

Research Article

Investigation on Aromaticity Index and Double-Bond Equivalent of Aromatic Compounds and Ionic Liquids for Fuel Desulphurization

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Aromaticity index (AI) and double-bond equivalent (DBE) were studied to seek a simpler approach in identifying suitable ionic liquids for the desulphurization process. Manifestation of interaction mechanism by COSMO-RS and Raman spectroscopy is discussed. The findings demonstrate that AI and DBE calculations can be used to analyze and arrogate potential combination of cation and anion for fuel desulphurization purposes.

1. Introduction

Due to the limited efficiency of hydrodesulphurization towards removing aromatic organosulphur compounds, a number of recent researches had focused on extracting them using ionic liquids [1, 2]. Notable characteristics of ionic liquids (ILs) are their nonmeasurable vapour pressure, thermal stability with wide liquid range, and solvating properties for diverse materials. Because of these notable characteristics, ILs have drawn great attention in which their properties are believed to leave minimal impact on the environment as well as human health [3–9].

The prospect of ILs in becoming an industrial solvent for the desulphurization process may be illustrated from the solute-solvent properties' point of view [7, 9–13]. These may include the polarity of the solute, the dipole moment, molecular size, and molar volume. As for the aromatic organosulfur functioning as a solute, its miscibility in ILs can mostly be described through its π -electron density. The solute with a strong π -electron density would be highly miscible in ILs and vice versa. This leads to our observation that π -electron density could be a vital point in screening a potential

IL for desulphurization [1, 11–14]. However, to determine the π -electron density is not simple whereby it needs to be calculated using the quantum chemical calculations [13, 14]. Thus, the quantification of the π -electron density for ILs using simple calculation needs immediate justification. Therefore, here, by suggesting a new complimentary method that estimates the aromaticity index and double-bond equivalent which are closely related to π -electron density, the possibility of using it to preliminarily select an appropriate IL for fuel desulphurization purposes shall be explored.

2. Experimental and Theory

From Conductor-like Screening Model for Realistic Solvents (COSMO-RS) database, 407 combinations of organic ILs (11 of cations and 37 of anions) were investigated, while metal-based ILs were excluded. First, three important parameters that determine the extractive ability of the ILs which are predicted using COSMO-RS were basically calculated from the estimated activity coefficient (γ) at infinite dilution. These three parameters are capacity (C), selectivity (S), and performance index (PI). Capacity is defined as the maximum

amount of solute that can be dissolved in ILs, whereby selectivity is simplified from the ratio of the composition of solute in the extract (ILs phase) and its composition in raffinate (model fuel phase), while the resultant of multiplication between capacity and selectivity is defined as performance index. Numerically, these three parameters can be expressed by (1), (2), and (3), respectively [13]. These parameters have been estimated for a preliminary data comparison study against reported desulphurization performances. The three parameters can be expressed as follows:

$$C^{\infty} = \left(\frac{1}{\gamma_1^{\infty}} \right)^{\text{IL Phase}}, \quad (1)$$

$$S_{ij}^{\infty} = \left(\frac{\gamma_2^{\infty}}{\gamma_1^{\infty}} \right)^{\text{IL Phase}} \cdot \left(\frac{\gamma_1^{\infty}}{\gamma_2^{\infty}} \right)^{\text{Model Fuel Phase}} \approx \left(\frac{\gamma_2^{\infty}}{\gamma_1^{\infty}} \right)^{\text{IL Phase}}, \quad (2)$$

$$\text{PI} = C^{\infty} \cdot S_{ij}^{\infty}. \quad (3)$$

Koch and Dittmar introduced an AI that can be calculated solely from the exact molecular mass of the organic compound. AI is a measure of the C–C double-bond “density” which additionally considers the contribution of π -bonds by heteroatoms. Since all heteroatoms are taken into account as potential contributors, the actual aromaticity in a molecule can be higher and AI must be regarded as the most conservative approach, according to (4) [15]:

$$\text{AI} = \frac{1 + \text{C} - \text{O} - \text{S} - 0.5\text{H}}{\text{C} - \text{O} - \text{S} - \text{N} - \text{P}}. \quad (4)$$

The number of each atom in the molecule, for example, carbon (C), oxygen (O), sulphur (S), hydrogen (H), nitrogen (N), and phosphorus (P), provided the value of AI. The atoms which are described in (4) are the most common elements in an organic compound [15].

