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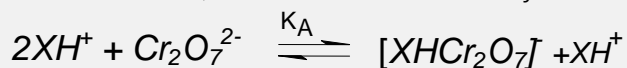
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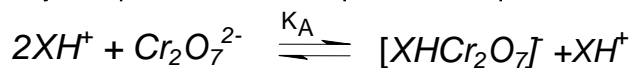


Conductance and Solvation Behavior of Some Onium Dichromates in Aqueous-Ethanol Mixtures

V Radhika ^α, M. Narsimha Reddy ^σ & P Manikyamba ^ρ

Abstract - The paper explores solvation behaviour of Nicotinium, Pyridinium and Quinolinium dichromates at 283K – 313K in ethanol, water and varying compositions (v/v) of water-ethanol mixtures. Analysis of conductance data to obtain Λ° is on the lines of Kraus-Bray and Shedlovsky equations. Λ° , the limiting molar ,varies with the composition of the solvent mixture. This is used in the interpretation of the preferential / discriminating solvation of cations by ethanol. The influence of mixed solvent composition on the solvation of ions is discussed in tune with the composition dependence of Walden product. The influence of the mixed solvent composition on the solvation of ions has been discussed with the help of 'R'-factor.

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I. INTRODUCTION

Quinolinium dichromate is a stable oxidant which was prepared and analyzed by Balasubramanian and coworkers [1]. This was used as an oxidant in the kinetic studies of oxidation of different functional groups [2-4]. Solvation behavior of this oxidant in Aq-DMF was presented in our earlier paper [5]. Pyridinium dichromate is a stable oxidant which was prepared and analyzed by Corey E J and Schmidt G[6], It is a very useful and versatile oxidant which can be used in many applications [7-9]. Nicotinium dichromate is a stable oxidant [10], which was prepared and analyzed by Lopez C and coworkers [11]. Though a large body of literature is available on kinetic aspects of these three oxidants, no information on the conductance behavior of these dichromates is these dichromates is available. Density, viscosity and dielectric constant of the medium, ion-solvent and

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dielectric constant of the medium, ion-solvent and solvent-solvent interactions influence the conductance behaviour of electrolytes in binary solvent mixtures. Ion-solvent interactions stabilize the ion by solvating it which is substantiated through vast information [12-21]. The present paper details the observations on conductance behaviour of Quinolinium, Pyridinium and Nicotinium dichromates in binary solvent mixtures of aqueous-ethanol.

II. EXPERIMENTAL SECTIONS

a) Chemicals Used

Quinolinium, Pyridinium and Nicotinium dichromates are prepared on the lines of the literature methods [1,6,11]. A stock solution of the reagent is prepared by dissolving a known weight of the sample in water and is standardized by iodometric method. A conductivity bridge (ELICO model-180) equipped with a glass conductivity cell of cell constant 1.103 cm^{-1} is used to measure the conductance of the solution. Conductivity cell is calibrated using 0.1M KCl solution. Deionised water is distilled and used for the preparation of the solution. The precision of the conductivity bridge used is $\pm 0.05 \text{ mS}$. Temperature is kept constant during the experiment using a thermostat with an accuracy of $\pm 0.1^\circ \text{C}$. To maintain the temperature below room temperature an ice bath equipped with a mechanical stirrer is used. Spectroscopic grade sample of acetone is procured from Sd-fine Chemicals Ltd., Bombay, India.

III. THEORY/CALCULATION

The solutions of Quinolinium, Pyridinium and Nicotinium dichromates are diluted to different concentrations in the range 0.1M to $5.0 \times 10^{-3} \text{ M}$ using different volumes of solvent / solvent mixture and their conductance is measured at 283-313K. The solvent systems used in this study have conductance values between 0.029 - 0.0315mS. The conductance values are found to be reproducible with $\pm 0.1\%$ error. The solvent conductance values are deducted from the conductance of the solution to get the conductance of the solute. The molar conductance is calculated using the relation $\Lambda = 1000 \times \mathbf{K}/\mathbf{C}$ where \mathbf{K} is the specific conductance and \mathbf{C} is the molarity of the solute in the solution The same procedure is followed at different

compositions of solvent mixtures and at different temperatures.

