Supporting Information

Investigation of Inclusion Complex formed by Ionic Liquid and β-Cyclodextrin through Hydrophilic and Hydrophobic Interactions

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The physical properties of binary mixtures in different mass fractions (w=0.001, 0.003, 0.005) of aqueous β-CD solutions at 298.15K have been reported in table S1. The values of density, viscosity, and refractive index of chosen ionic liquid in different mass fractions of aqueous β-CD mixture, as a function of concentration (molality) have been listed in tables given below.

Surface tension

The concentrations at which the inclusion occurred (the break point of the surface tension) have been calculated by solving the equation of two straight lines, and represented in table 1. For instance, in case of IL in w_2=0.001 mass fraction of β-cyclodextrin

$$\gamma = 1180.50\ c + 51.66$$

$$\gamma = 545.24\ c + 54.77$$

γ = 56.60 mN·m^{-1} and c = 3.00 millimolal

Conductance

The specific conductance (κ) of IL+aq.β-CD solutions under investigation in different mass fractions (w = 0.001, 0.003, 0.005) aq.β-CD were measured. The molar conductance (Λ) for the studied solutions has been calculated using following equation,[1] and given in Fig. 2.

$$\Lambda = 1000\ \boldsymbol{\kappa}\ /\boldsymbol{c} \qquad (1)$$

where c is the molar concentration of the studied solution.

Similarly the concentrations at which the inclusion occurred (the break point of the Conductance) have been calculated by solving the equation of two straight lines, and represented in table 2. For instance, in case of IL in w_2=0.001 mass fraction of β-cyclodextrin

$$\kappa = -21.971\ c + 1.9742$$

$$\kappa = -7.265\ c + 1.3462$$

κ = 1.21 S·m^{-1} and c = 3.00 millimolal

Apparent molar volume

The apparent molar volumes ϕ_V were determined from the solutions densities (Table S2) using the equation

$$\phi_V = M/\rho - 1000(\rho - \rho_o)/m\rho\rho_o \qquad (2)$$

where M is the molar mass of the IL, m is the molality of the solution, ρ and ρ_0 are the density of the solution and aq. β-CD mixture respectively. The limiting apparent molar volumes ϕ_V^0 were obtained by a least-square treatment to the plots of ϕ_V versus $\sqrt{m}$ using the Masson equation,[2] and shown in table S3.

$$\phi_V = \phi_V^0 + S_V^* \cdot \sqrt{m} \qquad (3)$$

Viscosity

The experimental viscosity data for the studied systems are listed in table S2. The relative viscosity (η_r) has been analyzed using the Jones-Dole equation, [3]

$$(\eta/\eta_o - 1)/\sqrt{m} = (\eta_r - 1)/\sqrt{m} = A + B\sqrt{m} \qquad (4)$$

where $\eta_r = \eta/\eta_o$, η and η_0 are the relative viscosities, the viscosities of the ternary solutions (IL+aq. CD) and binary aqueous mixture (aq. CD) and m is the molality of the IL in ternary solutions. A and B are empirical constants known as viscosity A and B-coefficients, which are specific to solute-solute and solute-solvent interactions, respectively, are estimated by least-square method by plotting $(\eta_r - 1)/\sqrt{m}$ against $\sqrt{m}$, and reported in table S3.

Refractive index

The molar refraction, R_M can be evaluated from the Lorentz-Lorenz relation,[4]

$$R_M = \{(n_D^2 - 1)/(n_D^2 + 2)\}(M/\rho) \qquad (10)$$

where R_M, n_D, M and ρ are the molar refraction, the refractive index, the molar mass and the density of solution respectively. The Limiting molar refraction (R_M^0) estimated from the following euation, [5]

$$R_M = R_M^0 + R_S\sqrt{m} \qquad (11)$$

References:

(1) D. Ekka and M. N. Roy, *Amino Acids*, 2013, **45**, 755-777.

(2) D.O. Masson, *Phil Mag.,* 1929, **8***,* 218-223.

(3) G. Jones and D. Dole*, J. Am. Chem. Soc.,* 1929, **51,** 2950-2964.

(4) V.Minkin, O. Osipov and Y. Zhdanov, *Dipole Moments in Organic Chemistry.* New York, Plenum Press, **1970**.

(5) M. N. Roy, P. Chakraborti and D. Ekka, *Mol. Phys.,* 2014, **112** (**17)**, 2215-2226.

