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Synthesis, Characterization, Solution Behavior, and Density Functional Theory Analysis of Some Pyridinium-Based Ionic Liquids

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Abstract Some picolinium ionic liquids (IL) $[\alpha/\gamma-\text{PicC}_n]$ [Br/NO₃] (n = 3, 5, 7) were synthesized and characterized by ¹H NMR data. The surface tension and density of all the IL were determined. The aggregation behavior of these IL in aqueous medium and in dichloromethane was assessed from the variation of electrical conductivity in these media. The critical aggregation concentrations of these IL in aqueous medium were found to decrease significantly by the addition of cetyltrimethylammonium bromide. The structural features and the conformation of these IL were further investigated by using density functional theory calculations. The bromide ion was found to be inclined asymmetrically to one side of the pyridinium nucleus, while the nitrogen of the nitrate group lies close to the nitronium ion of the pyridinium nucleus.

Keywords Room-temperature ionic liquid \cdot Contact ion pair \cdot Critical aggregation concentration \cdot DFT \cdot Alkyl pyridinium bromide

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Introduction

Room-temperature ionic liquids (RTIL) are generally organic salts with melting points at or below 373 K (Stark & Seddon, 2007). These are composed of a bulky organic cation with an alkyl chain and a variable number of carbon atoms, and an inorganic or organic anion. The electrostatic anion-cation interactions are relatively weak because of the inefficient packing of the large, irregular organic cation with the inorganic or organic counteranion, resulting in the existence of the salt in the liquid state at room temperature (Rilo, Vila, García-Garabal, Varela, & Cabeza, 2013). Compared to classical organic solvents, IL exhibit some typical properties like low melting point, low volatility and flammability, high chemical and thermal stability, high electrical conductivity, a broad electrochemical window, and high polarity (Rilo et al., 2013; Welton, 1999). Mjalli, Naser, Jibril, Alizadeh, and Gano (2014) reported the synthesis and characterization of some novel IL-based deep eutectic solvents from tetrabutylammonium chloride and polyhydroxy compounds. Because of the variety of side chains that can be connected to the central N⁺ ion, many quaternary ammonium IL could be prepared to tune the physical properties by the selection and modification of the anion and the cation. Numerous articles on IL describing general chemical aspects of their applications have already appeared in the literature (Benavides-Garcia & Monroe, 2009; Danten, Cabaço, & Besnard, 2010; Fujimori et al., 2007; Kiefer & Pye, 2010; Olivier-Bourbigou, Magna, & Morvan, 2010; Ong & Ceder, 2010; Verma & Banerjee, 2010; Xiao et al., 2010).

While synthesizing alkyl γ -picolinium bromides as precursors for the synthesis of some polymethine dyes, we observed that the salts with alkyl chains having an odd

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Scheme 1 Reaction of picoline with alkyl bromide

number of carbon atoms (propyl and amyl groups) are liquid at room temperature (Patel, Panda, Kuanar, & Mishra, 2004). Subsequently, many alkyl picolinium salts have been synthesized, mostly having an alkyl chain with an even number of carbon atoms, and established as IL (Cornellas et al., 2011; Singh & Kumar, 2007, 2008). Some novel ether-based pyridinium IL capable of absorbing SO₂ were synthesized by Wang et al. (2014). Blends of monoethanolamine and some pyridinium IL were found to be effective absorbents of carbon dioxide (Huang, Zhang, Zhang, Dong, & Zhang, 2014). Some of these compounds aggregate in an aqueous medium above a certain concentration, called the critical aggregation concentration (CAC) (Bandres, Meler, Giner, Cea, & Lafuente, 2009; Galgano & El Seoud, 2010; Sastry et al., 2012). Copolymerization of vinyl pyridinium IL has been carried out by immobilizing these IL on a magnetic core to obtain an effective catalyst for biodiesel synthesis (Liang, 2014). Cai, Huang, Chen, Hu, and Wu (2014) used an ion-exchange method to replace the halide by a hydroxide and obtained IL with high purity.

Here we report the synthesis of some picolinium IL from 2/4-methyl pyridine and alkyl bromides and their behavior in both organic and aqueous media. Structural characteristics of the IL were also investigated through density functional theory (DFT) analysis.