To find out the limiting molar conductance of Pyridinium dichromate two models, Kraus- Bray model [22], and Shedlovsky model [23] have been used. Kraus-Bray equation, Eq. 1, takes into consideration the dissociation constant (K_C) of the partially dissociated electrolyte and correlates molar conductance (Λ_m) and the limiting molar conductance (Λ^0) as

$$\frac{1}{\Lambda_m} = \frac{1}{\Lambda^0} + \frac{1}{K_C \Lambda^{0^2}} (\Lambda_m C) \quad (1)$$

Shedlovsky equation, Eq. 2, considers the association constant of the ion-pair formed from the dissociated electrolyte into consideration and correlates the molar and limiting molar conductance values according to the equation

$$\frac{1}{S \Lambda_m} = \frac{1}{\Lambda^0} + \frac{K_A}{\Lambda^{0^2}} (S f_{\pm}^2 \Lambda_m C) \quad (2)$$

where Λ_m is molar conductance of the solute in the solution at concentration C,

Λ_0 is the limiting molar conductance

K_A is the association constant of the ion- pair,

K_C is the dissociation constant,

f_{\pm} is the mean ionic activity coefficient,

S is a factor given by

$$S = \left[\frac{\beta \sqrt{C \Lambda}}{4 \Lambda^{0^3/2}} + \sqrt{1 + \frac{\beta^2 C \Lambda}{4 \Lambda^{0^3}}} \right]^2 \quad (3)$$

$$\log f_{\pm} = \left[\frac{-1.8246 \times 10^6 (C \alpha)^{1/2} / (\epsilon T)^{3/2}}{1 + 50.24 \times 10^8 q (C \alpha)^{1/2} (\epsilon T)^{1/2}} \right]^2 \quad (4)$$

$$\alpha = \frac{S \Lambda}{\Lambda^0} \quad (5)$$

$$\beta = \frac{8.20 \times 10^5 \Lambda^0}{(\epsilon T)^{3/2}} + \frac{82.5}{\eta (\epsilon T)^{1/2}} \quad (6)$$

Where q is Bjerrum's critical distance q given by

$$q = \frac{e^2}{2 \epsilon k T} = \frac{Z_+ Z_- e^2}{2 \epsilon k T} \quad (7)$$

ϵ is dielectric constant of the medium and η is viscosity of the solvent, $Z_+ e$ and $Z_- e$ are the charges on the ions. k is Boltzmann's constant, T is the temperature in degrees Kelvin. S is calculated using Λ^0 obtained from the Onsager model using the plot of Λ_m against \sqrt{C} . The least square analysis of the data (Λ_m and C)

using the above two eqs. 1, 2 is satisfactory with linear correlation coefficients in the range 0.95-0.97.

IV. RESULTS AND DISCUSSION

a) Limiting molar conductance

The limiting molar conductance values Λ^0 thus obtained with the two equations (eq. 1 and eq. 2) are presented in Table 1. These values increase with increase in the temperature as expected. This is attributed to increase in the mobility of the ions due to increase in the temperature. The Λ^0 values also depend on the composition of the binary solvent mixture. Addition of ethanol to water decreases Λ_0 value. This may be due to decrease in the dielectric constant of the medium.

It is observed that the conductivity of the solution in each solvent system is increased with increase in the temperature. It is supposed that this variation has to follow Arrhenius relation like rate process. So the energy of activation of the conducting process is obtained from the Arrhenius relationship

$$\text{i.e.,} \quad \Lambda^0 = A e^{-E_a/RT} \quad (8)$$

Where A is a constant

E_a is activation energy of the conducting process

R is gas constant

T is the temperature

E_a values are obtained by correlating $\log \Lambda^0$ values with $1/T$ by means of linear least square analysis. These values are presented in Table 2. These values indicate that they are highly dependent on the proportion of organic solvent in the medium. These values are maximum in 60% ethanol for Quinolinium dichromate and in 20% ethanol for Pyridinium dichromate. For Nicotinium dichromate the maximum E_a is observed in pure water.

b) Radii of solvated ions

The effective ionic radii (r_i) of the cation and anion in each solvent system used are calculated by using Stoke's radius equation modified by Gill [24]

$$r_i = \frac{0.820 |Z|}{\Lambda_+ \eta_o} + 0.0103 \epsilon + r_y \quad (9)$$

Where r_y is a parameter equal to 0.85 \AA^0 for non associated solvents and 1.13 \AA^0 for associated solvents. These values are tabulated in Table 3. These values which are radii of solvated ions vary with the solvent composition suggesting the operation of ion-solvent interactions.

