

Research Article

Exploration of Host Guest Inclusion Complex of β -Cyclodextrin with an Ionic Liquid ($[C_4mpy]Cl$) in Aqueous Media by Physicochemical Approach

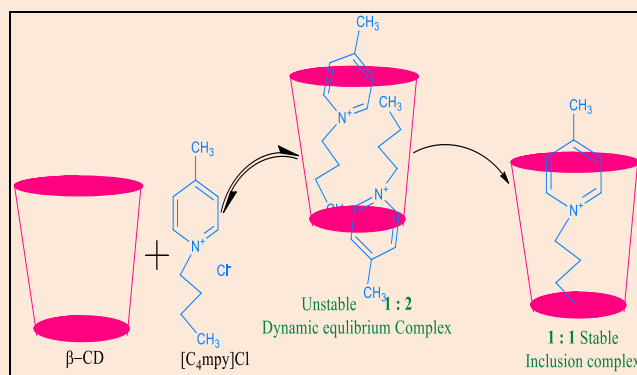
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Abstract

With the evidence of the experimental data evaluated from surface tension and conductance, the formation of inclusion complexes of β -Cyclodextrin with an Ionic Liquid, viz. N-butyl-4-methylpyridinium chloride ($[C_4mpy]Cl$) in aqueous media have been reported. The limiting apparent molar volume, viscosity B -coefficient and limiting molar refraction have been studied to derive the appropriate parameters for the formation of inclusion complexes prevailing in the investigated solvent systems.

Keywords: Inclusion complexes, N-butyl-4-methylpyridinium chloride ($[C_4mpy]Cl$), β -Cyclodextrin, solvation number.



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Introduction

From the X-ray structures it appears that in cyclodextrins the secondary hydroxyl groups (C2 and C3) are located on the wider edge of the ring and the primary hydroxyl groups (C6) on the other edge, and that the apolar C3 and C5 hydrogens and ether-like oxygens are at the inside of the torus-like molecules. This result in a molecule with a hydrophilic outside, and an apolar cavity, which provides a hydrophobic matrix, described as a 'micro heterogeneous environment' [1]. The favorable and best size of cavity diameter of the β -Cyclodextrin are as a host can form supramolecular and host-guest inclusion complexes [2] with a wide variety of hydrophobic guest molecules and have numerous applications in nanoscience, pharmaceutical industry, pesticides, foodstuffs, toilet articles, and textile processing [3–5]. Such successful flexible cavity also has the power of molecular recognition, self-assembly, selectivity, molecular encapsulation, chemical stabilization, and intermolecular interactions [6, 7]. Up to date, it has been seen that one or two guest molecules can be entrapped by one, two or three cyclodextrins.

It has been reported that ILs can form extended hydrogen bond systems in the liquid state and are therefore highly structured [8]. The pre-organized structure exhibits an extended network of cations–anions connected by hydrogen bonds. The soluble nature of cyclodextrin in ionic liquids has deduced to be associated with the extended hydrogen-bonded systems [9]. Palepu et al. determined the conductivity of solutions of sodium alkyl carboxylates in water with different alkyl groups and β -CD [10]. However, to the best of our knowledge, the study of the inclusion interaction between β -Cyclodextrin and N-butyl-4-methylpyridinium chloride ($[C_4mpy]Cl$) has not been reported so far. Considering the special structure and properties, it is of interest to investigate the complexation behavior between them using selected techniques. In the present study we have tried to attempt the formation of inclusion complexes between β -Cyclodextrin and $[C_4mpy]Cl$ as well as the stoichiometry of the inclusion complexes (ICs) formed.

Experimental

Materials and Reagents

The selected ionic liquid and β -Cyclodextrin of puriss grade were purchased from Sigma-Aldrich, Germany. The surface tension experiments were done by platinum ring detachment method using a Tensiometer (K9, KRÜSS; Germany) at the experimental temperature. The accuracy of the measurement was within $\pm 0.1 \text{ mN}\cdot\text{m}^{-1}$.

