Effect of temperature on solvation behaviour of diclofenac sodium salt in aqueous glycine and L-proline solutions

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ABSTRACT

Apparent molar volume ($V_{2,\phi}$) and apparent molar isentropic compressibility ($K_{s,2,\phi}$) of diclofenac sodium salt (DSS) drug within the concentration range of (0.001 to 0.008) mol · kg^{-1} in (0.01, 0.03 and 0.05) mol · kg^{-1} aqueous glycine and L-proline solutions are computed from the experimental density (ρ) and speed of sound (u) values at $T = (293.15$ to $313.15)$ K and atmospheric pressure. Derived parameters such as partial molar properties, transfer partial molar properties, hydration numbers and Hepler's constant are computed from the data of $V_{2,\phi}$ and $K_{s,2,\phi}$. These parameters have been used to understand the effect of temperature on interactions between DSS drug and aqueous glycine/L-proline solution. Furthermore, the structure making and breaking ability of DSS drug in probed solutions are analysed at experimental conditions.

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1. Introduction

Drug interactions as (drug + drug), (drug + food additives) and (drug + biomolecules) are having effect on the drug action which are clinically significant [1,2]. Drug actions, i.e., drug reaching to the blood stream, extent of distribution, binding to the receptors and finally producing the physiological action depend on various physicochemical properties of drug [3]. (Drug + protein) interactions are of great importance in drug discovery and can be studied through thermophysical experiments and computational simulations [4,5]. However, it is difficult to examine the (drug + protein) interactions directly but, as proteins are building blocks of amino acids, these interactions are possible to understand through (drug + amino acids) interactions. Thermophysical and thermodynamic properties are useful to understand the molecular interactions (hydrophilic, hydrophobic and ionic interactions) of drugs in aqueous and non-aqueous binary/ternary solutions, as observed by several researchers [6,7].

Diclofenac is a non-steroidal anti-inflammatory drug used mainly to treat musculoskeletal pain and chronic pain, besides several other medicinal uses [8]. Most biochemical processes are occurred in aqueous medium; this promoted us to investigate the volumetric and acoustic properties of diclofenac sodium salt (DSS) drug in investigated aqueous medium. This work is in continuation of our research interest on systematic investigation of volumetric and acoustic properties of drugs in solvent mixtures [9].

In the present work, the densities (ρ) and speeds of sound (u) of DSS drug in aqueous glycine/L-proline solutions at $T = (293.15$ to $313.15)$ K and atmospheric pressure have been measured. The experimental values are used to calculate the derived parameters such as apparent molar volume ($V_{2,\phi}$), partial molar volume (V_2^∞), transfer partial molar volume ($\Delta_t V_2^\infty$), apparent molar isentropic compressibility ($K_{s,2,\phi}$), partial molar isentropic compressibility ($K_{s,2}^\infty$), and transfer partial molar compressibility ($\Delta_t K_{s,2}^\infty$). These derived thermodynamic parameters are used to examine the effects of temperature, concentration and solvent composition on molecular interactions in (DSS drug + water + glycine/L-proline). The co-sphere overlap model is used to understand the values of $\Delta_t V_2^\infty$ and $\Delta_t K_{s,2}^\infty$. To the best of our knowledge from the literature survey, thermophysical properties of DSS drug in aqueous glycine/L-proline solutions have not been reported.

2. Experimental

2.1. Chemicals

For the investigation on the effect of temperature on density (ρ) and speed of sound (u) of DSS drug in aqueous glycine and L-proline solutions, chemicals used along with CAS number, supplier
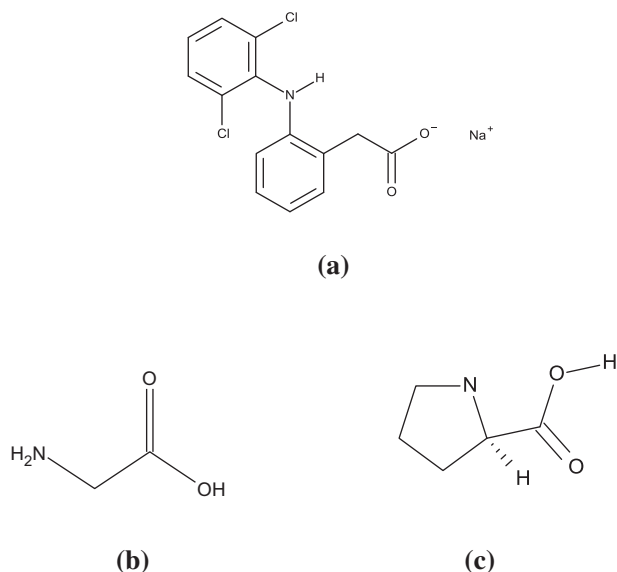
FIGURE 1. Structure of components studied in this work: (a) diclofenac sodium salt, (b) glycine and (c) L-proline.

TABLE 1
Provenance and mass fraction purity of the chemicals used in this work.

Compound*	CAS No.	Source	Purity mass fraction
Diclofenac sodium salt	15307-79-6	TCI Chemical (India) Pvt. Ltd	0.980
Glycine	56-40-6	Sd fine – Chem Limited (India)	0.995
L-proline	147-85-3	Spectrochem. India Pvt. Ltd	0.990

* All the compounds were used after drying over P_2O_5 in vacuum desiccators at room temperature for 48 h.

details and mass fraction purity are presented in table 1. All the compounds were used after drying over P_2O_5 in vacuum desiccators at room temperature for 48 h. The structures of the investigated compounds are given in figure 1.