DBE has been introduced through organic matters characterization studies and its calculation is a well-established tool in mass spectrometry. In short, DBE can be defined as a summation of the unsaturations plus rings in a molecule which basically can be calculated via a molecular formula, using (5), where N_i and V_i are the number of atom and valence of each atom, respectively [15]:

$$\text{DBE} = 1 + \frac{\sum_i^{\text{max}} N_i (V_i - 2)}{2}. \quad (5)$$

In order to identify the interaction mechanism, a vial containing a sample of BT/[BMIM][OSO₄] mixture was placed on the top of the laser spot. The total amount of the sample mixture was fixed accordingly for interaction purposes between benzothiophene (BT) and 1-butyl-3-methylimidazolium octylsulfate ([BMIM][OSO₄]). A series of BT/[BMIM][OSO₄] binary system $\{x \text{ BT} + (1 - x) [\text{BMIM}][\text{OSO}_4]\}$ with mole fraction in the range of $x = 0.22, 0.53, \text{ and } 0.72$ was studied.

The investigated ILs were synthesized in-house and some were purchased from Merck with stated halides content of less than 1%. Allowable water content in ILs for extraction

has to be maintained below 500 ppm. In the present extractive desulphurization process, a mixture of *n*-dodecane (*n*-C₁₂) and BT (1000 $\mu\text{g}/\text{mL}$) was used as model fuel. The extraction was carried out in 25 mL screw-cap vials. The mixture was vigorously stirred at room temperature for 10 min and another 10 min for settling to attain equilibrium, which has been previously identified [2]. The ILs have higher densities from the model fuel. The upper phase which is the model fuel could be withdrawn easily and analyzed for its sulphur content using the HPLC (DAD detector, reverser-phase ZORBAX SB-C18 column), and, based on the values, a material balance was calculated. At equilibrium, the sulphur partition coefficient determines the extent of the mobility of sulphur into ILs phase. The sulphur partition coefficient is defined as the ratio of equilibrium concentration of sulphur in ILs phase (S_a) to that in model fuel phase (S_b), as shown in (6) below. The details of the procedures and analysis are provided elsewhere [2]

$$K_d = \frac{S_a}{S_b}. \quad (6)$$

3. Result and Discussion

In the electroneutral mixture method of the COSMO-RS, in order to estimate the activity coefficient (γ), a mixture of ILs and solute was treated as ternary system (1:1 IL, cation + anion + solute) that can be converted into a binary system. The activity coefficient value is estimated for calculating the capacity and selectivity values. Later, the prediction extractability or rather known as performance index of the ILs at infinite dilution was determined using calculated capacity and selectivity values. Meanwhile, the experimental extractability which was collected from the literature is plotted against performance index for interaction mechanism identification, as shown in Figure 1. In general, it can be seen that the experimental extractability of sulphur compounds which are extracted from *n*-C₁₂ by [BMIM][OSO₄] decreased in the order of DBT > BT > 4-MDBT > 4,6-DMDBT > TS > tetrahydrothiophene > dodecanethiol while, on the other hand, the prediction extractability by COSMO-RS depicted a different order with TS > tetrahydrothiophene > BT > DBT > 4-MDBT > 4,6-DMDBT > dodecanethiol. In the experimental approach, the researchers have already explained that the order of sulphur compounds extracted mostly depended upon the π -electron density of the compounds but, for the prediction approach via COSMO-RS, the explanations came from the sigma profile plot, shown in Figure 2. On the left-hand side of the histogram is the hydrogen bond donor region ($\sigma < -\sigma_{\text{HB}}$; $\sigma_{\text{HB}} \sim 0.009 \text{ e}/\text{\AA}^2$) and on the right-hand side is the hydrogen acceptor region ($\sigma > \sigma_{\text{HB}}$; $\sigma_{\text{HB}} \sim 0.009 \text{ e}/\text{\AA}^2$). From this figure, it can be seen that the cation part of [BMIM][OSO₄] lies in the donor region while the anion part lies in the acceptor region. A small fraction of the sigma profile of all predicted sulphur compounds stretched out into the donor and acceptor region, thus indicating that these sulphur compounds favour a very weak hydrogen bonding. The overlapping of the sigma profile

