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Acoustical studies of pharmaceutical excipients in binary solvent mixtures

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ABSTRACT

Pharmaceutical excipients have gained a great importance due to their control of blood glucose level and sugar alternative. Thermodynamic methods provide an easy way for determination of solute-solute and solute-solvent interactions in solutions. Density and sound velocity for sugar alcohols have been measured in binary mixtures of Dimethyl Sulfoxide-Water at different percentage compositions (i.e. 10%–50%) at different temperatures. Density and sound velocity data have been used to calculate apparent molal volume, apparent molal isentropic compressibility, partial molal volume, partial molal isentropic compressibility, intermolecular free length, relative association, Rao's molar sound function and solvation number. Results have been discussed in terms of solvent-solvent, solute-solute and solvent-solute interactions. For all the systems studied, the density, sound velocity and apparent molal volume increase with increasing concentration of sugar alcohols which indicates the presence of solute-solvent interactions. The value of partial molal volume also increases with increasing temperature. The values of S_v are found positive while the values of apparent molal isentropic compressibility are negative which indicates the presence of solute-solvent interactions.

1. Introduction

Sugar alcohols are a kind of functional food. They are useful in many aspects like pharmacy, food, chemical engineering and cosmetics. They are used by diabetic patients because they are low caloric in nature. It has good taste and causes no tooth decay [1]. Xylitol occurs widely in nature and also a normal intermediate in human metabolism [2]. Sorbitol is a sweetening agent, plasticizer, capsule and tablet diluents. It is used in food industries as it has a sweet taste and about 50–60% the sweetness of sucrose [3]. With the continuous improvement of people's life standards, people come out with more necessities for good quality food [1]. Diets containing sugar alcohols have decreased levels of plasma triglyceride and cholesterol [4].

There are many techniques for the analysis of solute-solvent interactions like NMR, volumetric analysis, Densitometric and Molecular Dynamics Simulations [5]. Direct analysis of a complex biological system and macromolecular interaction is complicated. The most suitable approach to study the molecular interactions in solutions system is thermodynamic methods [6]. Thermodynamic methods provide an easy way for the determination of association between solute molecules as well as between solute and solvent in the solutions [7]. The measurement of viscosity, density and sound velocity of liquids and their mixture is valuable for determining the acoustical and thermodynamic properties that are sensitive to molecular interactions [8]. When a compound is being dissolved in the liquid, different kinds of attractions create. This includes attraction between ions and ions with solvent. The interactions are measured by sound velocity and density of the solution [9].

There are several reports in the literature concerning acoustic and volumetric studies. They confirm that the water–solute interactions depend on the molecular conformation and stereochemistry of the solute and solvent system [10]. Volumetric properties are being used for interpretation of electrostatic attraction and structure making/breaking capacity in aqueous systems [11]. Analytical chemists, biologists and medical researchers are interested in Dimethyl Sulfoxide (DMSO) as a solvent. It has many applications within pharmacy and biological systems. It has long been recognized as an important reaction solvent for the synthesis of numerous compounds [9]. The structures of sugar alcohols are shown in Fig. 1.

2. Experimental

2.1. Materials

D-Sorbitol (a Daejung product; CAS No. 50-70-4) and Xylitol (a BDH product; CAS No. 87-99-0) were utilized. These chemicals have high value of purity (>99%). The doubly distilled and deionized water were used for solution preparation and washing. The

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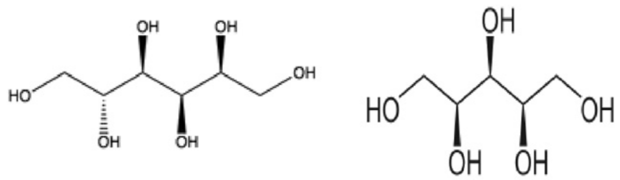

Structure of D-Sorbitol Structure of Xylitol

Fig. 1. Structure of sugar alcohols.

purity of water was checked by values of density, conductance and refractive index. The water is degassed before preparation of solutions. Highly pure Dimethyl sulfoxide (a Merck product; CAS No. 67-68-5) of purity >99% was used. Its purity was confirmed by comparing the experimental density and sound velocity with reported literature values.

2.2. Measurements

Mixtures of different percentage composition of Dimethyl sulfoxide in water (10, 20, 30, 40 and 50%) were prepared and Sugar alcohol (D-Sorbitol and Xylitol) was added to make the solution of 0.03, 0.06, 0.09, 0.12 and 0.15 molality by w/w method. All the solutions were prepared fresh before use. Weighing of the sugar alcohols was done by Electrical balance (Model: GC 2102 Sartorius) with a precision of ±0.001 mg. Three readings for each composition were taken and then averaged. Sound velocity and density were measured for different percentage solutions at different temperatures (293.15, 298.15, 303.15, 308.15 and 313.15 K) by density sound analyzer (DSA 5000) M. Calibration of (DSA 5000 M) was performed by measuring density and sound velocity of water and air at each temperature. The accuracy and repeatability of DSA 5000 M for density were 5×10^{-6} g/cm^3 and 1×10^{-6} g/cm^3 and that of temperature is 0.01 °C and 0.001 °C respectively.