Experimental

Materials and Methods

The α/γ -picoline and alkyl bromides were obtained from Spectrochem and Sisco Chemicals (Mumbai, India). Millipore water was used for the preparation of IL solutions. The melting points of compounds were measured by the open capillary method and the boiling points using Siwoloboff's method (Sahay, Mishra, Behera, & Shah, 1988). The structure of the products was established using NMR spectral data. The ¹H-NMR spectra were recorded on a 400-MHz Bruker NMR spectrometer in D₂O and CDCl₃ as solvents for the different compounds. Different concentrations of IL were prepared and their conductivities in the aqueous medium were recorded by a direct reading conductivity meter (type 303; SYSTRONICS, Ahmedabad, India) in the micro range. The surface tension of neat IL was measured by a manual tensiometer (model ST 500-man; Nima Technologies, Coventry, UK) using the Wilhelmy plate method with an uncertainty of ± 0.03 mN m⁻¹ at 302 K. Densities of the liquids were measured by a pycnometer.

Synthesis of the IL $[\alpha/\gamma$ -PicC_n][Br]

In a sealed tube, equimolar amounts of alkyl halide and α /- γ -picoline were heated in an oil bath for 24–30 h at different temperatures. After completion of the heating, a brown colored liquid was obtained, which was washed with ether several times till the ether extract did not contain the starting materials (Scheme 1). The compounds synthesized using this protocol are shown in Table 1.

Synthesis of IL $[\alpha/\gamma$ -PicC_n][NO₃]

To a solution of 0.5 mL α/γ -picolinium alkyl bromide in 5 mL Millipore water, a solution of 0.5 g AgNO₃ in 10 mL water was added slowly till the precipitation was complete. The solution was then warmed in a water bath for 30 min. The precipitate of silver bromide was filtered off, and the water from the filtrate was removed under reduced pressure. The syrupy liquid obtained was kept in a desiccator. The compounds synthesized by the above procedure are listed in Table 2.

Measurement of CAC

The CAC values were determined by the electrical conductance method. The conductivities of the solutions of the IL in water, dichloromethane (DCM), and an aqueous solution of cetyltrimethyl ammonium bromide (CTAB) were monitored at different concentrations, and the specific conductance values were plotted against the concentration of IL (Fig. 1). A break point in the plot of the conductance *versus* [IL] indicated the onset of formation of the aggregates, and this point of intersection was taken as as the CAC of the IL (Table 3).

Table 1 Structure, boiling point, density, and surface tension of $[\alpha/-\gamma-\text{PicC}_n][\text{Br}] \text{ IL}$

IL	Reaction temperature (°C)	Boiling point (°C)	Density (g cm ⁻³)	Surface tension (mN m ⁻¹)	
[y-PicC ₃][Br]	145	200-202	1.432	47.8	
[a-PicC ₃][Br]	130	190–192	1.42	56.2	
[y-PicC5][Br]	145	220-222	1.45	44.3	
[a-PicC ₅][Br]	130	210-212	1.5	42.6	
[y-PicC7][Br]	180	232-235	1.52	41.8	
[a-PicC ₇][Br]	180	210-213	1.47	37.9	

IL	Structure		Density (g cm^{-3})	Surface tension (mN m ⁻¹)	
[γ-PicC ₃][NO ₃]		148–150	1.36	52.8	
[α-PicC ₃][NO ₃]		145–148	1.42	50.7	
[γ-PicC ₅][NO ₃]		155–159	1.38	51.6	
[α-PicC ₅][NO ₃]		151–154	1.41	49.1	
[\gamma-PicC ₇][NO ₃]		174–177	1.40	48.5	
[α-PicC ₇][NO ₃]		169–172	1.41	47.3	

Table 2 S	tructure and	physical	characteristic	of $\left[\alpha \right]^{\prime}$	γ -PicC _n	INO ₃] IL
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Results and Discussion

Like imidazolium salts, pyridinium salts have relatively low melting points to be considered as RTIL. Substitution of the methyl group in the pyridinium moiety contributes to the lowering of the melting point by increasing the nonpolar characteristic of the molecule, thereby decreasing the intermolecular dipole–dipole interactions of the compound. *N*-Alkyl picolinium bromides were prepared by the Menchutkin reaction of picoline with an excess of neat alkyl bromide to ensure complete quaternization of the entire picoline (Scheme 1). The unreacted alkyl bromides were removed by washing with ethyl ether several times till a clear NMR spectrum of the molecule was obtained. Among a series of alkyl bromides, propyl, pentyl, and heptyl bromides alone could produce RTIL from the quaternization reaction.