c) Solvation Number

S_n , the solvation number, which is the number of solvent molecules in the solvent cover around the

species, is calculated from the effect of dielectric constant (ϵ) on Λ^0 . This is based on the equation

$$\log \Lambda^0 = \log \Lambda^{01} - \frac{Z_A Z_B e^2}{\epsilon d_{AB} k_B T} \quad (10)$$

Where, Λ^{01} is the limiting molar conductance in a solvent of infinite dielectric constant

$Z_A e$, $Z_B e$ are the ionic charges

k_B is Boltzmann constant

T is the temperature

d_{AB} is the distance between the centers of the two ions.

The plot of $\log \Lambda^0$ against $1/\epsilon$ is linear with negative slope from which, d_{AB} is calculated. S_n is computed using the relation.

$$S_n = \frac{d_{AB} - r_i}{r_{solvent}} \quad (11)$$

Where r_i is the Stokes radius of the ion calculated using Stoke's equation [25]

$$r_i = \frac{0.820|Z|}{\Lambda_o \eta_o} + 0.0103\epsilon + r_y \quad (12)$$

Where $r_y = 0.85 \text{ \AA}$ for dipolar unassociated solvents and 1.13 \AA for protic and associated solvents. These r_i values are tabulated in Table 3.

In order to understand the extent molecular interactions occurring in the solutions, solvation number was calculated.

Solvation numbers thus determined at 293K - 303K are presented in Table 4.

The variable solvation number indicates that the ion-pair is solvated to different extents depending on the composition of the solvent which reflects variable ion-solvent interactions.

d) Ionic conductances and Ion-solvation

As suggested by Hammamy [26] the ionic conductances Λ_+^0 and Λ_-^0 of the onium ion and the dichromate ion are computed in all the solvent systems used and presented in Table 3. Λ_+^0 is maximum in 100% water and decreases due to the addition of ethanol attaining a slight higher value in 100% ethanol. The ionic conductance of the anion slightly increases due to the initial addition of ethanol and gradually decreases attaining a minimum value in 100% ethanol. This variation in the ionic conductance suggests that the specific solvation of the anion is by water while ethanol from the solvent mixture selectively solvates the cation. The solvation behavior of the ions in mixed solvent systems can be better understood in terms of the ionic

Walden products, $\eta \Lambda_{\pm}^0$, of the electrolytes. The calculated values of these ionic Walden products are presented in fig. 1(A,B). These values are maximum in water and decrease gradually due to the addition of organic component in each system. According to Morinaga and coworkers [27] the ratio (R),

$$R = \frac{\eta \Lambda_{\pm}^0(\text{solvent})}{\eta \Lambda_{\pm}^0(\text{water})}$$

can be used to obtain information on the nature of solvation of an electrolyte and its constituent ions in aqueous solvent mixtures. The calculated values of these factors for both the ions are shown in Table 3. This ratio for the cation is less than one and decreases sharply with the increase in the proportion of organic component. According to Morinaga [27] this is a strong indication of selective solvation of the ion by the ethanol. Thus it may be concluded that the cation is more solvated by acetone from the solvent system. The 'R' factor of the dichromate ion increases up to 80% (v/v), indicating that the anion is selectively hydrated from the aqueous solvent mixture. The addition of organic solvent breaks the structure of water and makes the water molecules available for hydration of the anion. This type of behavior is observed by Morinaga [27] for alkali metal ions in water rich regions of water-acetonitrile and water-DMSO mixtures.

V. CONCLUSIONS

Among the three dichromates studied higher solvation number is observed for Pyridinium ion compared to Quinolinium and Nicotinium ions. This may be attributed to smaller size of the Pyridinium ion which increases the charge density.

VI. ACKNOWLEDGEMENTS

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Table 1 : Limiting molar conductance (Λ°) values in S cm² mol⁻¹ of Quinolinium , Pyridinium and Nicotinium dichromates in aqueous mixtures of ethanol at different temperatures.