The conductance measurements were carried out in a Systronics-308 conductivity bridge of accuracy $\pm 0.01\%$, using a dip-type immersion conductivity cell, CD-10 having a cell constant of approximately $(0.1 \pm 0.001) \text{ cm}^{-1}$ [11]. The densities were measured by means of vibrating *U*-tube Anton Paar digital density meter (DMA 4500M) with a precision of $\pm 0.00005 \text{ g cm}^{-3}$ maintained at $\pm 0.01 \text{ K}$. The viscosities were measured using a Brookfield DV-III Ultra Programmable Rheometer with fitted spindle size-42 [12].

Refractive index was measured with the help of a digital refractometer Mettler Toledo. The light source was light emitting diode (LED), $\lambda = 589.3 \text{ nm}$. The refractometer was calibrated twice using distilled water and calibration was checked after every few measurements. The uncertainty of refractive index measurement was ± 0.0002 units.

Result and Discussion

Surface tension

It was reported that the ionic liquids with an alkyl chain were surface active in aqueous solutions [13]. So, if the alkyl chain of ionic liquids C_4mpyCl , can form ICs with β -CD, and then the surface tensions of their solutions would be distinctly affected by the addition of β -CD. Therefore, surface tension measurements can be used to elucidate not only whether inclusion can happen or not but also the stoichiometry of inclusion complexes formed. The surface tensions of pure water and aqueous solutions of β -CD are almost constant, indicating that β -CD has no effect on the surface tensions of pure water. Surface tension of the IL- β -CD solution system has been obtained by dilution method. The reliance of the surface tensions on β -CD concentrations is shown in Figure 1. Thus, it may suppose that the noteworthy changes of surface tensions of ionic liquid solutions are attributed to the formation of the inclusion complex.

For C_4mpyCl aqueous solutions, the surface tensions increase gradually with increasing β -CD concentration (**Figure 1**), indicating the formation of inclusion complexes between β -CD and C_4mpyCl . Two perceptible breaks in the surface tension curves are 0.00053 M and 0.00055 for first break point and 0.00106 and 0.00108 for stable second break point respectively (**Table 1**), suggesting that the stoichiometry of the inclusion is $1.9:1$ and $1.8:1$ in first break point; $1.06:1$ and $1.08:1$ in stable second break point. The possible reason is that C_4mpyCl has a hydrophobic tail (13.68 \AA), thus a larger steric inhibition for penetrating into the cavity ($5.03\text{--}8.81 \text{ \AA}$) of β -CD. Therefore, at first break point approximately two hydrophobic tail groups of C_4mpyCl molecule include into the apolar cavity of one β -CD molecule (**Scheme 1**) through the narrow ($5.28\text{--}7.92 \text{ \AA}$) and wider ($7.60\text{--}8.53 \text{ \AA}$) rim and form $1:2$ complex in dynamic equilibrium. But after the addition of aqueous β -CD, the numbers of β -CD molecules are increasing with respect to the fixed number of ionic liquids. As a result, one β -CD molecule can pull or attract partially encapsulated hydrophobic tail of C_4mpy^+ and finally form stable equimolar $1:1$ inclusion complex. Thus, it can be deduced that hydrophobicity plays an important role in the formation of inclusion complexes. It is noted that the nature of the chloride ion also has the significant influence on the inclusion complexes, e.g., the Cl^- ion is most electronegative, and in the aqueous solution it pull the movable water molecules towards itself, as a result the C_4mpy^+ and β -CD molecules become free to interact with each other in the solution which form the inclusion complex.

In these complexes (**Scheme 2**), the C_4mpy^+ , a guest molecule is incorporated within the dimensionally fit host cavity of the β -cyclodextrin molecule, provides a microenvironment into which appropriately sized non-polar moieties enter and form stable inclusion complexes [14]. But, there is no any covalent bonds are breaking or forming during the formation of the inclusion complex [15]. The main driving force of complex formation is the release of enthalpy-rich water molecules from the cavity (Scheme 2). Water molecules are displaced by more hydrophobic guest molecules present in the solution to attain an apolar–apolar association and decrease of cyclodextrin ring strain

resulting in a more stable lower energy state [16]. The binding of C₄mpyCl molecule within the host cyclodextrin is not fixed or permanent but rather is a dynamic equilibrium and the binding strength compatible as well the stable 'host-guest' complex fits together, on specific local interactions between surface atoms.