In the typical NMR spectral data of $[\gamma$ -PicC_n][Br], *i.e.*, $[\gamma$ -PicC₃][Br], the characteristic doublets of two proton area

for the pyridinium protons were found at ~9.325 δ and 7.89 δ (Fig. S1) with J = 6.4. The singlet of the pyridinium methyl group appeared at 2.564 δ . With variation of chain length in the *N*-alkyl group, these peaks suffered slight upfield shift for the 2-proton and downfield shift for the 3-proton of the pyridinium ring. The singlet of the methyl group also showed an upfield shift. However, when the counterion changed from bromide to nitrate, the changes in the chemical shifts were significant around the probable localized site of the counterion. In [γ -PicC₃][NO₃], the peak for 2-proton was to an extent of 0.28 δ (Fig. S7). The peaks of pyridinium methyl protons were not affected much, with a shift of 0.07 δ only.

For 2-methyl substituted pyridinium moieties, four peaks appeared in the aromatic region, each one distinctive of each proton as two doublets and two triplets. The doublet at the extreme downfield region may be assigned to the 6proton of the pyridinium nucleus and appearing around



Fig. 1 Plots of conductance *versus* concentration of (a) [α-PicC₃][Br] and (b) [α-PicC₅][Br]

IL	CAC in water	CAC in DCM	CAC of mixed surfactant (CTAB:IL)						
			1:1	2:1	4:1	6:1	8:1	10:1	12:1
[y-PicC ₃][Br]	45.45	21.37	5.31	4.46	3.70	3.70	3.61	3.57	3.62
[a-PicC ₃][Br]	45.45	25.25	5.74	4.58	3.87	3.90	3.66	3.67	3.63
[γ-PicC ₅][Br]	45.25	25.26	5.32	4.31	3.90	3.79	3.73	3.62	3.60
[a-PicC ₅][Br]	38.46	18.50	5.10	4.33	4.06	3.70	3.87	3.76	3.64
[γ-PicC ₇][Br]	50.00	32.46	5.00	4.38	3.90	3.82	3.78	3.70	3.75
[\alpha-PicC ₇][Br]	50.00	11.47	5.26	4.42	3.93	3.90	3.78	3.70	3.76

Table 3 CAC of IL (in mM) in the absence and presence of CTAB

9.27 δ for bromide salts, while that around 8.55 δ was for corresponding nitrate salts. The peak for C-5 proton appeared as a triplet around 8.4 δ for bromide and 8.2 δ for the corresponding nitrate. The protons at C-3 and C-4 positions have chemical shift values of 7.67–8.00 δ for both bromide and nitrate salts.

The aliphatic protons of the *N*-alkyl chain also exhibited a typical triplet for the terminal methyl group at 0.98δ for the propyl chain and 0.81δ for the heptyl chain in 4-methyl pyridinium salts. The peak for the N-CH₂ proton appeared as a triplet at 4.82δ for the *N*-propyl group and at 4.86δ for *N*-heptyl group with bromide as the counterion. With change in the position of methyl group in the pyridinium nucleus, no significant change in the peak position was observed. The other methylene units showed peaks at ~1.3 δ and 1.9δ . The change in the counterion, *i.e.*, from bromide to nitrate, induced a significant upfield shift in the peak of N-CH₂.

The significant changes in the chemical shift values of proton at the 2- and 6-positions of picolinium units and the N-CH₂ group clearly suggest that the pyridinium salts exist as tight ion pair with the counterion. In 2-methyl pyridinium compounds, the 6-proton suffered more shift (0.72 δ) compared to the pyridinium methyl group (0.30 δ), indicating the closeness of the counterion toward the C-6 proton compared to the methylene group.

Physical Properties of IL

The density values of the IL were found to be in the range $1.4-1.5 \text{ g cm}^{-3}$. There was no specific trend for the change of density with the structure of the IL. The surface tension values were found to decrease with increase in the chain length of the pyridinium bromide salts. In a review on rheological behavior of IL, it was reported that with increasing chain length in the alkyl group linked to N or C of imidazo-lium groups, the surface tension of the corresponding IL decreases (Sedev, 2011). In the case of 4-methyl pyridinium compounds, a plot of surface tension *versus* the number of carbon atoms in the alkyl chain was found to be linear with $R^2 = 0.99$, while in case of 2-methyl pyridinium

IL R^2 was 0.93. The surface tension of $[\alpha-\text{PicC}_3][\text{Br}]$ was found to be more than that of the corresponding $[\gamma-\text{PicC}_3]$ [Br], while the trend was opposite for $[\text{PicC}_5][\text{Br}]$ and $[\text{PicC}_7][\text{Br}]$ IL.