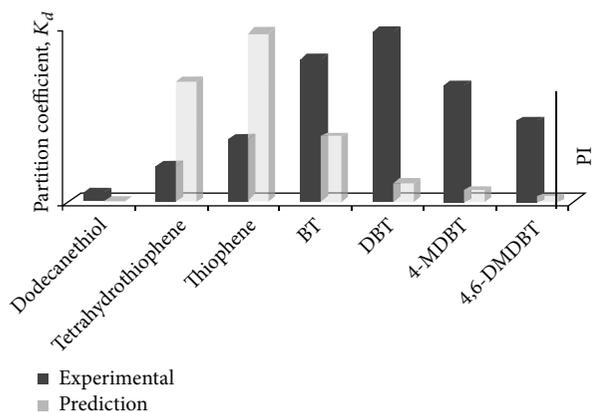


FIGURE 1: Comparison of extractability (K_d value) of the sulfur species from n -C₁₂ collected from the literature [8, 10] and COSMO-RS prediction.

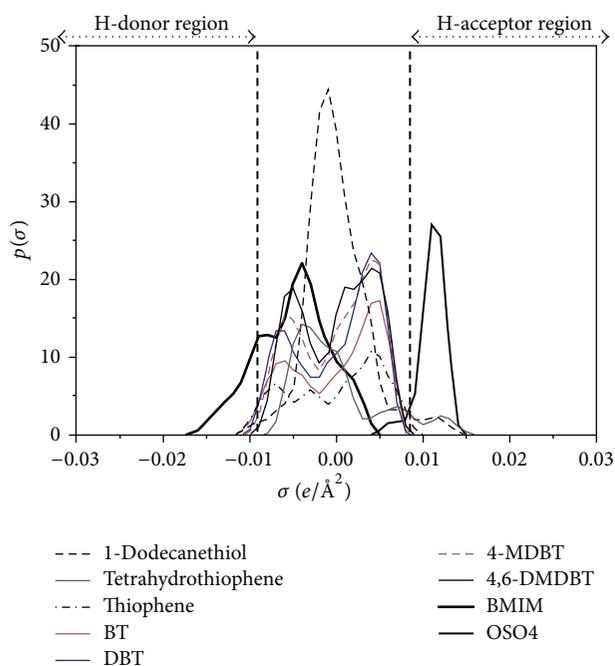


FIGURE 2: Sigma profile for [BMIM][OSO₄] and respective sulfur species.

between the sulphur compounds and [BMIM][OSO₄] represents that miscibility between these compounds is possible. However, thiophene (TS) showed more overlaps compared to the other sulphur compounds which proves that more thiophene will be extracted from n -C₁₂ as per estimated. With these inconsistent observations between experimental and prediction approach by COSMO-RS, we were determined to investigate the interaction mechanism between BT molecules and [BMIM][OSO₄] using Raman spectroscopy.