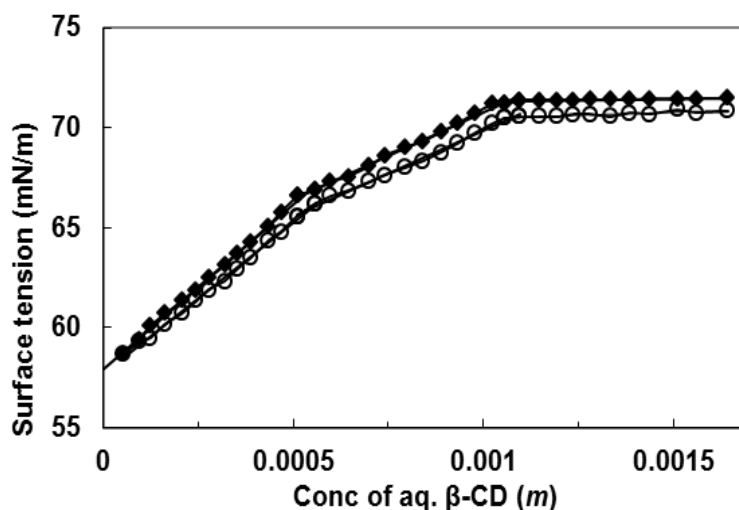


Figure 1 Variation of surface tension (γ) with concentration of [C₄mpy]Cl solution (0.001M) in aqueous β -Cyclodextrin

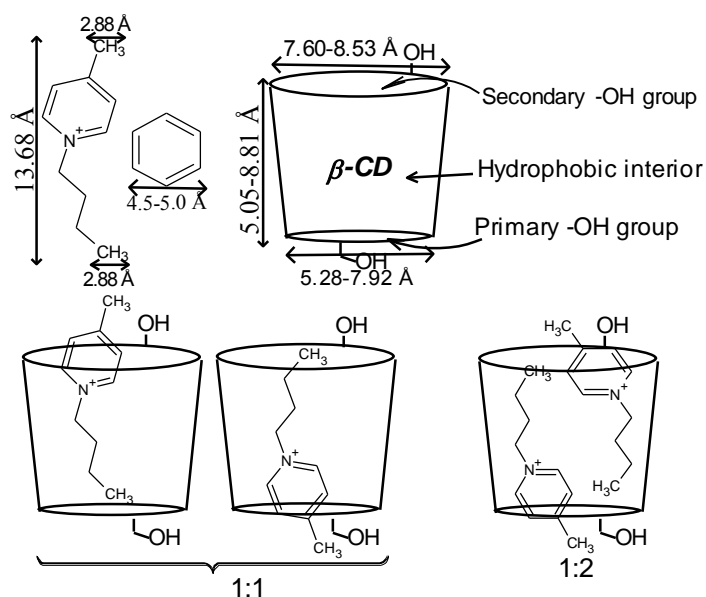
Table 1 Surface tension (γ) with corresponding concentration, and concentration ratio (ratio of inclusion IL: β -CD) at the first and second break point of 4-methyl-N-butylpyridinium chloride solution (0.001 M) in aqueous β -CD

	Conc (m)	γ (mN/m)	Conc ratio (IL: β -CD)	Conc (m)	γ (mN/m)	Conc ratio (IL: β -CD)
	at unstable first break point			at stable second break point		
Run I	0.00053	66.71	1.9 : 1	0.00106	71.32	1 : 1.06
Run II	0.00055	66.01	1.8 : 1	0.00108	70.52	1 : 1.08

