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Volumetric properties of betaine hydrochloride drug in aqueous NaCl and KCl solutions at different temperatures

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ABSTRACT

Densities (ρ) and speeds of sound (u) of betaine hydrochloride (B.HCl) drug (0.01–0.06) mol kg^{-1} in (0.10, 0.20 and 0.30) mol kg^{-1}aqueous NaCl and KCl solutions have been reported as a function of temperature at T = (293.15 –313.15) K and at atmospheric pressure. Using experimental data the 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 ($K_{s,2}^{\infty}$), transfer partial molar isentropic compressibility ($\Delta_t K_{s,2}^{\infty}$), partial molar expansion (E_2^{∞}) and Hepler's constant ($\partial^2 V_2^{\infty}/\partial T^2)_P$ were calculated. Further, all these parameters are employed to understand the temperature and cosolute effects on B.HCl drug–solvent interactions. Cosphere overlap model is used to analyze the hydrophilic/ionic-ionic interactions in (B.HCl drug + NaCl/KCl + H_2O) ternary mixture. The sign of Hepler's constant have been used to interpret the structure making or braking tendency of B.HCl drug in aqueous NaCl and KCl solutions at probed compositions and temperatures.

1. Introduction

The solvation behavior of drug molecules in solutions has a significant role to understand the activity of drugs in biological system. It is difficult to understand these drug–solvent interactions directly in biological system, these interactions can be altered by the cosolutes such as salt, polymer, carbohydrate, osmolytes, surfactant, amino acid, protein, peptide, alcohol, etc., furthermore, drug–solvent interactions also vary with the temperature of the solutions [1–3]. However, it is possible for some extent to examine cosolute and temperatures effects on drug–solvent interactions through thermophysical properties at various temperatures and compositions [4–6]. Most of the biochemical processes occur in aqueous media, the drug–water molecular interactions and their temperature dependence play an important role in finding the drug action across the biological membrane [7].

We are engaged in systematic study of solvation behavior of B. HCl drug in various solvents [8] through thermophysical property measurements since volumetric and acoustic properties have been used as potential tools to understand and analyze the solvation behavior of solutes in aqueous and non-aqueous solutions [9–12]. In this work, we have studied the volumetric properties of B.HCl drug in aqueous NaCl and KCl solutions, to understand the molecular interactions at different temperatures and compositions of solute and cosolute. Densities (ρ) and speeds of sound (u) of (0.01–0.06) mol kg^{-1} B.HCl drug in (0.10, 0.20 and 0.30) mol kg^{-1}aqueous NaCl and KCl solutions have been measured as a function of temperature at T = (293.15, 298.15, 303.15, 308.15 and 313.15) K and at atmospheric pressure. Results are interpreted in terms of ion–ion, hydrophilic-ionic, ion-hydrophobic, electrostatic interactions and structure making/breaking ability of B.HCl drug in aqueous NaCl and KCl solutions. To the best of our knowledge, densities and speeds of sound of B.HCl drug in aqueous NaCl and KCl solutions are not reported in the literature.

2. Experimental

2.1. Chemicals

For the investigation of thermophysical properties of B.HCl drug in aqueous NaCl and KCl solutions, the following chemicals have been used; betaine hydrochloride were obtained from Sigma–Aldrich Co. and the structure of B.HCl drug shown in Scheme 1, sodium chloride supplied by Himedia Laboratory, potassium

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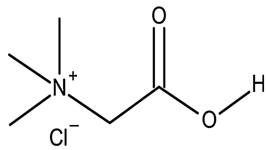

Scheme 1. Structure of betaine hydrochloride.

chloride have been received from Merck Chemicals. All the compounds were of ≥0.99 mass fraction purity and were used after drying over P_2O_5 in vacuum desiccators at room temperature for 48 h. The details of the chemical compounds used in this work are shown in the Table 1.

2.2. Equipment and procedure

The aqueous solutions were prepared by using the doubly distilled, degassed water with a specific conductance less than 1×10^{-6} S cm^{-1} at 298.15 K. All aqueous solutions were made at room temperature on the mass basis over a concentration range (0.01–0.06) mol kg^{-1} and these solutions kept in airtight bottles to avoid contamination of air and moisture. The weighting was performed by using an electronic analytical balance (Sartorius, Model CPA225D) with a precision of ±0.01 mg. The densities (ρ) and speeds of sound (u) have been measured using Anton Paar DSA 5000M instrument on the same day of sample preparation. The instrument was calibrated with doubly distilled water and dry air at the investigated temperatures; uncertainty in the measurements of density (ρ) and speed of sound at 3 MHz frequency are (u) is $\pm 5 \times 10^{-3}$ kg m^{-3} and ±0.5 m s^{-1}, respectively. The experiments were carried out at T = (293.15, 298.15, 303.15, 308.15 and 313.15) K with an accuracy of ±0.01 K. The temperature was controlled by a Peltier thermostat (PT 100) which is in-built on Anton Paar DSA 5000M instrument [13]. The instrument was calibrated with doubly distilled freshly degassed water and dry air in frequent intervals of time. Details about instrument calibration and measurement procedures are explained in our recent work [14].

Table 1
Specifications of the chemicals used in this work.