2.2. Equipment and procedure

Millipore quality freshly degassed water having specific conductance less than $5 \cdot 10^{-6}$ S $\cdot$ cm^{-1} was used as solvent for the preparation of binary mixtures such as (water + DSS drug), (water + glycine) and (water + L-proline). Further, (water + glycine) and (water + L-proline) binary mixtures are used as a solvent for the preparation of ternary mixture like (water + glycine + DSS drug) and (water + L-proline + DSS) drug. All solutions were prepared at room temperature on the mass basis over a concentration range (0.001 to 0.008) mol $\cdot$ kg^{-1} and kept in airtight bottles to avoid the air and moisture contamination. A digital analytical balance (Sartorius, Model CPA225D) with a precision of ±0.01 mg is used for the preparation of solutions. The density (ρ) and speed of sound (u) values of DSS drug in aqueous glycine and L-proline solutions were measured using the Anton Paar DSA 5000M instrument on the same day of the sample preparation. The experimental temperatures $T = (293.15, 298.15, 303.15, 308.15$ and $313.15)$ K with an accuracy of ±0.01 K are controlled by a Peltier thermostat (PT 100) which is in-built on Anton Paar DSA 5000M instrument. The instrument was calibrated with doubly distilled water and dry air at the probed temperatures; uncertainties in the measurements of density (ρ) and speed of sound (u) at 3 MHz frequency are $±5 \cdot 10^{-3}$ kg $\cdot$ m^{-3} and $±0.5$ m $\cdot$ s^{-1}, respectively. Standard uncertainties u are found as: $u(m) = 2 \cdot 10^{-5}$ mol $\cdot$ kg^{-1}, $u(T) = 0.01$ K, $u(p) = 0.01$ MPa, $u(u) = 0.5$ m $\cdot$ s^{-1} and $u(\rho) = 5 \cdot 10^{-3}$ kg $\cdot$ m^{-3}, here, m is the molality of the DSS drug in per kg of water or (water + amino acid). Molality of amino acids in per kg of water was prepared with standard uncertainty of $3 \cdot 10^{-5}$ mol $\cdot$ kg^{-1}.

3. Results and discussion

The density (ρ) and speed of sound (u) of (DSS drug + glycine/L-proline + water) at different temperatures and compositions are presented in table 2. The comparison of experimental values of density (ρ) and speed of sound (u) of pure water and binary mixtures are in good agreement with the corresponding literature

values as shown in supporting information as table ST1, and figures S1, S2 and S3. The relative deviation of experimental values with available literature values for density and speed of sound are within 0.03%, except for the densities of (DSS + water). Up to 0.1% relative deviations are observed for the densities of (DSS + water) with values obtained by Iqbal and Chaudhry [10]. The apparent molar volumes ($V_{2,\phi}$) and apparent molar isentropic compressibility ($K_{s,2,\phi}$) of DSS drug in aqueous glycine and L-proline solutions are computed from the values of density (ρ) and speed of sound (u) from equations (1) and (2), respectively and the values of $V_{2,\phi}$ and $K_{s,2,\phi}$ are reported in table 3. The change in the values of $V_{2,\phi}$ and $K_{s,2,\phi}$ with rise in temperature, molality of DSS drug and composition of glycine/L-proline suggests the effect of temperature, concentration and solvent composition on molecular interactions.

$$V_{2,\phi} = [M/\rho] - [1000(\rho - \rho_o)/(m\rho\rho_o)], \tag{1}$$

$$K_{s,2,\phi} = [\kappa_s M/\rho] - [1000(\kappa_s^o \rho - \kappa_s \rho_o)/(m\rho\rho_o)], \tag{2}$$

where M and m are molar mass and molality of DSS drug, ρ and ρ_o are the densities of solution and solvent (water or water + glycine/L-proline), κ_s and κ_s^o represent the isentropic compressibility of solution and solvent, respectively. Values of the isentropic compressibility (κ_s) are calculated from the values of density (ρ) and speed of sound (u) by using the relation

$$\kappa_s = 1/(u^2 \rho). \tag{3}$$

The plot of apparent molar volume ($V_{2,\phi}$) versus molality (m) of DSS drug in water at different temperatures is shown in Figure 2. The partial molar volumes (V_2^∞) and partial molar isentropic compressibility ($K_{s,2}^\infty$) for DSS drug in water, aqueous glycine and L-proline solutions have been reported by the least-square fitting of the linear plots of $V_{2,\phi}$ and $K_{s,2,\phi}$ against the molality (m) of DSS drug, respectively.

$$V_{2,\phi} = V_2^\infty + S_v \cdot m, \tag{4}$$

$$K_{s,2,\phi} = K_{s,2}^\infty + S_k \cdot m, \tag{5}$$

here S_v and S_k are the experimental slopes, which are used to understand the (solute + solute) interactions in binary or ternary mixtures. The values of S_v and S_k depends on solvent, solute, and temperature, for large organic or non-electrolytic solutes these values are not of much significance [10]. Furthermore, at infinite dilution the (solute + solute) interactions are negligible: therefore, the understanding of (solute + solvent) interactions at infinite dilutions are important which depends on temperature and composition of the mixtures and these (solute + solvent) interactions can be accomplish by partial molar properties such as partial molar volume (V_2^∞) and partial molar isentropic compressibility ($K_{s,2}^\infty$) [11,12]. In the present study, the values of V_2^∞ and $K_{s,2}^\infty$ (along with standard deviations) of DSS in aqueous glycine and L-proline solutions are given in table 4. The values of V_2^∞ and $K_{s,2}^\infty$ increases with increase in temperature of the solution, this may be attributed to decreasing of electrostriction or hydration from second solvation