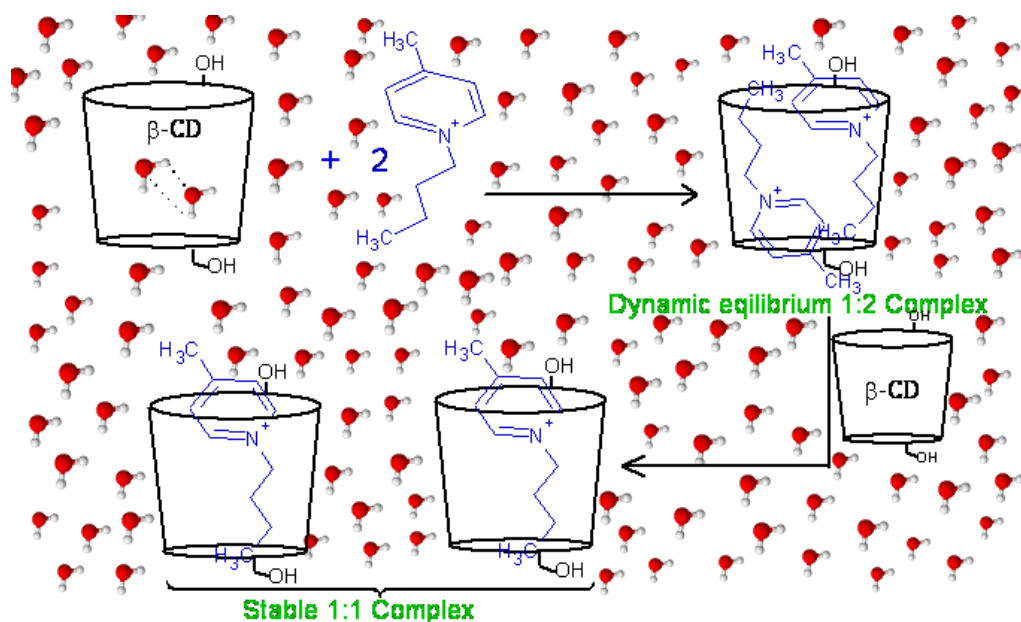
The stability of the formation of inclusion complexes can be described by the key factors. Since, the C₄mpyCl molecule is the spot on size; it fits properly into the cyclodextrin cavity and forms stable complex. In general, therefore, there are four energetically favourable interactions that help shift the equilibrium towards the forward (Scheme 2) to form the inclusion complex:

- The displacement of exits polar water molecules from the apolar cavity of β -cyclodextrin.
- The formation of extended hydrogen bonds by the primary and secondary hydroxyl (-OH) groups and rest water molecules that open a face for entering the guest molecule.
- A reduction of the repulsive interactions between the hydrophobic guest and the aqueous environment.
- An increase in the hydrophobic interactions as the guest inserts itself into the apolar cyclodextrin cavity.

Association of the inclusion complex is not a rapid process because large number of water molecules in the surrounding environment is trapped by Cl⁻ ion it has the high charge surface density. The resulting concentration gradient shifts the equilibrium in Scheme 2 towards the right.



Scheme 1 Plausible inclusion structures of the β -CD –C₄mpyCl in aqueous solution of stable 1:1 and dynamic equilibrium 1:2 stoichiometry (the cavity diameter, height of β -CD; chain length and group of C₄mpyCl have been determined from ref. [23])



Scheme 2 Schematic reorientation of the formation of inclusion complex in the solution

Conductance

Conductivity is a useful method for studying the inclusion phenomenon, and it can be used to elucidate not only whether inclusion can occur or not but also the stoichiometry of the inclusion complexes (ICs) formed. If it forms an inclusion complex with β -CD, the solution conductivity will be distinctly affected by the addition of β -CD. The

conductivity of various β -CD concentrations in ([C₄mpy]Cl) (0.001M), and the dependence of the conductivity on β -CD concentration have been done in many times and best three (Run I, II and III) is shown in **Table 2** and **Figure 2**.

Table 2 Conductance (Λ) with corresponding concentration, and concentration ratio (ratio of inclusion IL: β -CD) at the first and second break point of 4-methyl-N-butylpyridinium chloride solution (0.001 M) in aqueous β -CD

	Conc (m)	Λ (S m ² /mol)	Conc ratio (IL: β -CD)	Conc (m)	Λ (S m ² /mol)	Conc ratio (IL: β -CD)
	at first break point			at second break point		
Run I	0.00051	88.26	~2 : 1	0.00110	62.773	1 : 1.10
Run II	0.00051	85.06	~2 : 1	0.00107	61.456	1 : 1.07
Run III	0.00051	81.70	~2 : 1	0.00105	60.345	1 : 1.05