Tables

Table S1. Experimental values of density (*ρ*), viscosity (*η*), and refractive index (n_D) in different mass fraction of aqueous *β*-cyclodextrin mixtures

aq. solvent mixture	Temp /K[a]	$\rho\cdot10^{-3}$ /$kg\cdot m^{-3}$	η /mP·s	n_D
w_1=0.001[b]	298.15	0.99856	1.18	1.2940
	303.15	0.99601	0.92	-
	308.15	0.99256	0.89	-
w_1=0.003[b]	298.15	0.99904	1.22	1.3005
	303.15	0.99677	0.98	-
	308.15	0.99332	0.96	-
w_1=0.005[b]	298.15	0.99993	1.29	1.3110
	303.15	0.99737	1.04	-
	308.15	0.99423	1.01	-

[a] Standard uncertainties in temperature ***u*** (T) = 0.01 K, viscosity ***u*** *(η)* = 0.01 mPa·s. refractive index ***u***(n_D) =0.0002 [b] w_1 is the mass fractions of *β*-CD in aqueous mixture.

Table S2. Experimental values of densities (ρ) and viscosities (η) corresponding to concentration in different mass fractions of aq. β-cyclodextrin at different temperature

Conc (m)	$\rho \cdot 10^{-3}$ /kg·m^{-3}	η /mP·s	Conc (m)	$\rho \cdot 10^{-3}$ /kg·m^{-3}	η /mP·s	Conc (m)	$\rho \cdot 10^{-3}$ /kg·m^{-3}	η /mP·s
298.15 K[a]			303.15K[a]			308.15K[a]		
IL								
w_1=0.001 [b]								
0.01	0.99873	1.20	0.01	0.99616	0.94	0.01	0.99263	0.91
0.025	0.99879	1.24	0.025	0.99645	0.96	0.025	0.99294	0.93
0.040	0.99934	1.27	0.040	0.99672	0.98	0.040	0.99321	0.94
0.055	0.99945	1.30	0.055	0.99694	1.01	0.055	0.99349	0.97
0.070	1.00015	1.35	0.070	0.99749	1.03	0.070	0.99391	0.99
0.085	1.00064	1.41	0.085	0.99792	1.06	0.085	0.99431	1.02
w_1=0.003 [b]								
0.01	0.99923	1.22	0.01	0.99682	0.98	0.01	0.99333	0.96
0.025	0.99991	1.25	0.025	0.99714	1.01	0.025	0.99391	0.99
0.040	1.00034	1.33	0.040	0.99770	1.04	0.040	0.99423	1.03
0.055	1.00074	1.38	0.055	0.99808	1.07	0.055	0.99454	1.07
0.070	1.00110	1.45	0.070	0.99838	1.11	0.070	0.99479	1.09
0.085	1.00143	1.49	0.085	0.99871	1.15	0.085	0.99513	1.12
w_1=0.005 [b]								
0.01	0.99998	1.29	0.01	0.99778	1.04	0.01	0.99426	1.01
0.025	1.00056	1.34	0.025	0.99843	1.07	0.025	0.99489	1.05
0.040	1.00113	1.39	0.040	0.99881	1.11	0.040	0.99514	1.08
0.05	1.0014	1.46	0.05	0.9991	1.15	0.05	0.9957	1.12

5	5		5	0		5	6	
0.07	1.0019	1.51	0.07	0.9994	1.17	0.07	0.9960	1.15
0	3		0	7		0	6	
0.08	1.0025	1.59	0.08	0.9998	1.20	0.08	0.9967	1.17
5	6		5	5		5	9	

Standard uncertainties in temperature (T) = 0.01 K. viscosity ***u** (η)* = 0.01 mPa·s. [b] w_1 is the mass fractions of *β*-CD in aqueous mixture.