Raman spectroscopy is a vibrational molecular spectroscopy which derives from an inelastic light scattering process. In Raman spectroscopy, sample preparation is simpler

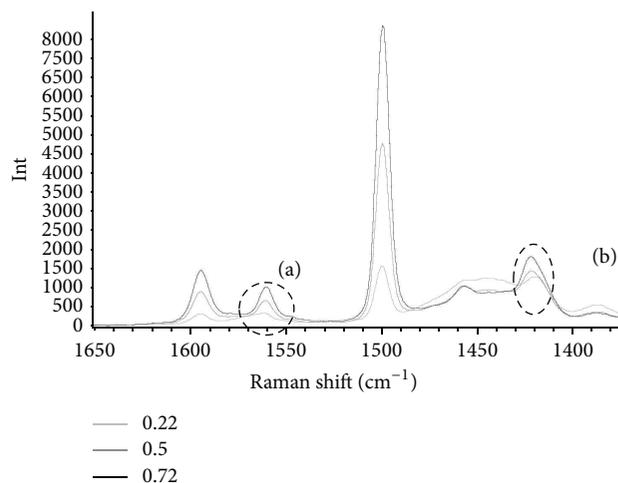


FIGURE 3: Raman spectra of $\{x \text{ BT} + (1 - x) [\text{BMIM}][\text{OSO}_4]\}$ over the range of 1600–1400 cm^{-1} with the mole fraction increasing from 0.22 to 0.72.

as compared to other Fourier transforms spectroscopy techniques. Basically, with Raman spectroscopy, a laser photon is scattered by a sample molecule and losses or gains of energy during the process. The amount of energy lost is seen as a change in energy (wavelength) of the irradiating photon. This energy loss is characteristic for a particular bond in the molecule. Figure 3 shows the comparison in Raman spectra in the 1600–1400 cm^{-1} region where shifting occurred for two identified peaks at 1560 and 1420 cm^{-1} , respectively. By observing these peaks, the shifted peaks have been assigned to C = C stretching and the C–H vibrations of the aromatic ring system were identified. It is probable that the interaction largely involved the π -bond between BT and C–H of imidazolium cation of [BMIM][OSO₄]. Irrevocably, it proved that π -electron density and aromaticity played a crucial role in extracting aromatic organosulphur which ruled out the conceptual observation explicated by the sigma profile of COSMO-RS. While looking at this mechanism which may fit any kind of aromatic compounds, we were driven to quantify potential ILs for fuel desulphurization by π -electron and aromaticity aspect using AI and DBE calculation approach, instead of relying on π -electron density calculations which are hard to be estimated and are complicated calculations. But first, preassessment is needed in order to justify this screening method.

The AI values of five aromatic organosulphurs (TS, BT, DBT, 4-MDBT, and 4,6-DMDBT) and three aromatic hydrocarbons (benzene, toluene, and xylene) were calculated using (4) and illustrated in Figure 4. With the aim of looking for some pattern within each aromatic species, the experimental extractability has been added for comparison study. The AI values of eight studied compounds were found to be relatively proportional with the experimental extractability whereby they followed the order of DBT > BT > TS > 4-MDBT > benzene > 4,6-DMDBT > toluene > xylene. For example, based on the miscibility study of aromatic hydrocarbons alone, as collected from the literature, the most miscible

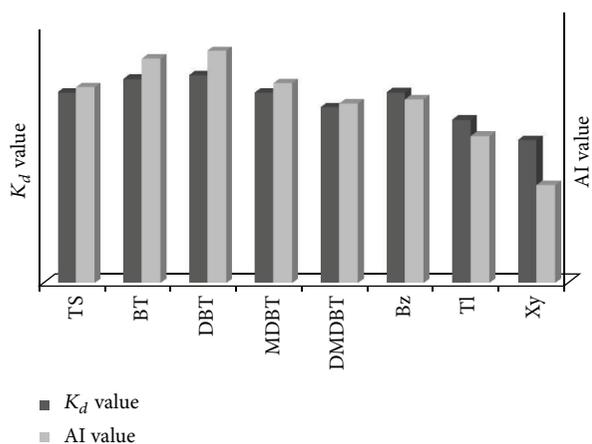


FIGURE 4: Comparison of extractability (K_d value) organosulphur and aromatic hydrocarbon compounds collected from the literature [8, 10–12] and AI value.

