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Apparent molar volumes and compressibilities of α- and β-cyclodextrin in aqueous sulfamethoxazole at different temperatures

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ABSTRACT

The apparent molar volumes, V_ϕ, apparent molar adiabatic compressibilities, $K_{\phi,s}$, apparent molar volumes at infinite dilution, V_ϕ^0, and apparent molar adiabatic compressibilities at infinite dilution, $K_{\phi,s}^0$ are evaluated from the measured densities, ρ, and speeds of sound, u values, for α-cyclodextrin and β-cyclodextrin in aqueous sulfamethoxazole solutions at T = (288.15, 293.15, 298.15, 303.15, 308.15) K. Further, transfer partial molar volume, ΔV_ϕ^0 at infinite dilution, transfer partial molar adiabatic compressibilities, $\Delta K_{\phi,s}^0$ at infinite dilution and pairwise and triplet interaction coefficients, are discussed in terms of solute–solute and solute–solvent occurring in the ternary solution of present study.

1. Introduction

In liquid phase a vast crowd of molecules gather closely, oscillating and rotating violently. Colliding with each other, they distinguish a kind of molecule from other ones. In particular, stereospecific interactions due to neighboring surfaces may play the leading role in, e.g., enzyme–substrate reactions, antigen–antibody reactions, some kinds of mechanisms of senses of smell and taste, and so on. Therefore, elucidating the role of asymmetric intermolecular interactions owing to the stereospecific structures of molecules is really important for understanding the mechanisms of chemical and biochemical reactions.

Cyclodextrins are well-known cyclic oligosaccharides formed of α(1–4) linkages of D(+)-glucopyranose units. Cyclodextrin molecules have a truncated cone shape, with the primary and secondary hydroxyl groups located at the edges of both bases, which results in a hydrophobic cavity and a hydrophilic exterior [1]. Their ability to form inclusion complexes with a large variety of substances has made them very useful as model compounds for the study of ligand binding processes. They have also found important applications as separation and catalysis agents, and in the pharmaceutical, food, cosmetic and agricultural industries [2]. van der Waals forces, hydrophobic effects, liberation of high-energy water molecules from the cyclodextrin cavity and hydrogen bonding, are considered the driving forces of complexation. The relative contribution of each of these interaction forces depends on the chemical and structural properties of the ligand, and on the cyclodextrin and ligand sizes [3].

Generally, the thermodynamic stability of inclusion compounds depends on three facts:

(i) The size of host and guest molecules
(ii) The dehydration of host molecules, and
(iii) The removal of water molecules from the cyclodextrin cavity.

The most common pharmaceutical application of cyclodextrins is to increase the solubility of poorly soluble drugs and to engineer slow-release delivery systems for drug molecules. There are some papers devoted to the investigation of the inclusion compounds of pyridine [13], pyridine derivatives [4], imidazole [5,6] and alcohol [7,8] with cyclodextrins in aqueous solutions. The complexation of different drugs with cyclodextrins (CDs) has been extensively studied in recent years [9–15].

The thermodynamic properties of solutes like volumetric and compressibility are known to be sensitive to the nature and degree of the solute salvation [16,17]. In the case of complex formation with CDs, the transfer of a guest molecule from water to the nonpolar cavity of a CD is expected to give rise to significant changes in its partial molar compressibility and/or volume. In recent years, a number of workers have determined the various thermodynamic properties of CDs in aqueous solutions containing organic and surfactant molecules [18–22].

Among these systems, we have focused on CD with aqueous sulfamethoxazole solutions. Measurements of density and speed of sound was used to determine the partial molar volume and partial

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molar compressibility data of α- and β-cyclodextrins in aqueous sulfamethoxazole at $T = (288.15, 293.15, 298.15, 303.15, \text{and } 308.15)$ K.