Quinolinium dichromate

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	1	2	1	2	1	2	1	2	1	2	1	2
283	121.66	122.27	101.03	10.614	80.45	80.24	64.19	64.17	76.91	77.32	45.73	44.53
293	143.89	138.02	128.21	126.94	109.15	108.83	98.06	98.31	92.66	93.07	46.96	48.74
303	154.66	154.93	146.91	139.55	125.52	139.30	115.94	116.93	98.54	98.62	49.49	49.33
313	196.67	196.40	159.95	160.66	167.67	154.71	156.67	147.51	124.84	123.57	55.38	55.04

Pyridinium dichromate

T(K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	1	2	1	2	1	2	1	2	1	2	1	2
283	205.55	205.67	126.06	132.50	108.5	108.41	95.50	95.35	75.05	78.58	69.61	69.85
293	221.58	222.80	176.98	175.56	140.35	137.35	112.05	112.25	95.80	90.65	72.08	71.73
303	253.42	259.61	225.41	226.76	159.62	158.32	122.84	123.24	104.34	98.09	76.24	76.61
313	303.43	307.27	252.61	254.71	219.88	219.19	158.29	159.57	128.85	121.30	85.42	84.81

Nicotinium dichromate

T(K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	1	2	1	2	1	2	1	2	1	2	1	2
283	127.77	127.27	115.03	113.14	98.45	97.24	84.19	84.17	79.91	79.32	48.31	47.86
293	154.66	154.93	138.21	136.94	119.15	118.83	108.06	108.31	99.66	97.07	55.56	55.75
303	173.71	179.40	156.76	155.53	145.52	139.30	123.94	123.93	104.76	104.56	60.24	60.25
313	199.66	198.50	169.49	169.57	158.67	158.51	151.51	154.84	124.42	132.56	67.11	67.24

1 = Kraus-Bray Model

2 = Shedlovsky model

Table 2: K_A and K_C values of Quinolinium, pyridinium and Nicotinium dichromates in aqueous-ethanol mixtures

Quinolinium dichromate

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C
283	54.67	0.02	31.60	0.03	21.12	0.05	35.33	0.04	35.57	0.03	61.65	0.02
293	70.07	0.01	22.03	0.06	20.55	0.04	21.39	0.09	29.69	0.03	54.90	0.02
303	28.24	0.02	13.56	0.04	19.90	0.05	16.20	0.13	29.86	0.05	45.61	0.02
313	21.89	0.05	45.14	0.23	19.41	0.05	18.70	0.16	29.10	0.04	44.91	0.02

Pyridinium dichromate

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C
283	7.58	0.13	4.07	0.21	19.10	0.05	7.00	0.14	8.76	0.13	13.89	0.03
293	15.20	0.11	6.73	0.15	19.88	0.05	6.59	0.16	10.29	0.12	7.73	0.03
303	37.65	0.28	8.91	0.11	12.66	0.08	38.09	0.26	8.40	0.15	31.08	0.03
313	38.61	0.27	4.77	0.21	19.23	0.08	50.00	0.19	10.64	0.12	36.11	0.03

Nicotinium dichromate

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C	K_A	K_C
283	11.95	0.059	10.98	0.091	11.33	0.077	9.09	0.11	10.98	0.092	17.30	0.057
293	10.78	0.091	11.24	0.081	12.00	0.088	8.89	0.12	15.87	0.082	32.80	0.031
303	12.77	0.077	12.55	0.079	8.75	0.113	15.43	0.066	12.5	0.07	30.1	0.033
313	5.76	0.174	6.34	0.1	12.01	0.084	11.33	0.088	13.16	0.075	33.82	0.030

K_A = Association constant from Shedlovsky equation.

K_C = Dissociation constant from Kraus-Bray equation.

Table 3 : Computed Values of E_a for Quinolinium, pyridinium and Nicotinium dichromates at different compositions (v/v) of aqueous-ethanol mixtures.