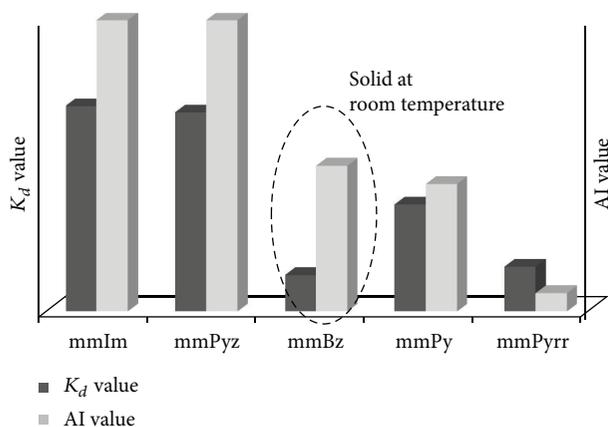


FIGURE 5: Comparison of AI value and desulphurization partition coefficient (K_d value) of cations solely with MSO_4 .

compound in imidazolium-based ILs is benzene followed by toluene and xylene. Apart from considering the molecular size or alkyl chain length, there is an alternative explanation in describing the miscibility of the aromatic hydrocarbons in imidazolium-based ILs: miscibility decreases as the value of calculated AI decreases. This fact indicates that calculating AI value could become a prediction tool for miscibility study of aromatic compounds in imidazolium-based ILs. Due to this, it is particularly exciting that the relationship between AI and the experimental extractability of aromatic compounds may open the possibility for guesstimating and perhaps screening potential ILs for the desulphurization process.

Table 1 shows the calculated AI and DBE values for common cation and anion. The AI values were calculated based on the root structure of cation alone by ignoring the alkyl chain attached prior to determine the pattern toward experimental extractability for extractive desulphurization process. Five ILs have been synthesized accordingly (refer to Table 2) and their desulphurization performance was determined in terms of sulfur partition coefficient (K_d value).

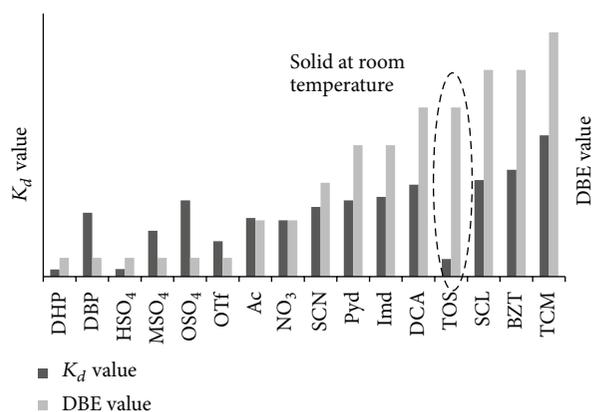


FIGURE 6: Comparison of DBE value and desulphurization partition coefficient (K_d value) of anions solely with BMIM.

Basically, it is apparent from the pattern of AI values that the order was as follows: imidazole \approx pyrazole $>$ benzimidazole $>$ pyridine $>$ pyrrolidone. Meanwhile, the results from extractive desulphurization depicted the order differently, as shown in Figure 5. The inconsistent order between AI and K_d value was found to be due to the physical phase of ILs whereby benzimidazole-based ILs are in the solid form at room temperature, resulting in poor desulphurization performance (K_d value = 0.124). As part of our study on screening the ILs for desulphurization, physical phase is an important aspect that should be considered first before evaluating AI value for cation selection.

In the second part of predicting ILs for extractive desulphurization, it should be noted that all of the ILs used are composed of relatively similar cations. Table 2 reports the K_d value of 16 ILs at room temperature of experimental conditions along with their respective calculated DBE values, which are also illustrated in Figure 6. DBE value was investigated instead of AI due to the limited number of anions that are currently available. The DBE value agrees reasonably well with the experimental findings if 1-butyl-3-methylimidazolium tosylate (TOS) is excluded. The solid phase of this IL attributes lavishly in decreasing the desulphurization ability on model fuel. Within the same root of two types of anions, namely, phosphate-based ILs (referred to as dihydrogenphosphate (DHP) and dibutylphosphate (DBP)) and sulfate-based ILs (referred to as hydrogensulfate (HSO_4), methylsulfate (MSO_4), and octylsulfate (OSO_4)), anions that have longer alkyl chains gave higher performances. Weakening of anions due to alkyl chain length can be correlated to the strength of cation-anion interactions whereby the shorter the alkyl chain, the stronger the interaction between cation and anion. Mochizuki and Sugawara [1] have observed a similar trend in their work where the extraction of sulphur compound increases linearly with the increase in alkyl chain length of imidazolium-based sulfate ILs. Among the ILs, tricyanomethane (TCM) stood out with a K_d value of 3.762. This is closely followed by benzoate and salicylate anion with K_d values of 2.846 and 2.571, respectively. This proves that, by