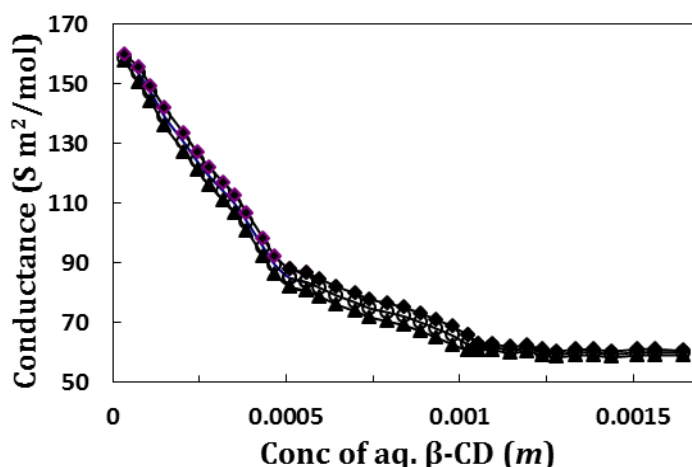


Figure 2 Variation of conductance (Λ) with concentration of [C₄mpy]Cl solution (0.001M) in aqueous β -Cyclodextrin

From the perusal of Figure 2 it is seen that the conductivity of the ionic liquid decreased remarkably with addition the concentration of β -CD. The decreasing tendency of the conductance-concentration curve clearly indicating that the β -CD molecules capture the ([C₄mpy]Cl) molecules one by one, as a results, the movement of the ionic liquid is restricted and which diminishes the conductivity. There are two noticeable breaks in the conductivity curve (Figure 2). The first break point is at the concentration of about 0.00051M β -CD, and the second one is at the concentration of 0.00110M, 0.00107M and 0.00105M (Table 2), arising a complicated situation in the discussion and the stoichiometry of the β -CD–([C₄mpy]Cl) inclusion complexes. This complicated problem can simply think and solve if we consider the concentration ratio of the ionic liquid and β -CD at the corresponding break point. At the first break point the concentration ratio ~2 : 1 of the ionic liquid and β -CD, is unstable and not an equimolar; but at the second break point the 1:1 ratio suggesting that the stoichiometry of the β -CD–[C₄mpy]Cl inclusion complex is stable and equimolar [17]. Thus, the result is in good agreement with the observation as observed from surface tension measurement.

Apparent molar volume, viscosity B -coefficient and refractive index

The remarkable behaviour of interaction or inclusion of chosen ionic liquid into β -CD has also been obtained from apparent molar volume and viscosity B -coefficient. Both the valuable parameters signify the solute-solvent interactions in the ([C₄mpy]Cl) +aq. β -CD ternary solution systems. The limiting molar volume (ϕ_v°) and viscosity B -

coefficient have been obtained from appropriate equation [18] using the experimental values of density (ρ) and viscosity (η) respectively and are presented in **Tables S2-S3** (supporting information) and **Figures 3 and 4**.

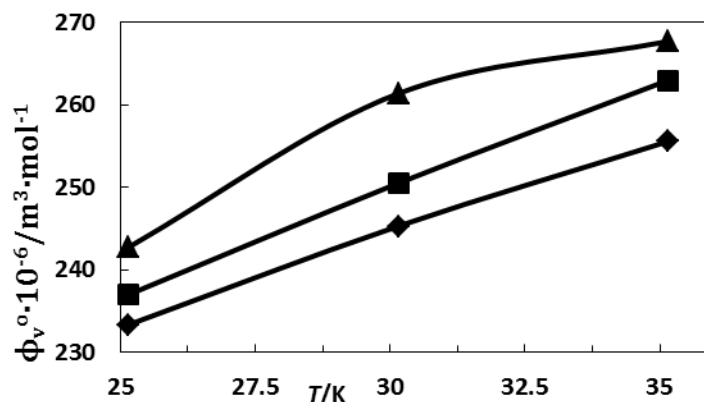


Figure 3 Variation of apparent molar volume (ϕ_v^o) with temp (T/K) of $[\text{C}_4\text{mpy}]\text{Cl}$ solution in 0.001(\blacklozenge), 0.003(\blacksquare), and 0.005(\blacktriangle) of aq. β -CD respectively

