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Volumetric behavior of glycine in aqueous succinic acid and sodium succinate buffer at different temperatures

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ABSTRACT

Apparent molar volume ($\varnothing_V$) of glycine in aqueous succinic acid and in aqueous sodium succinate buffer solutions have been determined from precisely measured density data at different temperatures ranging from 288.15 to 328.15 K. The $\varnothing_V$ values of glycine in aqueous succinic acid solutions increase with increase in molality of glycine and temperature whereas $\varnothing_V$ values of glycine in sodium succinate buffer shows different behavior as a function of molality and temperature at pH = 1.00, 7.40 and 14.00. Partial molar volume at infinite dilution ($\varnothing_V^o$) and partial molar volume of transfer (ΔV_{tr}) has been determined from$\varnothing_V$. Both positive and negative ΔV_{tr} values have been observed for glycine in the presence of sodium succinate buffer solutions, whereas only negative, ΔV_{tr} values have been observed in the presence of aqueous succinic acid solutions. Partial molar expansibilities $\left(\frac{\partial \varnothing_V^o}{\partial T}\right)_P$ determined from $\varnothing_V^o$ data, are higher in the presence of buffer solutions as compared to that of aqueous succinic acid solutions. Hydration numbers (n_H) for glycine in aqueous succinic acid solutions are higher than in aqueous sodium succinate buffer solutions at pH 7.40, which suggest a dehydration effect in later case.

1. Introduction

The physicochemical properties of amino acids in aqueous and mixed aqueous solutions of various additives have generated a great interest, as the studies on these basic building blocks of proteins provide an understanding of the effect of additive on biomolecules [1–8]. The interpretation of the behavior of these model compounds is quite helpful in understanding the water-protein interactions in solutions. The interactions of water with the various functional groups of proteins play a crucial role in determining the conformational stability of proteins [9–13]. In order to maintain the biological function and catalytic activity, it is desirous that proteins maintain their natively folded structure under physiological conditions. However, most proteins are sensitive to slightest change in cellular and environmental conditions such as temperature, pH, pressure and the presence of salts. The moderate change in solution pH and/or strength often results in drastic change in the conformational state of the protein and/or dissociation of protein complex [14].

The stabilization of native conformation of biological macromolecules is commonly related to several non-covalent interactions including hydrogen bonding, electrostatic and hydrophobic interactions. These interactions are affected by surrounding solutes and solvent in the immediate vicinity of macromolecules; for this reason, the physico-chemical behavior of proteins are strongly influenced by the presence of solutes, buffers etc. [15,16].

Buffers are compounds that undergo reversible protonation and, thus, aid in maintaining the pH of a solution [17]. Over the last 30 years a variety of buffers that are suitable for biological systems have been developed. Some of the criteria used for these buffers have included good solubility in water, low membrane permeability, minimum salt effect, low ion effect, good stability and high purity [18]. Succinic acid ($C_4H_6O_4$) also known as amber acid or butanedioic acid is a dicarboxylic acid with pk_a values of 4.21 and 5.64 at room temperature. It has been widely used in many fields, such as food, agriculture, pharmaceutical and polymer industries [19]. It combines with protein to rebuild muscle fibers, nerve endings and help fight infection. Several amino acids are metabolized to succinic acid, providing a source of anaerobic and aerobic energies and have been shown to be important in supplying the heart with fuel of myocardium contractions under low oxygen conditions [20,21]. Sodium Succinate dibasic hexahydrate has been used to study X-ray crystallography, protein structural analysis, proteomics and optimization reagents. It has also been used to determine the

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Table 1
Specification of chemical used.

Chemical name	CAS number	Provenance	Mass fraction purity
Glycine	56-40-6	S D Fine Chem. Limited	≥99.0
Succinic acid	110-15-6	LOBA Chemie, India	minimum 99.0
Sodium succinate dibasic hexahydrate	6106-21-4	S D Fine Chem. Limited	≥99.0

calorimetric and diffractometric evidence for the sequential crystallization of buffer components and the consequential pH swing in frozen solutions [22].

Thus, considering the importance of succinic acid and its salt, the densities (ρ) of glycine in (0.1, 0.3 and 0.5) M aqueous succinic acid (SA) and in (0.1 and 0.5) M aqueous sodium succinate buffer

Table 2
The densities (ρ) and apparent molar volumes ($\varnothing_V$) of glycine in water and in aqueous (0.1, 0.3 and 0.5) M succinic acid (SA) solutions at different temperatures, T = (288.15 to 328.15) K and P = 101.3 kPa.