TABLE 1: Calculated aromaticity index (AI) and double-bond equivalent (DBE) value for common cation and anion.

Cation (basic structure)		Anion	
Chemical formula	AI	Chemical formula	DBE
Benzimidazole, C ₇ H ₆ N ₂	1	Acetate, C ₂ H ₃ O ₂	1.5
Benzyltriphenylphosphine, C ₂₅ H ₂₁ P	0.6458	Benzoate, C ₇ H ₅ O ₂	5.5
Guanidine, CH ₅ N ₃	—	Bis(tpM)phos., C ₁₆ H ₃₄ O ₂ P	0.5
Imidazole, C ₃ H ₄ N ₂	2	Butylsulfate, C ₄ H ₉ O ₄ S	0.5
Oxazole, C ₃ H ₃ NO	1.5	Decanoate, C ₁₀ H ₁₉ O ₂	1.5
Piperidine, C ₄ H ₁₀ N ₂	0	DBP, C ₈ H ₁₈ O ₄ P	0.5
Pyrazole, C ₃ H ₄ N ₂	2	Dicyanamide, C ₂ N ₃	4.5
Pyridine, C ₅ H ₅ N	0.875	DEP, C ₄ H ₁₀ O ₄ P	0.5
Pyrrolidone, C ₅ H ₁₁ N	0.125	DHP, H ₂ O ₄ P	0.5
Quinoline, C ₉ H ₇ N	1.083	DMP, C ₂ H ₆ O ₄ P	0.5
Thiazole, C ₃ H ₃ NS	1.5	EESO ₄ , C ₄ H ₉ O ₅ S	0.5
		ESO ₄ , C ₂ H ₅ O ₄ S	0.5
		Hydrogensulfate, HSO ₄	0.5
		Methanesulfonate, CH ₃ O ₃ S	0.5
		MESO ₄ , C ₃ H ₇ O ₅ S	0.5
		MSO ₄ , CH ₃ O ₄ S	0.5
		Nitrate, NO ₃	1.5
		OSO ₄ , C ₈ H ₁₇ O ₄ S	0.5
		Salicylate, C ₇ H ₅ O ₃	5.5
		Thiocyanate, CNS	2.5
		TOS, C ₇ H ₇ O ₃ S	4.5
		TCM, C ₄ N ₃	6.5
		(ME)ESO ₄ , C ₅ H ₁₁ O ₆ S	0.5
		Imidazolidine or pyrazolidine, C ₃ H ₃ N ₂	3.5
		Bis(PFE)phos., C ₄ F ₁₀ O ₂ P	0.5
		Bis(PFES)ami., C ₄ F ₁₀ NO ₄ S ₂	0.5
		Bis(TFM)imi., C ₂ F ₆ N	0.5
		Bis(TFMS)meth., C ₃ HF ₆ O ₄ S ₂	0.5
		Perchlorate, ClO ₄	0.5
		HFB, C ₄ F ₇ O ₂	0.5
		IOPE, F ₄ NO ₂ P ₂	0.5
		pFBS, C ₄ F ₉ O ₃ S	0.5
		NTf ₂ , C ₂ F ₆ NO ₄ S ₂	0.5
		TFA, C ₂ F ₃ O ₂	1.5
		OTf, CF ₃ O ₃ S	0.5
		Tris(tFMS)meth., C ₄ F ₉ O ₆ S ₃	0.5

determining AI and DBE values, the appropriate ILs for fuel desulphurization can be classified.