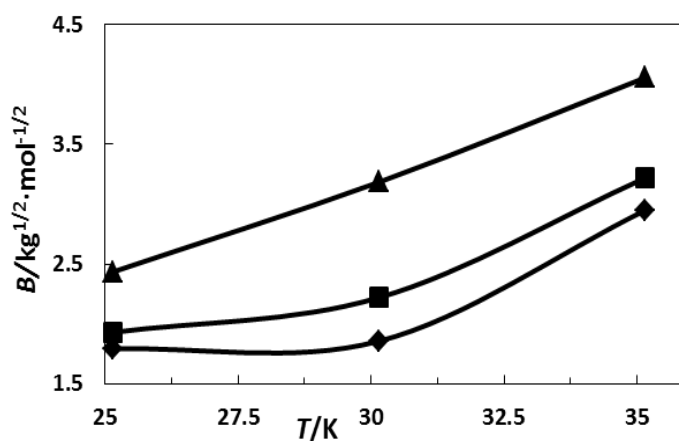


Figure 4 Plot of viscosity B -coefficient with temp (T/K) of $[\text{C}_4\text{mpy}]\text{Cl}$ solution in 0.001(\blacklozenge), 0.003(\blacksquare), and 0.005(\blacktriangle) of aq. β -CD respectively

The scrutiny of Figure 3 and 4 shows that the limiting molar volume (ϕ_v^o) and viscosity B -coefficient both raise regularly with increasing temperature, and these values are higher in $w=0.003$ than 0.001, which in turn higher in 0.005 mass fraction of aq. β -CD.

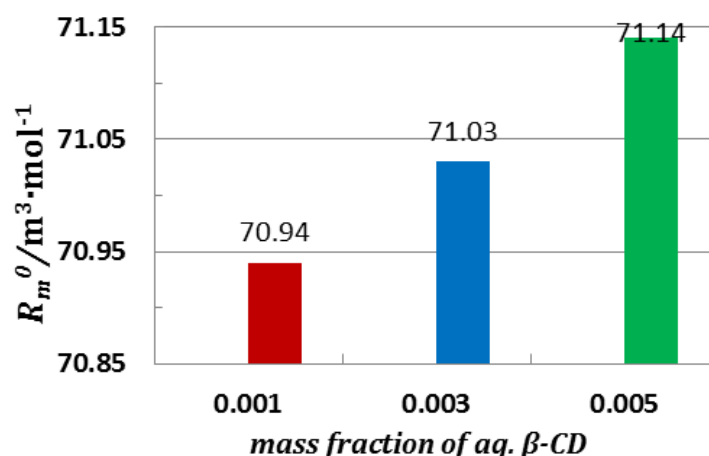
The trend shrugs the interactions between the ionic liquid and β -CD molecules are enhancing with increasing temperature and also with mass fraction of aq. β -CD. This is due to the fact that β -CD shows favorable interaction with pyrimidine based IL $[\text{C}_4\text{mpy}]\text{Cl}$. The facts support the data and results observed from surface tension and conductance that have been discussed earlier.

Solvation numbers (S_n) are evaluated from apparent molar volume and viscosity B -coefficient. S_n expresses the solvation of the ILs by the cyclodextrin molecule, *i.e.*, the interaction between the polar groups of the guest and the $-\text{OH}$ groups at the primary and secondary rims of cyclodextrin [19, 20]. In **Table 3** the solvation numbers are listed which show that after the formation of inclusion complex the ILs form H-bonds with the $-\text{OH}$ groups at the primary and secondary rims of cyclodextrin, which further stabilizes the inclusion complex.

Table 3 Solvation number (S_n), ionic apparent molar volume (ϕ_{\pm}°) in deferent mass fractions of aqueous β -cyclodextrin mixtures

Temp /K ^a	S_n	$\phi_v^{+}\times 10^6$	$\phi_v^{-}\times 10^6$
$w_I=0.001$			
298.15	7.68	142.08	91.27
303.15	7.97	152.91	92.39
308.15	11.54	162.02	93.54
$w_I=0.003$			
298.15	8.14	145.59	91.42
303.15	8.86	158.00	92.50
308.15	12.24	169.27	93.70
$w_I=0.005$			
298.15	10.03	151.18	91.57
303.15	12.19	168.65	92.72
308.15	15.16	173.70	93.99

The refractive index measurement is also a convenient method for investigating the interaction occurring in solution. Stated more simply, the refractive index of a compound describes its ability to refract light as it moves from one medium to another and thus, the higher the refractive index of a compound, the more the light is refracted [21]. The values of refractive index n_D , molar refraction R_M , limiting molar refraction R_M° are reported in Table S4 (supporting information) and **Figure 5**.