CAC of IL

The amphiphilic characteristics of the IL are due to the hydrophilic pyridinium group and the hydrophobic alkyl group. Characteristically, amphiphilic compounds assemble in an aqueous medium at a particular concentration known as the critical micelle concentration (CMC) when the assemblies lead to the formation of micelles. The possibility of aggregation of these IL was explored through conductivity measurements. In the aqueous solution, the conductivity of the IL increased with increasing concentration of the IL, and the corresponding plot was found to be bilinear. The transition point of the bilinearity may be considered as the CAC of the IL. In most of cases, CAC appeared at around 0.06 M of the IL (Fig. 1). The CAC values of 4-methyl IL increased with increase in the alkyl chain length, while that of 2-methyl IL decreased significantly.

The addition of CTAB (CTAB:CMC = 0.9 mM) to the aqueous solution of IL was found to decrease the CAC significantly. At equimolar concentration of both CTAB and IL, the CAC values decreased from ~50 to 5 mM. The nonideal change in the CAC may be ascribed to a mixed aggregation process in which CTAB played the dominant role. Rodrigues, Ito, and Sabadini (2011) observed a similar nonideal change in the CMC of CTAB with other small cationic surfactants and attributed the result to a synergistic effect.

Quantum Mechanical Calculations

The physical and chemical properties of IL are highly dependent on their molecular structure (Fumino, Wulf, & Ludwig, 2009). For example, in imidazolium-type IL, the position and length of alkyl chains or type of the inorganic anion affect the ability to form hydrogen bonding, and

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Alkyl chain	Energy (a.u.)	E_{HOMO} (a.u.)	E_{LUMO} (a.u.)	ΔE (kCal)	λ_{\max} (nm)	M (Debye)
C3	-2977.8470	-0.1615	-0.0982	39.746	720.92	13.68
C5	-3056.4770	-0.1612	-0.0981	39.659	682.08	13.55
C7	-3135.1023	-0.1617	-0.0949	41.918	684.33	13.52
C3	-2977.8491	-0.1617	-0.0951	41.780	692.34	13.73
C5	-3051.3761	-0.1612	-0.0954	41.300	682.08	13.68
C7	-3129.4455	-0.1617	-0.0949	41.918	719.33	13.56
C3	-686.4124	-0.1738	-0.0876	54.0976	528.51	10.797
C5	-765.0411	-0.1739	-0.0849	55.8609	511.82	11.303
C7	-843.6686	-0.1738	-0.0869	54.4741	524.85	11.330
C3	-686.4237	-0.1727	-0.0832	56.1558	509.14	11.512
C5	-765.0427	-0.1721	-0.0824	56.3064	507.77	11.485
C7	-843.6687	-0.1719	-0.0822	56.3253	507.60	11.498
	Alkyl chain C3 C5 C7 C3 C5 C7 C3 C5 C7 C3 C5 C7 C3 C5 C7 C3 C5 C7 C7	Alkyl chain Energy (a.u.) C3 -2977.8470 C5 -3056.4770 C7 -3135.1023 C3 -2977.8491 C5 -3051.3761 C7 -3129.4455 C3 -686.4124 C5 -765.0411 C7 -843.6686 C3 -686.4237 C5 -765.0427 C7 -843.6687	Alkyl chainEnergy (a.u.) E_{HOMO} (a.u.)C3-2977.8470-0.1615C5-3056.4770-0.1612C7-3135.1023-0.1617C3-2977.8491-0.1617C5-3051.3761-0.1612C7-3129.4455-0.1617C3-686.4124-0.1738C5-765.0411-0.1739C7-843.6686-0.1727C5-765.0427-0.1721C7-843.6687-0.1719	Alkyl chainEnergy (a.u.) E_{HOMO} (a.u.) E_{LUMO} (a.u.)C3-2977.8470-0.1615-0.0982C5-3056.4770-0.1612-0.0981C7-3135.1023-0.1617-0.0949C3-2977.8491-0.1617-0.0951C5-3051.3761-0.1612-0.0954C7-3129.4455-0.1617-0.0949C3-686.4124-0.1738-0.0876C5-765.0411-0.1739-0.0849C7-843.6686-0.1727-0.0832C5-765.0427-0.1721-0.0824C7-843.6687-0.1719-0.0822	Alkyl chainEnergy (a.u.) E_{HOMO} (a.u.) E_{LUMO} (a.u.) ΔE (kCal)C3-2977.8470-0.1615-0.098239.746C5-3056.4770-0.1612-0.098139.659C7-3135.1023-0.1617-0.094941.918C3-2977.8491-0.1617-0.095141.780C5-3051.3761-0.1612-0.095441.300C7-3129.4455-0.1617-0.094941.918C3-686.4124-0.1738-0.087654.0976C5-765.0411-0.1739-0.084955.8609C7-843.6686-0.1738-0.086954.4741C3-686.4237-0.1727-0.083256.1558C5-765.0427-0.1721-0.082456.3064C7-843.6687-0.1719-0.082256.3253	Alkyl chainEnergy (a.u.) E_{HOMO} (a.u.) E_{LUMO} (a.u.) ΔE (kCal) λ_{max} (nm)C3-2977.8470-0.1615-0.098239.746720.92C5-3056.4770-0.1612-0.098139.659682.08C7-3135.1023-0.1617-0.094941.918684.33C3-2977.8491-0.1617-0.095141.780692.34C5-3051.3761-0.1612-0.095441.300682.08C7-3129.4455-0.1617-0.094941.918719.33C3-686.4124-0.1738-0.087654.0976528.51C5-765.0411-0.1739-0.084955.8609511.82C7-843.6686-0.1738-0.082256.1558509.14C5-765.0427-0.1721-0.082456.3064507.77C7-843.6687-0.1719-0.082256.3253507.60

