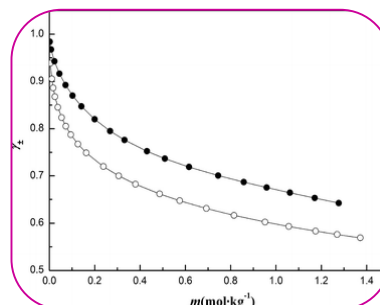


**ACTIVITY COEFFICIENT OF UREA IN TERNARY SYSTEM****Sopan K. Kushare**

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ABSTRACT

The binary (urea + water) system, using experimental osmotic coefficient data, the activity and activity coefficient of urea and water are calculated, and further activity data are processed to obtain the Gibbs free energy change of mixing and excess Gibbs free energy change of mixing. The water activities for the studied ternary system were calculated and used to obtain the activity coefficient of PEG-4000 and urea.

KEYWORDS : Urea, PEG, Activity Coefficients**1. INTRODUCTION**

Recently, we reported an analysis related to Kirkwood–Buff integrals using activity and activity coefficient data for aqueous solutions of polyethylene glycol (PEG) solutions.¹ We interpreted the free-energy integral for solute–solute (polymer–polymer molecules) affinity for aqueous PEG-4000 solution in terms of an increase in solute–solute, that is, hydrophobic interaction effect. The polyethylene glycols (PEGs), that is, HO–(CH₂–CH₂–O)_n–OH (where n is the number of repeating units), have high affinity for water. These are used in protein crystallization and cell fusion processes.² PEGs are known to form gel-like structures in solution containing cyclodextrins.³ The properties of aqueous solutions of PEGs are generally interpreted in terms of hydrogen bonding and polymer–polymer interactions.^{1,4-6} We thought that aqueous PEG-4000 solution properties in the of urea presence (a protein denaturing agent) may serve as a model system to study both effects due to the hydrophobic and hydrophilic interaction. Therefore, for urea in the water (binary system) and ternary system (urea + 0.10065 mol·kg⁻¹ PEG-4000 + H₂O), the measurements of osmotic coefficients are made at 298.15 K. The previously reported osmotic coefficient data for binary PEG-4000–H₂O system at 298.15 K. The water activity data have been used for analysis.¹ The water activity data of the studied ternary system have been obtained and processed to calculate activity coefficients of the individual components in the solution phase.

2. EXPERIMENTAL:

The details of chemical name, source, purity, and molar mass of the studied compounds are Chemical name source purity molar mass (kg·mol⁻¹) urea Merck ≥98% 0.06006 polyethylene glycol-4000 (PEG- 4000)a Merck ≥97% 4.131, HO–(CH₂–CH₂–O)_n–OH, n being the number of a repeating unit equal to 89.5. The actual molecular weight estimated by using osmometry was found to be 4.131 g·mol⁻¹ for PEG-4000.¹ Chemicals were used as received. All the solutions were freshly prepared on molality basis in quartz doubly distilled water by using high precision analytical balance (Mettler Toledo AB204-S) having the capacity to weigh a minimum of 10 mg and maximum of 220 mg and with a readability of 0.1 mg.

3. RESULT:

Binary System (Urea + H₂O). By using a vapour pressure osmometer, the osmotic coefficient (ϕ_2^0) values were determined for the aqueous solutions of urea in the concentration range of 0.11400 to 1.03192 mol·kg⁻¹ at 298.15 K by using the equation m osmolality. The data of ϕ_2^0 are collected in Table 2, and the variation of ϕ_2^0 as a function of the molality of urea at 298.15 K is shown in Figure 1 along with literature data. Using the ϕ_2^0 data, the water activity (a_w^0) values for aqueous urea solutions have been calculated. Further, a_w^0 values were utilized to calculate the solvent activity coefficient (γ_1^0).

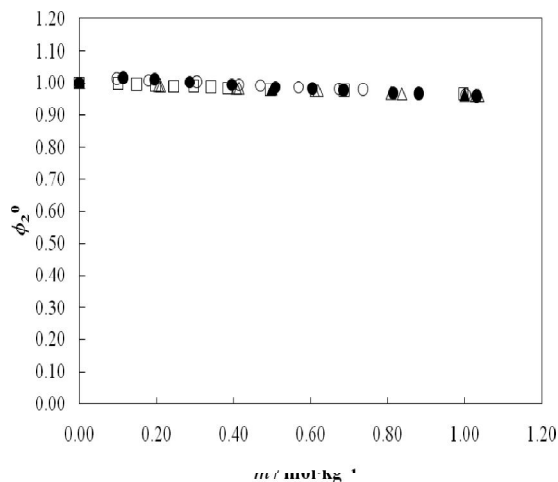


Figure 1. Variation of osmotic coefficient (ϕ_2^0) as a function of the molality of urea in aqueous solutions at 298.15 K: solid circle, experimental; open square, open triangle, ref 7; solid triangle, ref 8; open circle.