**Figure 5** Plot of limiting molar refraction (R_m°) of $[C_4\text{mpy}]Cl$ solution with mass fraction of aq. β -CD respectively

As also stated by Deetlefs et al. [22] the refractive index of a substance is higher when its molecules are more tightly packed or in general when the compound is denser. The refractive index is directly proportional to molecular polarizability, scrutiny of Table S4 and Figure 5 reveals the n_D and R_M values increases with an increasing concentration of mass fraction aq. β -CD into the solution, suggesting that the $[C_4\text{mpy}]Cl$ and β -CD are more tightly packed and more solvated. This is also in good agreement with the results obtained from apparent molar volume and viscosity B -coefficient and viscosity parameters discussed above.

Conclusion

The exceptional inclusion behaviour of β -CD and ([C₄mpy]Cl) in aqueous solution has been studied by surface tension and conductance measurements. The results point out that β -CD and ([C₄mpy]Cl) finally form stable inclusion complexes (ICs) with a 1:1 stoichiometry. They both are promoting to each other due to hydrophilic and hydrophobic interactions among them. The experimental values obtained from the volumetric, viscometric and refractometric studies also support the data and results observed from surface tension and conductance measurements.

Supporting information

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

$$\gamma = 16536.87c + 57.91$$

$$\gamma = 8677.58c + 62.09$$

$$\gamma = 66.71 \text{ mN} \cdot \text{m}^{-1} \text{ and } c = 0.00053 \text{ (M)}$$

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.

$$\Lambda = 1000 \kappa / c \quad (1)$$

Where, c is the molar concentration of the studied solution.

Apparent molar volume

The apparent molar volumes ϕ_V were determined from the solutions densities (Table S3) using the equation

$$\phi_V = M / \rho - 1000(\rho - \rho_0) / m \rho \rho_0 \quad (2)$$

Where, M is the molar mass of the nucleosides, 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 S4.

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

Viscosity

The experimental viscosity data for the studied systems are listed in table S3. The relative viscosity (η_r) has been analyzed using the Jones-Dole equation,[3]

$$(\eta/\eta_0 - 1)/\sqrt{m} = (\eta_r - 1)/\sqrt{m} = A + B \sqrt{m} \quad (4)$$

where $\eta_r = \eta/\eta_0$, η and η_0 are the relative viscosities, the viscosities of the ternary solutions (IL+aq. β -CD) and binary aqueous mixture (aq. β -CD) and m is the molality of the nucleosides 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 S4.

Refractive index

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

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

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 equation [5],

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

References:

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Table S1-S4 has been given in supporting information.

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

aq. solvent mixture	Temp /K ^a	$\rho \cdot 10^{-3}$ /kg·m ⁻³	η /mP·s	n_D
$w_I = 0.001^b$	298.15	0.99752	1.30	1.3040
	303.15	0.99620	1.20	-
	308.15	0.99440	1.10	-
$w_I = 0.003^b$	298.15	0.99817	1.31	1.3115
	303.15	0.99680	1.21	-
	308.15	0.99510	1.11	-
$w_I = 0.005^b$	298.15	0.99893	1.32	1.3220
	303.15	0.99750	1.22	-
	308.15	0.99575	1.12	-

^aStandard uncertainties in temperature (T) = 0.01 K. ^b w_I 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 (<i>m</i>)	$\rho \cdot 10^{-3}$ /kg·m ⁻³	η /mP·s	Conc (<i>m</i>)	$\rho \cdot 10^{-3}$ /kg·m ⁻³	η /mP·s	Conc (<i>m</i>)	$\rho \cdot 10^{-3}$ /kg·m ⁻³	η /mP·s
298.15 K ^{<i>a</i>}			303.15K ^{<i>a</i>}			308.15K ^{<i>a</i>}		
[C ₄ mpy]Cl								
<i>w</i> ₁ =0.001 ^{<i>b</i>}								
0.0100	0.99732	1.31	0.0101	0.99603	1.21	0.0101	0.99419	1.11
0.0252	0.99764	1.34	0.0252	0.99623	1.23	0.0253	0.99435	1.14