Table S3. Limiting apparent molar volume (ϕ_v^o), experimental slope (S_v^*), viscosity *B* and *A*-coefficient in different mass fractions of aqueous *β*-cyclodextrin mixtures

Temp /K[a]	$\phi_v^o \times 10^6$	S_v^*	*B*	*A*
		[moim]BF_4		
		w_1=0.001[b]		
298.15	223.35	-287.83	1.62	-0.084
303.15	225.30	-320.43	1.65	-0.106
308.15	235.56	-358.36	2.84	-0.218
		w_1=0.003[b]		
298.15	227.01	-290.19	1.86	-0.103
303.15	230.50	-345.52	2.62	-0.132
308.15	242.97	-395.24	3.11	-0.219
		w_1=0.005[b]		
298.15	232.75	-326.70	2.32	-0.142
303.15	241.37	-351.01	3.54	-0.227
308.15	247.69	-432.90	3.98	-0.301

[a] Standard uncertainties in temperature (T) = 0.01 K. [b] w_1 is the mass fractions of *β*-CD in aqueous mixture.

Table S4. Measured parameters for IL ([moim]BF4) in 0.001(M), 0.003(M)and 0.005(M) aquous beta CD solutions at 298.15 K temperature.

c /mol·dm^{-3}	n_D	R_m	R_{m0}
	[moim]BF_4		
	w_1=0.001[b]		
0.010	1.3232	70.0945	69.14
0.025	1.3237	70.1963	

0.040	1.3242	70.2623	
0.055	1.3249	70.3111	
0.070	1.3254	70.3667	
0.085	1.3258	70.4094	
		w_1=0.003[b]	
0.010	1.3241	70.1823	
0.025	1.3246	70.2854	
0.040	1.3252	70.3389	70.23
0.055	1.3257	70.3934	
0.070	1.3261	70.4412	
0.085	1.3265	70.4766	
		w_1=0.005[b]	
0.010	1.3249	70.2826	
0.025	1.3253	70.3659	
0.040	1.3257	70.4116	70.94
0.055	1.3262	70.4658	
0.070	1.3267	70.5079	
0.085	1.3274	70.5498	

[b] w_1 is the mass fractions of β-CD in aqueous mixture.

Figures:

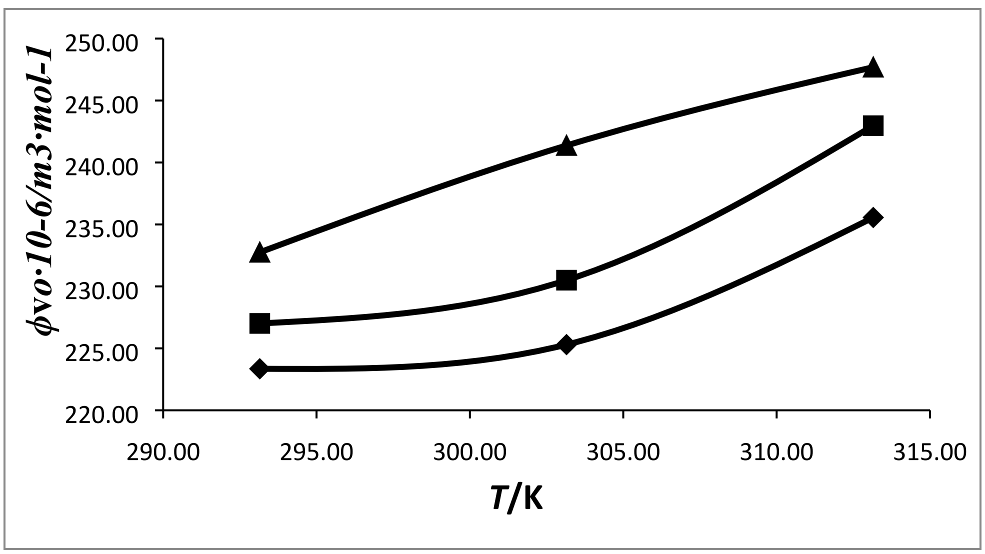

Fig. 3 Variation of apparent molar volume (ϕ_v^o) with temp (*T/K*) of IL solution in 0.001(♦), 0.003(■), and 0.005(▲) of aq. β-CD respectively