2. Experimental

The oligosaccharides: α-cyclodextrin (CAS No. 10016–20-3) and β-cyclodextrin (CAS No. 7585-39-9) from (HiMedia, Mumbai) were used after drying at 333.15 K in a vacuum oven for a minimum of 48 h. The solutions were prepared by mass on the molality concentration scale with an accuracy of $\pm 1 \times 10^{-5}$ using an A&D Company, Limited electronic balance (Japan, Model GR-202) with a precision of ± 0.01 mg. The solutions were prepared using double distilled water (specific conductance 10^{-6} S cm^{-1}). The uncertainties in the solution molalities were in the range $2 \cdot 10^{-5}$ mol·kg^{-1}. Densities and speeds of sound of α-cyclodextrin and β-cyclodextrin in aqueous sulfamethoxazole solutions at different temperatures and at pressure $p = 0.1$ MPa were measured simultaneously and automatically at 3 MHz, using an Anton Paar (model DSA 5000) vibrating-tube densimeter. Both the speed of sound and the density are extremely sensitive to temperature and hence, it was controlled to $1 \cdot 10^{-2}$ K by a built-in solid state thermostat. The apparatus was also tested with the density of a known molality of aqueous NaCl using the data given by Pitzer et al. [22]. The uncertainty of the density and speed of sound estimates was found to be less than $5 \cdot 10^{-3}$ kg·m^{-3} and $5 \cdot 10^{-2}$ m·s^{-1}. Before each series of measurements, the instrument was pre-calibrated with doubly distilled, deionized, degassed water, and dry air for the temperature range investigated.

3. Results and discussion

3.1. Apparent molar properties

The values of densities, ρ, and speeds of sound, u, of α-cyclodextrin and β-cyclodextrin in aqueous solutions of sulfamethoxazole (0.0005–0.002 mol kg^{-1}) at T = (288.15, 293.15, 298.15, 303.15, and 308.15) K are reported in Table 1. The experimentally measured densities, ρ, and speeds of sound, u, were used to calculate apparent molar volumes, V_ϕ, and apparent molar adiabatic compressibilities, $K_{\phi,s}$, of α-cyclodextrin and β-cyclodextrin in aqueous solutions of sulfamethoxazole by using the following Eqs. (1) and (2)and are given in Table 2.

$$V_\phi = [(M/\rho) - \{1000(\rho - \rho_0)/(m_A \rho\ \rho_0)\}] \tag{1}$$

$$K_{\phi,s} = [(M\ \beta_S/\rho) - \{1000(\beta_{S,0}\rho - \beta_S\rho_0)/(m_A\rho\rho_0)\}] \tag{2}$$

where M is the molar mass of α-cyclodextrin and β-cyclodextrin, and ρ, ρ_o, β_S and $\beta_{S,0}$ are the densities and coefficient of adiabatic

Table 1
Densities, ρ (kg m^{-3}) and speeds of sound, u (m s^{-1}) of α-cyclodextrin and β-cyclodextrin in aqueous solutions of sulfamethoxazole (mol kg^{-1})) at different temperatures (K) and at pressure $p = 0.1$ MPa.