4. Conclusion

Systematic investigations on AI and DBE of ILs have been presented. The predicted values obtained using COSMO-RS did not converge well with values obtained from the literature due to the interaction theory consideration. Using Raman spectroscopy, interaction mechanism has been revealed where the extractability of BT by [BMIM] [OSO₄] is through aromaticity and π -electron density. Further study then confirmed that the extractability of aromatic compounds is proportionate to π -electron which was closely related to AI

and DBE. In short, directly simple AI and DBE calculations can be used to analyze and arrogate potential combination of cation and anion ILs for fuel desulphurization purposes.

Abbreviations

AI:	Aromaticity index
BT:	Benzothiophene
Bz:	Benzene
COSMO-RS:	Conductor-like Screening Model for Realistic Solvents
DBT:	Dibenzothiophene
DBE:	Double bond equivalent
IL:	Ionic liquid

TABLE 2: Selected combination of cation and anion for ionic liquids with their respective calculated AI and DBE value.

Cation	Anion	K_d value
1, 3-Dimethylimidazolium, AI = 2	MSO ₄ , DBE = 0.5	0.409
1, 2-Dimethylpyrazolium, AI = 2	MSO ₄ , DBE = 0.5	0.366
1, 3-Dimethylbenzimidazolium, AI = 1	MSO ₄ , DBE = 0.5	0.124
1, 4-Dimethylpyridinium, AI = 0.875	MSO ₄ , DBE = 0.5	0.334
1, 1-Dimethylpyrrolidinium, AI = 0.125	MSO ₄ , DBE = 0.5	0.306
1-Butyl-3-methylimidazolium, AI = 2	DHP, DBE = 0.5	0.191
1-Butyl-3-methylimidazolium, AI = 2	DBP, DBE = 0.5	1.703
1-Butyl-3-methylimidazolium, AI = 2	HSO ₄ , DBE = 0.5	0.205
1-Butyl-3-methylimidazolium, AI = 2	MSO ₄ , DBE = 0.5	1.222
1-Butyl-3-methylimidazolium, AI = 2	OSO ₄ , DBE = 0.5	2.030
1-Butyl-3-methylimidazolium, AI = 2	OTf, DBE = 0.5	0.942
1-Butyl-3-methylimidazolium, AI = 2	Acetate, DBE = 1.5	1.564
1-Butyl-3-methylimidazolium, AI = 2	NO ₃ , DBE = 1.5	1.500
1-Butyl-3-methylimidazolium, AI = 2	CNS, DBE = 2.5	1.857
1-Butyl-3-methylimidazolium, AI = 2	Imidazolid, DBE = 3.5	2.125
1-Butyl-3-methylimidazolium, AI = 2	Pyrazolid, DBE = 3.5	2.030
1-Butyl-3-methylimidazolium, AI = 2	TOS, DBE = 4.5	0.471
1-Butyl-3-methylimidazolium, AI = 2	Dicyanamide, DBE = 4.5	2.448
1-Butyl-3-methylimidazolium, AI = 2	Benzoate, DBE = 5.5	2.846
1-Butyl-3-methylimidazolium, AI = 2	Salicylate, DBE = 5.5	2.571
1-Butyl-3-methylimidazolium, AI = 2	TCM, DBE = 6.5	3.762

mmBz:	1,3-Dimethylbenzimidazolium
mmim:	1,3-Dimethylimidazolium
mmPy:	1,4-Dimethylpyridinium
mmPyrr:	1,1-Dimethylpyrrolidinium
mmPyz:	1,2-Dimethylpyrazolium
Tl:	Toluene
TS:	Thiophene
Xy:	Xylene
[BMIM][OSO ₄]:	1-Butyl-3-methylimidazolium octylsulfate
4-MDBT:	4-Methyldibenzothiophene
4,6-DMDBT:	4,6-Dimethyldibenzothiophene.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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