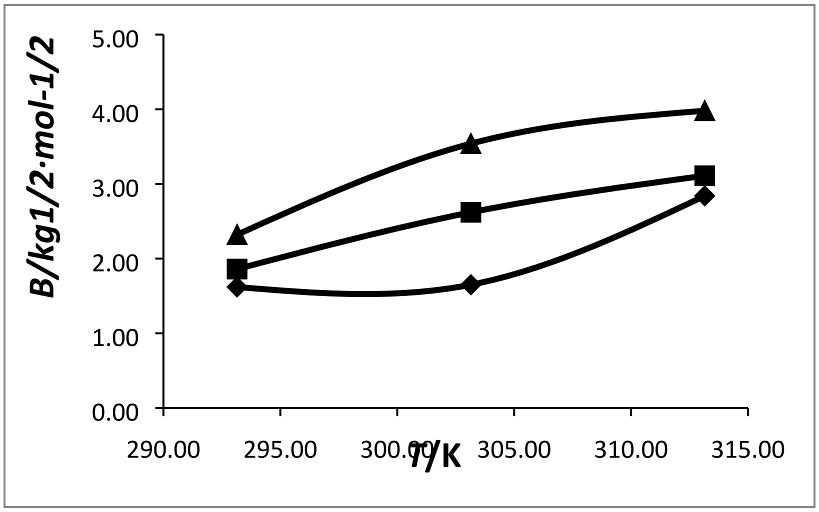

Fig. 4 Plot of viscosity *B*-coefficient with temp (*T/K*) of ILsolution in 0.001(♦), 0.003(■), and 0.005(▲) of aq. β-CD respectively

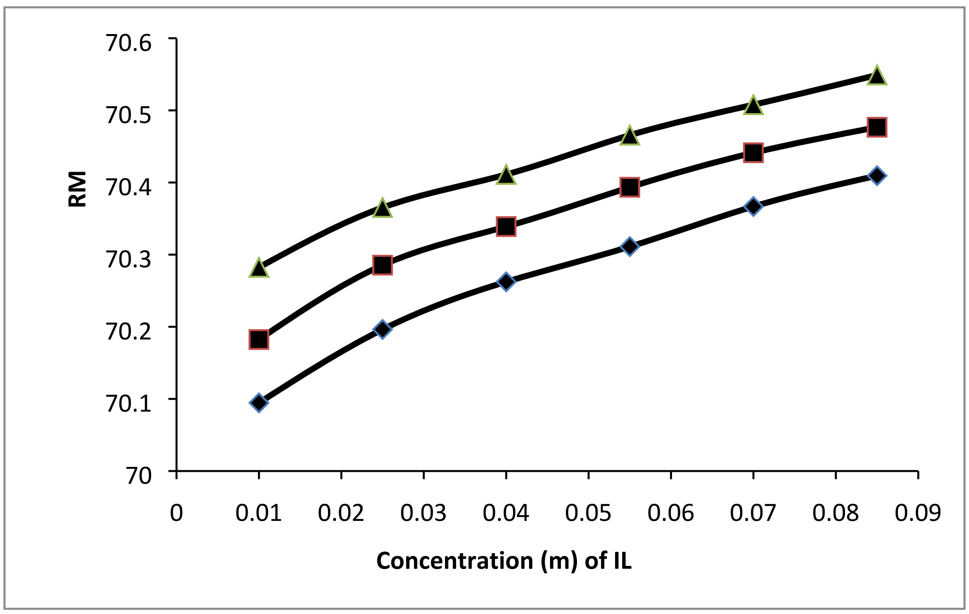

Fig. 5 Plot of molar refraction with concentration of IL solution in 0.001(♦), 0.003(■), and 0.005(▲) of aq. β-CD respectively