Table 4 Energy, absorbance, and dipole moment of $[\alpha/\gamma-\text{PicC}_n][\text{Br/NO}_3]$ IL

consequently affect their physical and chemical properties (Huddleston et al., 2001). Thus, investigation of their interactions at the molecular level with counterion and with various solutes is of great importance to develop new applications. Molecular dynamics simulation is a powerful tool for correlating the physical and chemical properties with structural parameters. However, the result quality of every simulation depends on the force field, which should reproduce system properties accurately enough over a wide range of thermodynamic states. Theoretical calculations were also performed to explore the structure and interactions of the counterion in the synthesized IL. Recently, Kirchner (2009) reviewed the theoretical investigations of IL. Combined with the experimental work, these studies have encouraged researchers to make more informed decisions regarding the properties to be expected for a given class of IL.

The synthesized RTIL structures were drawn using the GaussView program. The geometries of the compounds were optimized by using DFT considering the Becke's three-parameter hybrid exchange functional and the Lee–Yang–Parr correlation functional (B3LYP) (Becke, 1993; Lee, Yang, & Parr, 1988) by using 6-31G (d) basis set. All calculations were carried out with the Gaussian 03 program (Frisch et al., 2003).

After optimizing the molecular structure with Gaussian 03, the quantum chemical parameters were obtained from the output file (Table 4). Typically, the van der Waals force increases as the molecular weight increases. The electric charge on individual atoms and the shortest hydrogen-bond distance can be predicted from quantum mechanical calculations. The common quantum chemical descriptors such as dipole moment (μ), energy of the highest occupied molecular orbital ($E_{\rm HOMO}$), and energy of the lowest unoccupied molecular orbital ($E_{\rm LUMO}$) were determined. A thorough hydrogen-bonding analysis involving the geometry of the

molecule and the interactions of functional groups was conducted. Optimized geometries of IL and the type and possible positions for hydrogen bonds from van der Waals atomic radii overview are shown in Figs. 2 and S8A–J. Hydrogen bonds are denoted by dashed lines, and the corresponding $H \cdots X$ and $O \cdots H$ distances are labeled.

