

Molecular interaction studies on binary mixture of lysine and adenosine at different temperatures

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Ultrasonic velocity, density and viscometric measurements have been performed on lysine and binary mixture of lysine and adenosine at 25, 30 and 35°C. These measurements have been used to evaluate some useful ultrasonic and thermodynamic parameters viz. apparent molal volume ϕ_v , apparent molal compressibility ϕ_k and isentropic compressibility β_s . The results have been discussed in the light of solute-solvent interactions. Effect of temperature variation on these interactions has been discussed.

Nucleic acids are the fundamental structural units of compounds of biological relevance¹. Adenosine is one of the most important class of nucleosides in molecular biology². Ultrasonic and volumetric studies of the conformational properties of these molecules, the interactions of their different chemical groups with water molecules in aqueous solution and with each other in solution and the temperature dependence of these interactions play a very important role in understanding the thermodynamic behaviour of biochemical processes in living cells. Extensive studies of the temperature variation of ultrasonic velocity and allied parameters of non-electrolytes as a function of concentration have been made by many workers^{3,4}. Recently Pandey *et al.*⁵⁻⁷ have reported the ultrasonic and thermodynamic studies on adenosine and its allied compounds in aqueous and non-aqueous solutions. An extensive study of thermodynamic properties of amino acids have been carried out by many workers⁸⁻¹⁰, but such investigations in binary mixtures are scanty. Hence, in order to investigate solute-solvent and solute-solute interactions in binary mixtures of lysine and adenosine in aqueous solutions, in the present work volumetric, viscometric and ultrasonic velocity measurements of lysine and lysine-adenosine mixture in aqueous solution at 25, 30 and 35°C have been carried out and the results are reported herein.

Experimental

Lysine and adenosine used were of AR grade. Purity was checked by paper and thin layer chromatography with accuracy of 0.01%. Triply distilled water was used to prepare stock solutions of lysine and adenosine. All the measurements have been carried out on a water bath thermostatically controlled within $\pm 0.01^\circ\text{C}$. The density measurements were performed with pycnometer at 25, 30 and 35 $\pm 0.01^\circ\text{C}$. The apparent molal volume¹¹ (ϕ_v) is the linear function of the concentration term and is in good agreement with Masson's equation¹².

$$\phi_v = \phi_v^\circ + S_v \sqrt{m} \quad \dots (1)$$

where ϕ_v° is the partial molal volume at infinite dilution and is a measure of solute-solvent interactions. It is obtained from the linear plot of ϕ_v versus $\sqrt{m}$ using the least squares method. S_v is the experimental slope, a measure of ion-solvent interaction¹³.

The ultrasonic velocity (U) was measured by single crystal variable path ultrasonic interferometer operating at 1 MHz frequency at different temperatures with accuracy of the interferometer is $\pm 0.5 \text{ ms}^{-1}$.

The viscosity of the solution was measured by using calibrated Ostwald viscometer at 25, 30 and 35°. Uncertainties in the measured viscosities were with $\pm 0.01\%$.

The adiabatic compressibility β_s of aqueous solutions was determined from the sound velocity using the relation,

$$\beta_s = 1/U^2 \rho \quad \dots (2)$$

The apparent molal compressibility of the system has been computed using the relation

$$\phi_k = \frac{1000 (\beta_s - \beta_o)}{m \rho_o} + \beta_s \phi_v \quad \dots (3)$$

where β_o and β_s are the compressibility of the solvent and solution respectively, m is the molality, ρ_o is the density of the solvent and ϕ_v is the apparent molal volume. ϕ_k is the apparent molal compressibility which is the linear function of concentration and found to be in good agreement with Masson's equation¹²

$$\phi_k = \phi_k^\circ + S_k \sqrt{m} \quad \dots (4)$$

where ϕ_k^0 is the apparent molal compressibility at infinite dilution and is a measure of solute-solvent interaction. S_k is the experimental slope and a measure of ion-solvent interaction.

Results and discussion

Lysine

The experimental values of ultrasonic velocity, density, viscosity and compressibility have been recorded in Table 1. The values of ultrasonic velocity of lysine solution decreases with decrease in concentration and increases with increase in temperature. This indicates that the velocity data can be made fit in the relation.

$$(U - U_0) = f m \quad \dots (5)$$

where U_0 is the velocity of the solvent (water) and U is the velocity of the system at concentration m . It is found that the values of $U - U_0$ varies linearly with increase in molar concentration. It has been found that the adiabatic compressibility increases continuously with decrease in concentration and decreases continuously with increase in temperature. The variation of adiabatic compressibility with concentration can be represented by the relation deduced by Bachem¹⁴,

$$\beta_s = \beta_s^0 + A m + B m^{3/2} \quad \dots (6)$$

where m is the molar concentration, β_s^0 is the adiabatic compressibility of the pure solvent (water), A and B are constants. An attempt has been made to evaluate $(\beta_s - \beta_s^0)/m$ from the