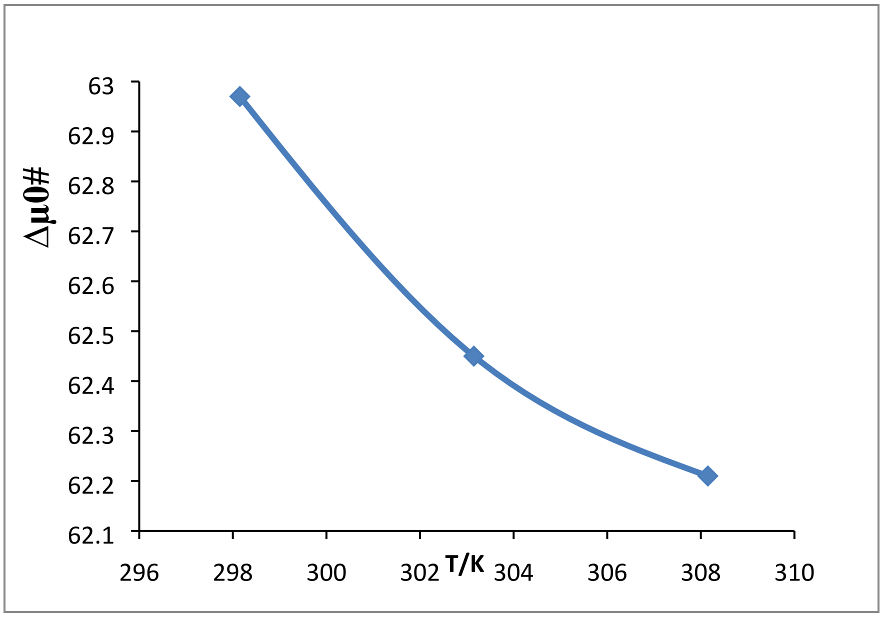

Fig. 6: Plot of $\Delta\mu^{0\#}$ versus Temperature of IL in 0.001 m conc. Of β-CD

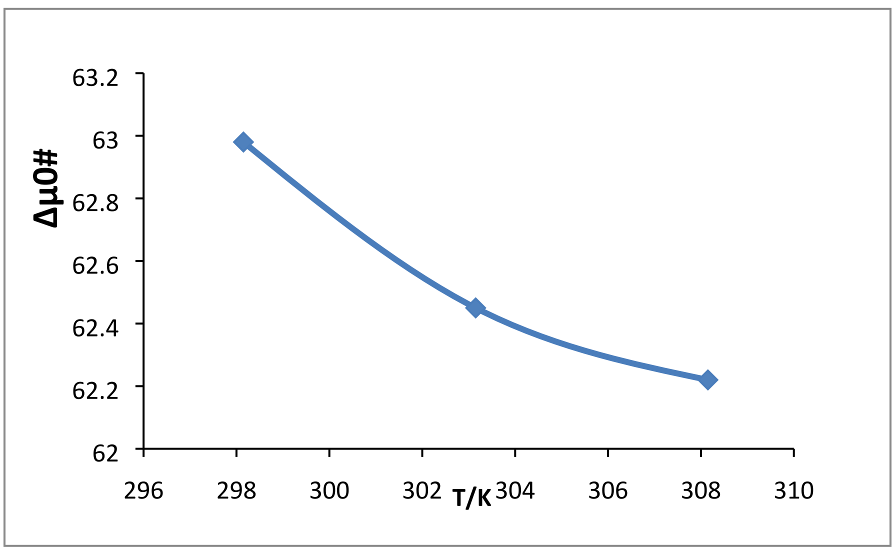

Fig. 7: Plot of $\Delta\mu^{0\#}$ versus Temperature of of IL in 0.003 m conc. Of β-CD

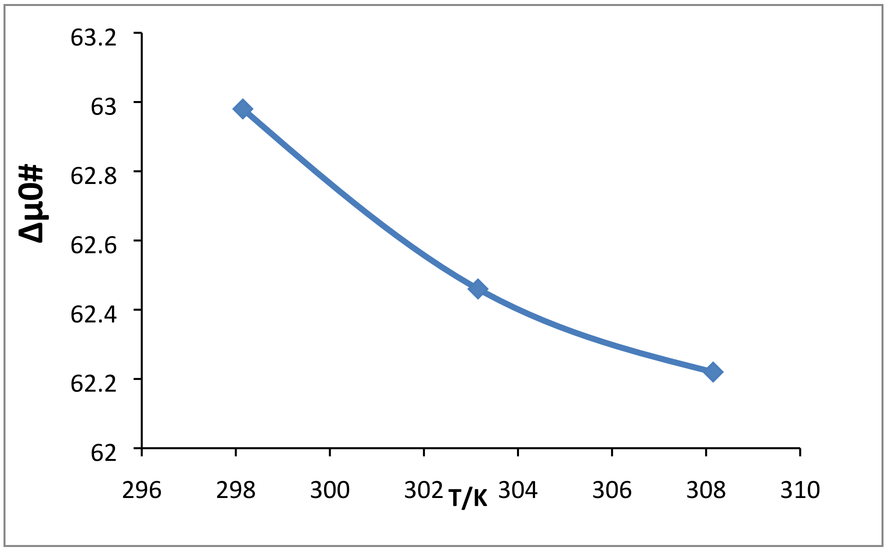

Fig. 8: Plot of $\Delta\mu^{0\#}$ versus Temperature of IL in 0.005 m conc. Of β-CD