From the calculations, it was found that the variation of chain length and the position of the methyl group in the pyridine ring have no significant effect on the dipole moment. The Br⁻ ion remains on one side of the pyridine ring with the dihedral angle of 20–22° (–N–C–H–Br). The dipole moments of the picolinium nitrates are found to be less than those of the corresponding bromide salts, which may be due to the position of the nitrate ion with respect to pyridinium nucleus. In $[\gamma-PicC_3][Br]$, there are weak nonconventional hydrogen bonds between Br and C-H(7) and C-H(11) with the atomic distance of 2.302 and 2.531 Å, respectively. In $[\alpha$ -PicC₃][Br], there are three hydrogen bonds with bond distances 2.3, 2.498, and 3.068 Å for C-H(7), C-H(11), and C-H(18),



Fig. 2 Optimized structure of [γ-PicC₃][Br]

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respectively. The proximity of -NC-H in $[\alpha-PicC_3]$ [Br] when compared to $[\gamma-\text{PicC}_3]$ [Br] may be ascribed to the steric effect of the 2-methyl group, which repels the flexible terminal methyl group toward Br-. This is supported by the increase in bond angle of C-N-C in $[\alpha$ -PicC₃][Br] than $[\gamma$ -PicC₃][Br]. In the corresponding nitrate salt, the central nitrogen atom is found to remain above the plane of the picolinium (bond angles of C-N-N being 76–105°) aligned to the π -electron cloud with slight distortion. The oxygen atoms of nitrate ion in $[\gamma-\text{PicC}_3]$ [NO₃] may be linked to C-H(8), C-H(13), and C-H (12) with interatomic distances of 2.230, 2.229, and 2.816 Å, respectively. The liquid characteristics, thus, may be ascribed to the spatial orientation of the anion, which deviates from the symmetry, leading to the relatively weak packing of molecules.

The molecular charge distributions on individual atoms of the IL are tabulated in Table S1. The charge on the adjacent C of N in the pyridine ring is assumed to have a positive value, while that of alkyl chain has a negative value. The reasoning seems to be obvious because the former atoms are connected to the electron-deficient N through π -bond and the electron clouds are polarized away from the C atoms, while in the latter case, due to the σ -bond, the inductive effect increases the electron cloud on the carbon atom connected to the quaternary N atom. The charge distribution on the hydrogen atoms close to the counterion supports the sidedness of the counterion. In a symmetrical compound like $[\gamma$ -PicC₃] [Br] (Fig. 2), the charge on 7H and 8H are found to be same (0.14) for 4-methyl pyridine, while on formation of the salt the charges are found to be 0.264 (7H) and 0.196 (8H), the former being more close to the counterion. The charge on the distant hydrogen like 9H is also influenced by the counterion. It assumes a relatively high charge of 0.015 than 6H. Though nitrate ion is found to be oriented on the π -electron cloud of the pyridine ring, there exists a sidedness in the orientation of the counterion, which was proposed earlier from the structural parameter. The unequal charge distribution on the carbon and hydrogen atoms also supports the existence of sidedness. The difference in the charge between 7H and 8H is found to be 0.029, while that between 3C and 4C is 0.019, the closed one having the higher charge.

In the case of $[\alpha$ -PicC_n] salts, the sidedness is obvious because of the bulky 2-methyl group, which forces the counterion to the other side of the ring. However, the effect of the methyl group is not very evident, as the charge on 7H is same as that in the $[\gamma$ -PicC_n] salts. The sidedness in the salt with nitrate ion is also supported by the charge distribution.

The HOMO–LUMO gaps of the IL are found to be reasonably high, indicating the significant stability of these molecules (Table 4). The absorption maxima determined for the vapor phase are found to be in the range of 682–721 nm for the bromide salts and 507–528 nm for the nitrate salts. The change in counterion from bromide to nitrate increases the bandgap significantly. Bai, Zhu, and Chen (2011) have also observed the HOMO–LUMO gap for imidazolium bromide and nitrate salts to be almost in the same range.

Conclusion

N-Alkyl pyridinium salts are found to be IL, but with relatively high melting temperatures compared to imidazolium IL. Furthermore, the alkyl chain with an odd number of carbon atoms is found to have low melting points compared to those with an even number of carbon atoms. Quantum mechanical studies suggest the orientation of the counterion to be unsymmetrical with respect to the organic cation. The odd number of carbon atoms in the alkyl chain and the asymmetric orientation of the counterion probably contribute to the liquid characteristics of the molecules. Pyridinium ions are more promising substrates than imidazolium ions, with the possibility of different types of substitution reactions of the pyridinium nucleus, and hence can be considered for task-specific IL.

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