0.0404	0.99802	1.37	0.0404	0.99682	1.26	0.0405	0.99497	1.17
0.0556	0.99863	1.40	0.0557	0.99738	1.29	0.0558	0.99521	1.22
0.0709	0.99965	1.43	0.0711	0.99811	1.32	0.0712	0.99602	1.26
0.0863	1.00097	1.46	0.0865	0.99886	1.35	0.0866	0.99711	1.31
$w_1=0.003^b$								
0.0100	0.99806	1.32	0.0101	0.99661	1.22	0.0101	0.99487	1.12
0.0252	0.99805	1.35	0.0252	0.99683	1.25	0.0252	0.99506	1.16
0.0404	0.99868	1.38	0.0404	0.99732	1.28	0.0405	0.99558	1.20
0.0556	0.99922	1.41	0.0557	0.99823	1.32	0.0558	0.99614	1.25
0.0709	0.99987	1.45	0.0710	0.99887	1.35	0.0711	0.99703	1.29
0.0863	1.00098	1.48	0.0864	0.99937	1.39	0.0865	0.99801	1.34
$w_1=0.005^b$								
0.0100	0.99879	1.33	0.0100	0.99732	1.23	0.0101	0.99551	1.13
0.0251	0.99883	1.37	0.0252	0.99706	1.27	0.0252	0.99572	1.18
0.0403	0.99912	1.41	0.0404	0.99749	1.31	0.0405	0.99629	1.23
0.0556	0.99980	1.45	0.0557	0.99834	1.36	0.0557	0.99705	1.29
0.0709	1.00059	1.49	0.0710	0.99905	1.41	0.0711	0.99791	1.35
0.0862	1.00192	1.53	0.0864	0.99989	1.47	0.0865	0.99898	1.40

Standard uncertainties in temperature (T) = 0.01 K. ^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, Solvation number (S_n), ionic apparent molar volume (ϕ_{\pm}^o) in deferent mass fractions of aqueous α and β -cyclodextrin mixtures

Temp /K ^a	$\phi_v^o \times 10^6$	S_v^*	B	A	S_n	$\phi_v^+ \times 10^6$	$\phi_v^- \times 10^6$
[C ₄ mPy]Cl							
$w_1=0.001^b$							
298.15	233.35	-297.83	1.79	-0.09	7.68	142.08	91.27
303.15	245.30	-340.43	1.86	-0.12	7.57	152.91	92.39
308.15	255.56	-368.36	2.95	-0.23	11.54	162.02	93.54
$w_1=0.003^b$							
298.15	237.01	-300.19	1.93	-0.12	8.14	145.59	91.42
303.15	250.50	-365.52	2.22	-0.14	8.86	158.00	92.50
308.15	262.97	-409.24	3.22	-0.23	12.24	169.27	93.70
$w_1=0.005^b$							
298.15	242.75	-336.70	2.44	-0.16	10.03	151.18	91.57
303.15	261.37	-371.01	3.19	-0.25	12.19	168.65	92.72
308.15	267.69	-442.90	4.06	-0.31	15.16	173.70	93.99

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

Table S4 Refractive index (n_D), molar refraction (R_m), and limiting molar refraction (R_m^0) for [(C₄mPy)Cl] in different mass fraction of aqueous β -CD at 298.15 K.^a

$c / \text{mol} \cdot \text{dm}^{-3}$	n_D	R_m	R_m^0
0.001 ^b			
0.010	1.3314	71.0998	70.94
0.025	1.3320	71.1938	
0.040	1.3325	71.2640	
0.055	1.3330	71.3177	
0.070	1.3336	71.3614	
0.085	1.3343	71.4030	
0.003 ^b			
0.010	1.3321	71.1833	71.03

0.025	1.3326	71.2813	
0.040	1.3331	71.3336	
0.055	1.3336	71.3921	
0.070	1.3341	71.4428	
0.085	1.3347	71.4798	
0.005 ^b			
0.010	1.3329	71.2868	71.14
0.025	1.3333	71.3617	
0.040	1.3337	71.4187	
0.055	1.3342	71.4672	
0.070	1.3347	71.5076	
0.085	1.3354	71.5482	

^aStandard uncertainties in temperature (T) = 0.01 K. ^b w_I is the mass fractions of β -CD in aqueous mixture respectively.

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