m_A	T									
	288.15		293.15		298.15		303.15		308.15	
	$\rho \cdot 10^{-3}$	u	$\rho \cdot 10^{-3}$	u	$\rho \cdot 10^{-3}$	u	$\rho \cdot 10^{-3}$	u	$\rho \cdot 10^{-3}$	u
0.0005 m_B Sulfamethoxazole + α-cyclodextrin										
0.00000	0.999135	1466.92	0.998196	1483.24	0.997056	1497.51	0.995654	1509.89	0.994035	1521.6
0.00205	0.999816	1467.73	0.99887	1484.04	0.997726	1498.31	0.996322	1510.69	0.994698	1522.27
0.00501	1.000780	1468.64	0.999823	1484.96	0.998675	1499.23	0.99727	1511.61	0.99564	1523.56
0.00802	1.001737	1469.25	1.000767	1485.63	0.999619	1499.85	0.998215	1512.26	0.99658	1524.31
0.00997	1.002343	1469.48	1.001366	1485.91	1.000218	1500.13	0.998816	1512.52	0.997179	1524.45
0.001 m_B Sulfamethoxazole + α-cyclodextrin										
0.00000	0.999152	1466.87	0.998205	1483.16	0.997091	1497.49	0.995704	1509.84	0.994452	1520.57
0.00201	0.999817	1467.65	0.998860	1483.93	0.997743	1498.26	0.996353	1510.58	0.995096	1521.31
0.00501	1.000794	1468.56	0.999816	1484.87	0.998700	1499.13	0.997304	1511.41	0.996039	1522.08
0.00798	1.001743	1469.16	1.000737	1485.53	0.999630	1499.65	0.998225	1511.90	0.996951	1522.47
0.01002	1.002385	1469.37	1.001355	1485.83	1.000257	1499.83	0.998847	1512.05	0.997562	1522.53
0.002 m_B Sulfamethoxazole + α-cyclodextrin										
0.00000	0.999167	1466.48	0.998236	1482.72	0.997126	1496.96	0.995735	1509.42	0.994605	1520.69
0.00200	0.999821	1467.53	0.998884	1483.77	0.997768	1497.99	0.996373	1510.46	0.995239	1521.44
0.00500	1.000781	1468.62	0.999831	1484.83	0.99871	1499.01	0.997309	1511.39	0.996164	1522.21
0.00809	1.001746	1469.11	1.000778	1485.23	0.999656	1499.33	0.998248	1511.58	0.997088	1522.54
0.00994	1.002313	1469.19	1.001335	1485.29	1.000213	1499.36	0.998799	1511.62	0.997627	1522.57
0.0005 m_B Sulfamethoxazole + β-cyclodextrin										
0.00000	0.999100	1468.46	0.998212	1484.81	0.997053	1499.05	0.995644	1511.48	0.994025	1521.07
0.00191	0.999738	1468.82	0.998845	1485.14	0.997682	1499.37	0.996271	1511.76	0.994671	1521.36
0.00508	1.000872	1469.45	0.999969	1485.75	0.998801	1499.98	0.997384	1512.35	0.995752	1521.91
0.00798	1.001992	1470.06	1.001082	1486.39	0.999904	1500.63	0.998483	1513.04	0.996851	1522.54
0.01001	1.002825	1470.52	1.001911	1486.87	1.000720	1501.16	0.999292	1513.60	0.997664	1523.18
0.001 m_B Sulfamethoxazole + β-cyclodextrin										
0.00000	0.999123	1466.87	0.998218	1483.16	0.997044	1497.49	0.995611	1509.84	0.99391	1520.57
0.00204	0.999745	1467.27	0.998831	1483.52	0.997653	1497.83	0.996215	1510.15	0.994509	1520.86
0.00482	1.000656	1467.86	0.999731	1484.09	0.998537	1498.40	0.997094	1510.71	0.995381	1521.39
0.00797	1.001779	1468.58	1.000841	1484.84	0.999614	1499.20	0.998161	1511.52	0.996443	1522.2
0.00989	1.002511	1469.06	1.001558	1485.37	1.000314	1499.75	0.998849	1512.11	0.9971237	1522.77
0.002 m_B Sulfamethoxazole + β-cyclodextrin										
0.00000	0.999185	1466.48	0.998280	1482.72	0.997111	1496.96	0.995700	1509.42	0.99409	1520.69
0.00241	0.999761	1466.84	0.998853	1483.04	0.997679	1497.26	0.996267	1509.67	0.994651	1520.9
0.00543	1.000735	1467.44	0.999819	1483.61	0.998639	1497.81	0.997219	1510.17	0.995595	1521.31
0.00849	1.001772	1468.11	1.000851	1484.27	0.999668	1498.43	0.998236	1510.75	0.996599	1521.81
0.01047	1.002547	1468.59	1.001618	1484.75	1.000426	1498.93	0.998992	1511.21	0.997345	1522.23