Table 1—Experimental density, viscosity, ultrasonic velocity, adiabatic, lowering and relative compressibilities data of lysine at different temperatures

C (mol)	T (°C)	ρ ($\text{kg}\cdot\text{m}^{-3}$)	$\eta \times 10^{-3}$ ($\text{kg}\cdot\text{m}^{-1}\text{s}^{-1}$)	U ($\text{M}\cdot\text{s}^{-1}$)	$\beta_s \times 10^{10}$ (N^{-1}m^2)	$\Delta\beta_s \times 10^{12}$ (N^{-1}m^2)	$\beta_r \times 10^{12}$ (N^{-1}m^2)
0.010	25	998.10	0.8833	1497.00	46.9455	15.75	35.70
	30	996.50	0.8082	1511.00	46.1265	10.50	23.10
	35	994.50	0.7489	1517.00	45.9270	10.50	25.20
0.013	25	998.10	0.8841	1498.00	46.8825	22.05	50.40
	30	996.67	0.8087	1512.00	46.0740	16.80	39.90
	35	994.70	0.7507	1520.00	45.8955	13.65	31.50
0.014	25	998.20	0.8854	1499.00	46.8090	29.40	66.15
	30	996.90	0.8096	1512.66	46.0320	22.05	43.05
	35	994.80	0.7519	1520.66	45.6435	38.85	88.20
0.016	25	998.30	0.8865	1499.25	46.7785	31.50	69.30
	30	996.90	0.8101	1513.33	45.9900	26.25	59.85
	35	995.00	0.7527	1523.33	45.8640	16.80	39.90
0.020	25	998.40	0.8814	1501.00	46.6830	43.05	95.55
	30	996.80	0.8111	1513.75	45.9580	29.40	67.20
	35	995.10	0.7537	1527.33	45.7485	28.35	66.15
0.025	25	998.40	0.8881	1501.75	46.6305	47.25	106.05
	30	997.00	0.8142	1514.00	45.9480	31.50	70.35
	35	995.30	0.7551	1530.33	44.7300	26.25	27.30
0.033	25	998.80	0.8975	1503.33	46.7880	32.55	72.45
	30	997.60	0.8201	1517.25	45.7100	53.55	120.75
	35	995.50	0.7579	1533.66	44.5830	16.80	278.25
0.050	25	1000.30	0.9208	1506.25	46.2630	84.00	123.90
	30	997.60	0.8296	1521.00	45.4860	81.90	174.30
	35	996.20	0.7592	1537.66	44.5830	40.95	332.85
0.100	25	1001.40	0.9278	1508.25	46.0950	100.80	225.75
	30	999.80	0.8581	1523.50	46.2945	48.30	229.95
	35	998.00	0.7719	1542.00	43.9630	205.90	473.55
0.200	25	1005.70	0.9817	1516.00	45.3800	172.00	384.30
	30	1003.20	0.8946	1529.00	44.7720	148.05	337.05
	35	1001.80	0.8005	1547.00	43.7955	223.65	510.30

above equation and show variation with $\sqrt{m}$. A linear relation has been observed in each case. The variation of ϕ_v against $\sqrt{m}$ is found to be almost linear within the concentration range studied at each temperature. In general, the apparent molal volume increases with increase in concentration and also with increase in temperature. This indicates the applicability of Masson's empirical relation. The positive values of ϕ_v (intercept) and S_v (slope) decrease with the increase in temperature in all systems, supporting the view that lysine cannot behave as structure maker in aqueous solution. In the present investigation, values of ϕ_k are negative at all concentrations and temperatures. The plots of ϕ_k versus $\sqrt{m}$ follows a linear relationship. The negative values of ϕ_k indicate electrostriction and hydrophobic interaction¹⁵ as well as the loss of structural compressibility of solvent molecules due to the increased population of four bonded water molecules showing

that the structural disruption is much more effective in water.

Lysine-adenosine mixture

The experimental values of speed of sound, densities, viscosities, relative viscosities (η_r), inentropic compressibilities (β_s), relative change in isentropic compressibilities ($\Delta\beta/\beta_0$) and relative change in sound velocity ($\Delta U/U_0$) for binary solution of lysine and adenosine in different proportions have been recorded in Table 2. The objective of the present work is to investigate the interaction between adenosine and lysine moieties in aqueous solution. During protein synthesis one codon (base triplet) designs only one amino acid. Since the codon triplet AAA designs lysine exclusively, it was thought that the precise interaction study between adenosine base and lysine at molecular level in terms of any measurable parameter may prove informative. The values deter-

Table 2—Experimental data for binary mixture of lysine and adenosine at various temperatures