m/ (mol·kg^{-1})	ρ/ (g·cm^{-3})	$\varnothing_V$/ (cm^3·mol^{-1})	ρ/ (g·cm^{-3})	$\varnothing_V$/ (cm^3·mol^{-1})	ρ/ (g·cm^{-3})	$\varnothing_V$/ (cm^3·mol^{-1})	ρ/ (g·cm^{-3})	$\varnothing_V$/ (cm^3·mol^{-1})	ρ/ (g·cm^{-3})	$\varnothing_V$/ (cm^3·mol^{-1})
Glycine in water										
	288.15 K		293.15 K		298.15 K		303.15 K		308.15 K	
0.00000	0.99909		0.99820		0.99704		0.99564		0.99403	
0.09982	1.00230	42.78	1.00137	43.20	1.00017	43.61	0.99875	43.83	0.99712	44.05
0.19877	1.00543	42.91	1.00446	43.33	1.00323	43.69	1.00178	43.97	1.00013	44.19
0.39340	1.01152	42.95	1.01047	43.37	1.00918	43.72	1.00767	44.02	1.00598	44.25
0.49581	1.01462	43.09	1.01354	43.49	1.01222	43.83	1.01069	44.11	1.00897	44.36
0.84908	1.02509	43.33	1.02388	43.73	1.02246	44.05	1.02085	44.32	1.01907	44.55
0.98821	1.02893	43.59	1.02769	43.96	1.02624	44.27	1.02460	44.54	1.02279	44.77
	310.15 K		313.15 K		318.15 K		323.15 K		328.15 K	
0.00000	0.99332		0.99221		0.99021		0.98803		0.98569	
0.09982	0.99640	44.17	0.99528	44.28	0.99326	44.51	0.99107	44.64	0.98873	44.68
0.19877	0.99940	44.30	0.99828	44.37	0.99624	44.60	0.99404	44.73	0.99169	44.82
0.39340	1.00524	44.33	1.00409	44.45	1.00203	44.64	0.99981	44.77	0.99745	44.86
0.49581	1.00823	44.43	1.00707	44.55	1.00500	44.72	1.00276	44.88	1.00039	44.97
0.84908	1.01829	44.65	1.01707	44.80	1.01419	44.92	1.01267	45.13	1.01027	45.24
0.98821	1.02201	44.86	1.02081	44.97	1.01869	45.12	1.01638	45.29	1.01401	45.36
Glycine in 0.1 M aqueous SA										
	288.15 K		293.15 K		298.15 K		303.15 K		308.15 K	
0.00000	1.00282		1.00183		1.00062		0.99917		0.99824	
0.01128	1.00320	41.33	1.00221	41.34	1.00100	41.35	0.99955	41.36	0.99862	41.37
0.07318	1.00530	41.06	1.00432	40.93	1.00309	41.21	1.00160	41.77	1.00066	41.92
0.10153	1.00617	41.91	1.00515	42.21	1.00390	42.62	1.00241	42.03	1.00146	43.24
0.19931	1.00932	42.16	1.00827	42.47	1.00699	42.83	1.00548	43.15	1.00450	43.41
0.30076	1.01244	42.64	1.01133	43.05	1.01000	43.47	1.00850	43.65	1.00750	43.90
0.39638	1.01539	42.79	1.01425	43.18	1.01292	43.50	1.01134	43.84	1.01035	44.01
0.49580	1.01833	43.09	1.01705	43.68	1.01574	43.90	1.01421	44.08	1.01307	44.52
0.85672	1.02906	43.27	1.02770	43.72	1.02631	43.95	1.02467	44.19	1.02340	44.61
1.00209	1.03313	43.47	1.03181	43.81	1.03029	44.14	1.02859	44.42	1.02745	44.64
	310.15 K		313.15 K		318.15 K		323.15 K		328.15 K	
0.00000	0.99802		0.99731		0.99614		0.99580		0.99347	
0.01128	0.99840	41.37	0.99769	41.37	0.99652	41.38	0.99618	41.39	0.99385	41.40
0.07318	1.00044	41.92	0.99972	42.06	0.99851	42.62	0.99815	42.90	0.99582	42.93
0.10153	1.00122	43.44	1.00058	42.75	0.99938	43.06	0.99901	43.36	0.99667	43.49
0.19931	1.00424	43.62	1.00369	42.82	1.00237	43.59	1.00202	43.64	0.99968	43.72
0.30076	1.00726	43.97	1.00669	43.51	1.00524	44.46	1.00483	44.70	1.00248	44.80
0.39638	1.01011	44.06	1.00936	44.17	1.00806	44.52	1.00768	44.63	1.00518	45.10
0.49580	1.01280	44.63	1.01226	44.29	1.01070	45.11	1.01030	45.23	1.00767	45.89
0.85672	1.02312	44.68	1.02255	44.53	1.02075	45.29	1.01978	46.05	1.01745	46.09
1.00209	1.02714	44.74	1.02642	44.76	1.02419	45.86	1.02348	46.25	1.02058	46.87
Glycine in 0.3 M aqueous SA										
	288.15 K		293.15 K		298.15 K		303.15 K		308.15 K	
0.00000	1.00956		1.00839		1.00687		1.00527		1.00402	
0.07111	1.01232	36.18	1.01107	37.28	1.00950	37.98	1.00789	38.12	1.00632	42.59
0.10412	1.01332	38.78	1.01213	38.98	1.01058	39.26	1.00894	39.65	1.00734	42.99
0.19634	1.01622	40.81	1.01503	40.92	1.01350	40.98	1.01170	42.00	1.01019	43.33
0.29510	1.01922	41.84	1.01799	42.05	1.01641	42.27	1.01462	42.92	1.01307	43.95
0.39562	1.02236	42.08	1.02109	42.34	1.01950	42.53	1.01773	42.98	1.01610	43.95
0.49806	1.02532	42.65	1.02402	42.92	1.02250	42.94	1.02060	43.55	1.01897	44.33
0.84000	1.03543	43.04	1.03403	43.33	1.03245	43.42	1.03062	43.71	1.02878	44.43
1.00206	1.04017	43.08	1.03873	43.36	1.03711	43.48	1.03518	43.84	1.03333	44.46
	310.15 K		313.15 K		318.15 K		323.15 K		328.15 K	
0.0000	1.00295		1.00198		1.00071		0.99765		0.99521	
0.07111	1.00523	42.88	1.00425	43.03	1.00296	43.32	0.99988	43.64	0.99743	43.81
0.10412	1.00628	42.91	1.00529	43.11	1.00396	43.67	1.00088	43.94	0.99843	44.06
0.19634	1.00906	43.65	1.00819	43.15	1.00673	44.13	1.00361	44.48	1.00115	44.62

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