Quinolinium dichromate

	0% Ethanol	20% Ethanol	40% Ethanol	60% Ethanol	80% Ethanol	100% Ethanol
E_a	9.12	11.06	17.68	19.74	10.75	4.77

Pyridinium dichromate

	0% Ethanol	20% Ethanol	40% Ethanol	60% Ethanol	80% Ethanol	100% Ethanol
E_a	9.12	17.06	16.12	11.83	10.08	4.88

Nicotinium dichromate

	0% Ethanol	20% Ethanol	40% Ethanol	60% Ethanol	80% Ethanol	100% Ethanol
E_a	9.12	14.03	15.44	17.01	12.37	8.45

Table 4 : Computed change in free energy (ΔG_a) and transfer (ΔG_t) Quinolinium, Pyridinium and Nicotinium dichromate in aqueous mixtures of ethanol at different temperatures in kJ mol^{-1} .

Quinolinium dichromate

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t
283	-4.76	-	-3.89	0.87	-5.73	-0.18	-4.92	-0.030	-4.51	0.05	-5.34	0.58
293	-4.03	-	-5.15	1.47	-10.08	0.09	-5.21	0.25	-4.73	0.34	-5.69	-0.17
303	-9.15	-	-5.39	3.76	-6.54	2.61	-5.68	0.60	-5.21	0.68	-5.44	0.64
313	-9.51	-	-5.92	3.59	-6.89	2.62	-5.89	0.61	-5.86	0.61	-6.38	0.52

Pyridinium dichromate

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t
283	-4.94	-	-8.03	-0.16	-8.05	-3.02	-8.46	-2.69	-13.05	9.27	-9.41	-1.94
293	-8.07	-	-7.74	-3.86	-8.06	2.30	-6.94	-2.69	-8.95	-1.41	-8.68	-1.68
303	-7.99	-	-7.48	-2.01	-7.18	-1.22	-7.37	-1.03	-7.51	-0.89	-7.18	-1.22
313	-8.74	-	-7.24	-2.60	-5.77	-2.24	-7.07	-2.14	-7.90	-0.12	-10.23	2.21

Nicotinium dichromate

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t	ΔG_a	ΔG_t
283	-4.760	-	-5.52	-0.758	-8.17	-2.65	-8.24	-2.54	-8.24	-3.48	-5.57	-0.81
293	-4.032	-	-9.13	-5.10	-8.59	-4.56	-8.51	-3.27	-8.51	-4.48	-5.88	-1.85
303	-9.151	-	-10.25	-1.10	-8.57	+0.58	-9.33	-0.18	-9.90	-0.75	-5.91	+3.24
313	-9.513	-	-9.63	-0.12	-6.70	+2.81	-9.21	+0.30	-8.91	+0.60	-8.91	+0.60

Table 5 : Ionic conductances and radii of solvated ions of Quinolinium, pyridinium and Nicotinium dichromate in aqueous-ethanol mixtures.

Quinolinium dichromate

T = 293K

Composition (v/v) ethanol	Λ_+^0 (S cm ² mol ⁻¹)	Λ_-^0 (S cm ² mol ⁻¹)	$r_+(A^0)$	$r_-(A^0)$	$r_+ + r_-(A^0)$
0%	48.98	94.94	3.11	2.71	5.82
20%	44.87	82.07	3.83	2.36	6.19
40%	32.43	76.72	3.67	2.57	6.24
60%	31.32	66.74	3.99	1.42	5.41
80%	29.72	62.94	5.27	1.38	6.65
100%	10.63	36.32	2.07	0.95	3.02

T = 303K

Composition (v/v) ethanol	Λ_+^0 (S cm ² mol ⁻¹)	Λ_-^0 (S cm ² mol ⁻¹)	$r_+(A^0)$	$r_-(A^0)$	$r_+ + r_-(A^0)$
0%	59.74	94.92	3.09	2.82	5.83
20%	50.60	88.17	2.99	2.52	6.23
40%	37.52	87.99	3.62	2.24	5.86
60%	33.33	82.65	3.38	2.24	7.07
80%	33.78	64.76	5.06	3.20	5.87
100%	3.91	45.59	7.31	2.95	10.36

Pyridinium dichromate

T = 293K

Composition (v/v) ethanol	Λ_+^0 (S cm ² mol ⁻¹)	Λ_-^0 (S cm ² mol ⁻¹)	$r_+(A^0)$	$r_-(A^0)$	$r_+ + r_-(A^0)$
0%	126.64	94.94	2.52	2.71	5.23
20%	94.91	82.07	2.53	2.36	6.33
40%	60.63	76.72	2.61	2.57	4.89
60%	45.51	66.74	3.15	1.42	4.57
80%	27.71	62.94	1.65	1.38	3.03
100%	35.41	36.32	1.85	0.95	3.68