The Activity Coefficients for ternary systems are calculated using McMillan–Mayer theory of solutions and found to be.

Activity Coefficient	Urea + PEG + Water
A_{01}	-46.456419
A_{11}	-3.775230
A_{02}	177.516621
A_{03}	-301.677660
A_{21}	0.497720
A_{12}	24.402391
A_{31}	0.928282
A_{22}	3.438661
A_{12}	-45.147686
A_{04}	174.806596

4. REFERENCES:

1. Kushare, S. K.; Shaikh, V. R.; Terdale, S. S.; Dagade, D. H.; Kolhapurkar, R. R.; Patil, K. J. Thermodynamics of Aqueous Polyethylene-Glycol (PEG) Solutions at 298.15 K: Activity, Activity Coefficients and Application of Molecular Theories. *J. Mol. Liq.* 2013, 187, 129–136.
2. Patel, B. A.; Debenedetti, P. G.; Stillinger, F. H.; Rosky, P. J. A Water-Explicit Lattice Model of Heat-, Cold-, and Pressure-Induced Protein Unfolding. *Biophys. J.* 2007, 93, 4116–4127.
3. Patel, S.; Cudney, B.; McPherson, A. Polymeric Precipitants for the Crystallization of Macromolecules. *Biochem. Biophys. Res. Commun.* 1995, 207, 819–828.

4. Wang, J.; Li, L.; Zhu, Y.; Liu, P.; Guo, X. Hydrogels Assembled by Inclusion Complexation of Poly(ethylene glycol) with Alpha-Cyclodextrin. *Asia-Pac. J. Chem. Eng.* 2009, 4, 544–550.
5. Ayranci, E.; Sahin, M. Interactions of Polyethylene Glycols with Water Studied by Measurements of Density and Sound Velocity. *J. Chem. Thermodyn.* 2008, 40, 1200–1207.
6. Patil, P. D.; Shaikh, V. R.; Gupta, G. R.; Hundiwale, D. G.; Borse, A. U.; Patil, K. J. Studies of Viscosity Coefficient and Expansivity Properties of Aqueous Solutions of Ethylene Glycol and Polyethylene Glycols at 293.15, 298.15 and 303.15 K and at Ambient Pressure. *J. Solution Chem.* 2016, 45, 947–969.
7. Terdale, S. S.; Dagade, D. H.; Patil, K. J. Thermodynamic Studies of Molecular Interactions in Aqueous α -Cyclodextrin Solutions: Application of McMillan-Mayer and Kirkwood-Buff Theories. *J. Phys. Chem. B* 2006, 110, 18583–18593. *Journal of Chemical & Engineering Data Article*
8. Patil, K.; Dagade, D. Studies of Activity Coefficients for Ternary Systems: Water + 18-Crown-6 + Alkali Chlorides at 298.15 K. *J. Solution Chem.* 2003, 32, 951–966.
9. Shaikh, V. R.; Dagade, D. H.; Terdale, S. S.; Hundiwale, D. G.; Patil, K. J. Activity and Activity Coefficient Studies of Aqueous Binary Solutions of Procaine, Lidocaine, and Tetracaine Hydrochloride at 298.15 K. *J. Chem. Eng. Data* 2012, 57, 3114–3122.
10. Shaikh, V. R.; Terdale, S. S.; Hundiwale, D. G.; Patil, K. J. Thermodynamic Studies of Drug- α -Cyclodextrin Interactions in Water at 298.15 K: Procaine Hydrochloride/Lidocaine Hydrochloride/ Tetracaine Hydrochloride/Ranitidine Hydrochloride + α -Cyclodextrin + H₂O systems. *J. Chem. Thermodyn.* 2014, 68, 161–168.
11. Ellerton, H. D.; Dunlop, P. J. Activity Coefficients for the Systems Water-Urea and Water-Urea-Sucrose at 25° from Isopiestic Measurements. *J. Phys. Chem.* 1966, 70, 1831–1837.
12. Stokes, R. H. Thermodynamics of Aqueous Urea Solutions. *Aust. J. Chem.* 1967, 20, 2087–2100.
13. Tomar, P. Studies on Complexation between Urea and 18-Crown-6 in Aqueous Solutions at 298.15 K. *Ind. J. Chem.* 2009, 48A, 1247–1250.