3. Result and discussion

The density and speed of sound data for pure DMSO and water at different temperatures have been given in Tables 1a and 1b. Binary solvent

Table 1a
Experimental density values ($D_o \times 10^{-3}$ kg m^{-3}) of pure solvents (Water and DMSO) and literature values.

Temperature (T) K	This work		Literature	
	Water	DMSO	Water	DMSO
293.15	0.998202	1.102224	0.998220 [12]	1.100410 [12]
298.15	0.997748	1.095243	0.997100 [12]	1.095191 [9]
303.15	0.997025	1.090241	0.995640 [12]	1.090166 [9]
308.15	0.994258	1.086422	0.994058 [12]	1.086070 [9]
313.15	0.992567	1.080986	0.992210 [12]	1.080640 [12]

Table 1b
Experimental sound velocity (u_o/m s^{-1}) of pure solvents (Water and DMSO) and literature values.

Temperature (T) K	This work		Literature	
	Water	DMSO	Water	DMSO
293.15	1483.35	1493.18	1483.10 [12]	1502.60 [12]
298.15	1497.12	1485.98	1497.00 [12]	1484.51 [12]
303.15	1509.51	1473.95	1509.40 [12]	1474.00 [12]
308.15	1520.17	1461.31	1519.83 [12]	1460.35 [13]
313.15	1529.89	1449.92	1529.10 [12]	

Table 2
Density ($D_o \times 10^{-3}$ kg m^{-3}) of binary solvent mixtures (DMSO + Water) of different percentage composition at different temperatures.

DMSO wt (%)	Temperatures (T) K				
	293.15	298.15	303.15	308.15	313.15
0	0.998202	0.997748	0.997025	0.994258	0.992567
10	1.011001	1.009281	1.007531	1.005791	1.004041
20	1.012741	1.011011	1.009281	1.007561	1.005831
30	1.014469	1.012741	1.011031	1.009331	1.007631
40	1.016191	1.014471	1.012761	1.011061	1.009371
50	1.018291	1.016581	1.014891	1.013211	1.011531
100	1.102224	1.095243	1.090241	1.086422	1.080986

Table 3
Speed of sound (u_o/m s^{-1}) of binary solvent mixtures (DMSO + Water) of different percentage composition at different temperatures.

DMSO wt (%)	Temperatures (T) K				
	293.15	298.15	303.15	308.15	313.15
0	1483.35	1497.12	1509.51	1520.17	1529.89
10	1527.12	1536.68	1545.72	1555.72	1564.32
20	1539.55	1544.38	1559.02	1570.14	1582.32
30	1551.51	1563.28	1575.56	1586.19	1595.76
40	1562.51	1574.18	1585.56	1596.13	1605.71
50	1572.34	1583.87	1592.23	1603.13	1612.71
100	1493.18	1485.98	1473.95	1461.31	1449.92

Table 4
Molality (m), density (D_s), apparent molal volume (V_Φ), speed of sound (u_s) and apparent molal isentropic compressibility (K_Φ) of D-Sorbitol in (10%) of DMSO-water solution at different temperatures.

Molality of solutions (m) (mol kg^{-1})	Density of solutions $D_s \times 10^{-3}$ (kg m^{-3})	Apparent molal volume $V_\Phi \times 10^6$ (m^3 mol^{-1})	Speed of sound of solutions (u_s) (m s^{-1})	($K_\Phi \times 10^{-4}$) (m^3 mol^{-1} Pa^{-1})
293.15 K				
0.00	1.011001		1527.12	
0.03	1.012945	116.60	1536.67	−1.51
0.06	1.014817	117.52	1546.09	−1.48
0.09	1.016634	118.29	1555.19	−1.44
0.12	1.018406	118.94	1564.21	−1.40
0.15	1.020128	119.57	1572.49	−1.35
298.15 K				
0.00	1.009281		1536.68	
0.03	1.011214	117.02	1546.90	−1.60
0.06	1.013099	117.58	1557.01	−1.57
0.09	1.014915	118.38	1566.71	−1.53
0.12	1.016691	119.00	1576.04	−1.48
0.15	1.018427	119.55	1584.85	−1.43
303.15 K				
0.00	1.007531		1545.72	
0.03	1.009437	118.00	1556.51	−1.67
0.06	1.011299	118.50	1566.91	−1.62
0.09	1.013111	119.07	1576.91	−1.56
0.12	1.014879	119.61	1586.61	−1.52
0.15	1.016601	120.16	1596.29	−1.48
308.15 K				
0.00	1.005791		1555.72	
0.03	1.007691	118.29	1566.99	−1.73
0.06	1.009549	118.76	1577.85	−1.67
0.09	1.011365	119.24	1587.99	−1.60
0.12	1.013129	119.80	1597.41	−1.52
0.15	1.014869	120.21	1606.42	−1.46
313.15 K				
0.00	1.004041		1564.32	
0.03	1.005917	119.18	1576.35	−1.83
0.06	1.007755	119.59	1587.81	−1.76
0.09	1.009554	120.01	1598.76	−1.69
0.12	1.011311	120.47	1608.81	−1.61
0.15	1.013021	121.97	1617.59	−1.52