C (mol)		Temp. (°C)	U ($M s^{-1}$)	ρ ($kg m^{-3}$)	$\eta \times 10^{-3}$ ($kg m^{-1} s^{-1}$)	$\beta \times 10^{10}$ ($N^{-1} m^2$)	$\Delta\beta/\beta_0$	η_r	$\Delta U/U_0$
A	L								
0.005+0.005		25	1530.80	999.70	0.8932	44.8245	5.0865	1.0030	0.023830
		30	1548.33	994.80	0.8077	44.0365	5.0578	1.0128	0.025384
		35	1562.66	991.30	0.7553	43.3755	6.0658	1.0498	0.031636
0.004+0.006		25	1509.80	997.20	0.8856	46.2420	1.9267	0.9938	0.009250
		30	1527.50	995.70	0.8053	46.2210	2.4118	1.0097	0.011590
		35	1551.00	994.80	0.7577	43.8795	4.9171	1.0532	0.023940
0.003+0.007		25	1526.00	997.30	0.9027	51.5130	4.2199	1.0120	0.020620
		30	1538.75	994.10	0.9999	44.6040	3.7474	1.0031	0.019040
		35	1556.50	993.50	0.7465	43.6275	5.4915	1.0376	0.027570
0.002+0.008		25	1507.40	996.90	0.8924	46.4415	1.4815	1.0015	0.004060
		30	1526.25	996.00	0.8055	45.2550	2.2680	1.0100	0.010760
		35	1542.00	995.00	0.7583	44.3835	3.7674	1.0429	0.017990
0.001+0.009		25	1501.25	996.10	0.8838	46.7670	0.7549	1.9918	0.004060
		30	1523.00	995.90	0.8025	45.4545	1.8154	1.0062	0.008610
		35	1544.60	995.00	0.7485	44.2995	4.1023	1.0404	0.019710
0.006+0.004		25	1522.00	996.50	0.8928	45.7695	2.9788	1.0019	0.017940
		30	1538.50	995.80	0.8068	44.5515	3.8661	1.0116	0.018870
		35	1560.75	995.00	0.7529	43.3230	2.7121	1.0467	0.030370
0.007+0.003		25	1517.00	996.80	0.8935	45.7695	2.9799	1.0026	0.014600
		30	1533.33	996.00	0.8091	44.8870	3.2224	1.0146	0.015450
		35	1551.00	995.10	0.7546	43.8585	4.9644	1.0489	0.023940
0.008+0.002		25	1542.50	997.30	0.8954	44.2470	6.3724	1.0048	0.031660
		30	1556.30	996.30	0.8112	43.5120	6.2254	1.0171	0.030660
		35	1568.66	995.20	0.7520	42.8715	7.2156	1.0453	0.034240
0.009+0.001		25	1518.20	998.00	0.8900	45.6435	3.2602	0.9988	0.015400
		30	1533.00	997.90	0.8092	44.7720	3.3652	1.0147	0.005430
		35	1546.80	995.57	0.7509	44.0790	4.4614	1.0438	0.021170

A = Adenosine, and L = lysine

Table 3—Ultrasonic velocity, isentropic compressibility, $\Delta\beta/\beta_0$, $\Delta U/U_0$, viscosity, relative viscosity and density values of aqueous 0.01 M adenosine and 0.01 M lysine at different temperatures

Solution	Temp. (°C)	U (M s ⁻¹)	$\beta \times 10^{10}$ (N ⁻¹ m ²)	$\Delta\beta/\beta_0$	$\Delta U/U_0$	$\eta \times 10^{-3}$ (kg m ⁻¹ s ⁻¹)	η_r	ρ (kg m ⁻³)
0.01 M adenosine	25	1500	46.7460	0.802935	0.003230	0.89217	1.001200	998.30
	30	1515	45.8944	0.817539	0.003311	0.81347	1.020030	996.79
	35	1520	45.6939	0.799365	0.003473	0.75088	1.043760	994.60
0.01 M lysine	25	1497	46.9455	0.452655	0.001223	0.88330	0.991200	998.10
	30	1511	46.1517	0.233625	0.000662	0.80823	1.013500	996.50
	35	1517	45.9291	0.241920	0.001492	0.74873	1.040770	994.54

mined of sound velocities, densities, viscosities, isentropic compressibilities of the binary mixture of adenosine and lysine have been found to vary as compared to that of pure adenosine and lysine solutions. This clearly shows significant interaction between these two molecules in solution.

A convenient parameter for describing the inter and intramolecular interactions in solution is the relative change in sound velocity per unit concentration, $A = (1/U_0) \partial U / \partial C$, which for very dilute solutions is equal to $(U - U_0)/U_0 C$, where U is the sound velocity at concentration C and U_0 is the velocity of the solvent (Table 2). The values of $(\Delta U/U_0)$ have been found to be quite different from that of 0.01 M lysine and 0.01 M adenosine separately (Table 3) giving indication of significant interaction between the two molecules¹⁶.

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