T = 303K

Composition (v/v) ethanol	Λ_+^0 (S cm ² mol ⁻¹)	Λ_-^0 (S cm ² mol ⁻¹)	$r_+(A^0)$	$r_-(A^0)$	$r_+ + r_-(A^0)$
0%	164.69	94.92	2.14	2.82	4.96
20%	137.24	88.17	2.07	2.52	4.59
40%	60.32	87.99	2.62	2.24	4.86
60%	33.59	82.65	3.08	2.24	5.32
80%	33.33	64.76	1.57	3.20	4.77
100%	30.65	45.59	1.96	2.95	4.91

Nicotinium dichromate

T = 293K

Composition (v/v) ethanol	Λ_+^0 (S cm ² mol ⁻¹)	Λ_-^0 (S cm ² mol ⁻¹)	$r_+(A^0)$	$r_-(A^0)$	$r_+ + r_-(A^0)$
0%	59.72	94.94	1.02	2.71	3.73
20%	54.14	82.07	1.23	2.36	3.59
40%	42.43	76.72	1.32	2.57	3.89
60%	52.09	66.74	1.66	1.42	3.08
80%	45.12	62.94	1.69	1.38	3.07
100%	19.24	36.32	2.02	0.95	2.97

T = 303K

Composition (v/v) ethanol	Λ_+^0 (S cm ² mol ⁻¹)	Λ_-^0 (S cm ² mol ⁻¹)	$r_+(A^0)$	$r_-(A^0)$	$r_+ + r_-(A^0)$
0%	78.79	94.92	2.03	2.82	4.85
20%	68.59	88.17	1.64	2.52	4.16
40%	57.53	87.99	1.61	2.24	3.85
60%	41.29	82.65	1.55	2.24	3.79
80%	40.00	64.76	1.17	3.20	4.37
100%	14.65	45.59	1.05	2.95	4.00

Table 6 : Solvation number values of Quinolinium, Pyridinium and Nicotinium dichromates in aqueous-ethanol mixtures at 293 and 303K.

Quinolinium dichromate

T(K)	0% Ethanol	20% Ethanol	40% Ethanol	60% Ethanol	80% Ethanol	100% Ethanol
293	5.02	4.78	4.48	4.38	4.34	3.19
303	5.93	5.83	5.31	4.70	4.63	2.59

Pyridinium dichromate

T(K)	0% Ethanol	20% Ethanol	40% Ethanol	60% Ethanol	80% Ethanol	100% Ethanol
293	6.34	5.86	5.44	5.36	4.52	3.63
303	6.15	5.84	5.62	4.65	4.42	3.72

Nicotinium dichromate

T(K)	0% Ethanol	20% Ethanol	40% Ethanol	60% Ethanol	80% Ethanol	100% Ethanol
293	0.79	1.06	1.01	1.49	1.23	1.02
303	1.64	1.39	1.90	1.78	1.37	1.32

Table 7: Computed change in free energy of solvation (ΔG_{i-s}^+) and (ΔG_{i-s}^-) for Quinolinium, P yridinium and Nicotinium dichromate in aqueous-ethanol mixtures at 293,303K in kJ mol^{-1} .

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-
293	3.1	3.2	2.6	4.3	3.3	4.7	3.9	10.8	3.9	14.8	30.8	18.0
303	3.0	3.0	3.7	3.9	3.6	4.3	4.8	5.9	4.4	7.3	4.7	16.4

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-
293	3.4	3.2	4.0	4.3	4.7	4.7	4.9	10.8	6.9	14.8	17.8	18.0
303	4.2	3.2	5.2	4.3	5.0	4.7	5.3	10.9	14.0	14.8	17.6	18.0

T (K)	0% Ethanol		20% Ethanol		40% Ethanol		60% Ethanol		80% Ethanol		100% Ethanol	
	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-	ΔG_{i-s}^+	ΔG_{i-s}^-
293	4.1	3.20	5.95	4.30	7.30	4.74	11.67	10.80	20.03	14.80	32.42	17.98
303	4.4	3.89	6.64	4.27	8.04	5.79	10.50	7.30	18.75	16.40	33.00	11.71