}V_{\phi}^{0}$, but the side group of amino acid is responsible for the difference of $\Delta_{tr}V_{\phi}^{0}$.

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