Compound[a]	Mass fraction purity	CAS no.	Source	Purification method
Betaine HCl	≥0.99	590-46-5	Sigma–Aldrich Co.	None
NaCl	≥0.99	7647-14-5	Himedia laboratory	None
KCl	≥0.99	7447-40-7	Merck chemicals	None

[a] Used as received from source, without further purification.

The standard uncertainties (u) of molalities, density, speed of sound, temperature and pressure are shown in respective table as a foot notes. Doubly distilled freshly degassed water is used for the preparation of binary mixtures and water + salt solution is used for the preparation of ternary mixtures.

3. Results and discussion

3.1. Partial molar properties

The experimental results of densities (ρ) and speeds of sound (u) for B.HCl drug in aqueous NaCl/KCl solutions are presented in Tables 2 and 3, respectively. Experimentally measured density, ρ and speed of sound, u of aqueous NaCl and aqueous KCl solutions are in good agreement with the corresponding available literature values as presented in Supporting material (Table S1 and Figs. S1 and S2). It can be seen from Tables 2 and 3, the values of density (ρ) and speed of sound (u) are varying with temperature, compositions of cosolute and solute at a given pressure, which furnish the effect of temperature and composition of additives on the solvation behavior of solute in probed solutions. Furthermore, the apparent molar volumes ($V_{2,\phi}$) and apparent molar isentropic compressibility ($K_{s,2,\phi}$) for ternary mixtures are calculated from the densities (ρ) and speeds of sound (u) of solutions by using Eqs. (1) and (2), respectively.

Table 2
Densities (ρ) and apparent molar volumes ($V_{2,\phi}$) of B.HCl inaqueous NaCl and KCl solutions at T = (293.15–313.15) K and pressure p = 0.1 MPa.[a]

m/ (mol kg^{-1})	$\rho \times 10^{-3}$/ (kg m−3) 293.15 K	$V_{2,\phi} \times 10^6$/ (m3 mol−1)	$\rho \times 10^{-3}$/ (kg m−3) 298.15 K	$V_{2,\phi} \times 10^6$/ (m3 mol−1)	$\rho \times 10^{-3}$/ (kg m−3) 303.15 K	$V_{2,\phi} \times 10^6$/ (m3 mol−1)	$\rho \times 10^{-3}$/ (kg m−3) 308.15 K	$V_{2,\phi} \times 10^6$/ (m3 mol−1)	$\rho \times 10^{-3}$/ (kg m−3) 313.15 K	$V_{2,\phi} \times 10^6$/ (m3 mol−1)
(B.HCl + 0.10 mol kg^{-1}NaCl)										
0	1.00242		1.00121		0.99977		0.99812		0.99628	
0.00949	1.00275	118.59	1.00153	119.12	1.00009	119.77	0.99844	120.33	0.99659	121.02
0.01968	1.00309	118.87	1.00188	119.38	1.00043	120.01	0.99877	120.56	0.99693	121.13
0.02922	1.00342	119.09	1.00219	119.61	1.00074	120.24	0.99908	120.77	0.99723	121.34
0.03906	1.00374	119.37	1.00252	119.86	1.00106	120.47	0.9994	121.03	0.99754	121.58
0.05026	1.0041	119.63	1.00287	120.16	1.00141	120.76	0.99974	121.31	0.99788	121.87
0.05896	1.00438	119.84	1.00315	120.4	1.00168	120.98	1.00001	121.56	0.99815	122.1
(B.HCl + 0.20 mol kg^{-1}NaCl)										
0	1.00667		1.00541		1.00393		1.00225		1.00038	
0.00968	1.007	118.93	1.00573	119.54	1.00425	120.18	1.00257	120.74	1.00069	121.42
0.02043	1.00736	119.28	1.00609	119.82	1.0046	120.39	1.00291	120.92	1.00103	121.53
0.02942	1.00765	119.47	1.00638	120.01	1.00489	120.58	1.0032	121.1	1.00131	121.71
0.03792	1.00793	119.66	1.00665	120.26	1.00516	120.76	1.00346	121.25	1.00158	121.92
0.04799	1.00825	119.85	1.00697	120.46	1.00547	120.98	1.00377	121.48	1.00188	122.11
0.05952	1.00862	120.1	1.00732	120.76	1.00582	121.31	1.00412	121.83	1.00222	122.42
(B.HCl + 0.30 mol kg^{-1} NaCl)										
0	1.01064		1.00934		1.00781		1.0061		1.0042	
0.0097	1.01096	119.46	1.00965	119.97	1.00813	120.62	1.00641	121.07	1.00451	121.75
0.02097	1.01133	119.7	1.01002	120.28	1.00848	120.93	1.00676	121.42	1.00485	122.11
0.03052	1.01163	119.92	1.01032	120.55	1.00878	121.17	1.00705	121.65	1.00514	122.28
0.04055	1.01195	120.21	1.01063	120.83	1.00908	121.43	1.00736	121.9	1.00544	122.49
0.04969	1.01223	120.49	1.0109	121.04	1.00936	121.68	1.00762	122.17	1.0057	122.79
0.06009	1.01254	120.73	1.01121	121.34	1.00966	121.9	1.00793	122.42	1.006	123.03