

Screening of Metal Chloride Anion-based Ionic Liquids for Direct Conversion of Hydrogen Sulfide by COSMO-RS

Muhammad Syahir Aminuddin¹, Zakaria Man¹, Mohamad Azmi Bustam @Khalil¹ and Bawadi Abdullah^{1,*}

¹Universiti Teknologi PETRONAS, Chemical Engineering Department, 32610 Bandar Seri Iskandar, Perak, Malaysia

Abstract. In order to identify the best possible reaction media for performing H₂S conversion, a total number of 300 different ILs from a combination of 20 cations and 15 anions were screened via COSMO-RS model simulations. By COSMO-RS method, thermodynamic and physicochemical properties of 300 ILs such as Henry's law constants, activity coefficient, selectivity, capacity and performance index are obtained and analyzed. Thus, by comparing the performance of ILs via COSMO-RS, a series of TSILs containing cation of [P₆₆₆₁₄] with metal chloride anions such as Fe, Ga and Sn were chosen and selected for synthesis based on their performance predicted by COSMO-RS and their economic values. Consequently, the physicochemical properties such as density, viscosity, thermal properties, as well as H₂S absorptive oxidation performances in those TSILs will be systematically investigated.

Keywords—Task Specific Ionic Liquids; Conversion of H₂S; H₂S; Sour Natural Gas

1 Introduction

Hydrogen sulfide (H₂S) is a poisonous gas commonly found in natural gas fields, crude oil, biogas and syngas [1]. H₂S is highly toxic and its hazardous effects towards living organisms could be seen as low as at 10 ppm of concentration and could cause death after exceeding 500 ppm [2]. It is also very corrosive to carbon steel [3], which is usually used in the pipelines and production such as storage tanks in oil and gas industry [4]. Therefore, the removal of H₂S is very important for safety and economic purposes.

Industrially, there are different methods involved in natural gas desulphurization processes such as absorption, adsorption and conversion of H₂S into elemental sulfur. Among these processes, LO-CAT and Claus process possess remarkable advantages of converting H₂S to elemental sulfur, (S₈) at higher efficiencies [5]. However, these commercial technologies are energy intensive processes and suffer with degradation and catalyst deactivation, resulting in lower sulfur production output and high cost of conversion [6].

Ionic liquids (ILs) are salts with melting point below 100°C. It is a new class of green solvents with a potential use in natural gas sweetening processes [7]. ILs are widely known as “designer solvents” due to its tunable physicochemical properties such as density, viscosity, hydrophobicity, polarity and etc. by interchanging the cation and anion of the ILs [8]. These unique properties can be harnessed for H₂S conversion processes.

In recent years, a lot of studies have been carried out focusing on conversion of H₂S into elemental sulfur by using ILs [9]. Many studies have reported the potential use

and candidacies of conventional room temperature ILs (RTILs) for H₂S conversion experimentally [10, 11]. However, it is found out that the solubility and capacity of H₂S in these ILs are still low at low pressure and thus, unable to perform their tasks efficiently [12-16]. Therefore, a new kind of ILs, Task Specific ILs (TSILs) such as metal chloride anion based ILs has been proposed in this research for conversion of H₂S [17, 18]. By considering the conversion efficiency achievable with such TSILs, it is expected that such TSILs can potentially promote faster conversion of H₂S to S₈ [19, 20].

However due to limitless combinations possibility between cations and metal chloride anions that are available for the synthesis, the evaluation of the most appropriate metal chloride anion based ILs for oxidative absorption or direct conversion of H₂S is very expensive and time consuming if carried out experimentally [21, 22], and also impossible to be performed. The opportunities to identify and select new ILs will also be wasted [23]. Hence, to select the best ILs with desired properties efficiently, all possible ILs must be screened systematically and thoroughly by changing the respective cations and anions [24].

The potential ILs were screened by using a quantum chemical based, Conductor-like Screening Model for Real Solvents (COSMO-RS) developed by Klamt *et al.* [25] for the prediction of liquids thermodynamic properties. The main advantage of COSMO-RS for screening ILs is its ability to predict the properties of the mixtures' components without any prior experimental data needed. Specifically, COSMO-RS is used for predicting solvent selectivity and capacity for H₂S in ILs at infinite dilution.

* Corresponding author: bawadi_abdullah@utp.edu.my ; bawadi73@gmail.com

Based on the selectivity and capacity of H₂S, the performance of ILs in conversion of H₂S can be predicted. There were a few previous studies that reports the screening of ILs for desulfurization of H₂S [26-30]. The novelty of this study compared to previous studies is this is the first study that emphasize the screening of metal chloride anions based ILs for direct conversion of H₂S.

2 Computational methods

2.1 COSMO-RS method

COSMO-RS is used to predict the thermophysical properties in various type of systems. For example in COSMO calculations, ILs are treated as equimolar mixtures consisting of cations and anions [31]. Therefore by using the TURBOMOLE program package [32], various COSMO files were generated for cations and anions using Becke and Perdew (BP) functional [33] with triple zeta valence polarized (TZVP) basis set [34].

2.2 Property calculation

The mixture properties for ILs and H₂S are set at room temperature and pressure condition. All the COSMO-RS calculations were implemented with the COSMOtherm program [35], which offers an efficient performance of the COSMO-RS method.

2.2.1 Henry's law constant

Henry's law states that at a constant temperature, the solubility of a gas in a liquid is directly proportional to the pressure of the gas. Thus, the solubility of a gas at a unit pressure is equal to Henry's constant [36]. Solubility of H₂S for 300 ILs can be predicted directly by using the Henry's law constants values for all obtained from COSMO-RS screening. A lower prediction value of Henry's law constant indicates a higher solubility of H₂S in ILs.

2.2.2 Activity coefficient

Activity coefficient is the ratio of the chemical activity of any substance to its molar concentration. In this particular research, COSMO-RS has been used intensively to predict the activity coefficient at infinite dilution, (γ^∞) values of H₂S in various ILs from combinations of multiple cations and anions. γ^∞ values are important because it quantifies the differences of the strength between the molecular interactions and thus providing clear insights of the complex ILs-based system at the molecular levels. Besides, the measurement of γ^∞ data are cheaper and more convenient compared to liquid-liquid equilibria (LLE) and vapour-liquid equilibria (VLE) diagrams [37].

Activity coefficient at infinite dilution prediction by COSMO-RS is significant for evaluating the selectivity and capacity of ILs for oxidative absorption of H₂S [38]. Selectivity and capacity are two crucial parameters in determining the extractive strength of the solvent. The predictions of activity coefficient by COSMO-RS only require molecular structures of the chemical species

involved in the reaction. In order to predict the activity coefficient at infinite dilution, (γ^∞) by COSMO-RS, the ILs are treated to have equimolar concentrations of cations and anions. The activity coefficient (γ) of H₂S at infinite dilution in 300 ILs at 298.15 K is calculated from the COSMO-RS prediction results.

2.2.3 Selectivity

Selectivity of H₂S in ILs that acts as a reaction media or catalyst is the ability of the ILs to direct a reaction which favors H₂S over O₂ to yield a particular product which is elemental sulfur. Selectivity is calculated as the ratio of composition of O₂ and H₂S in IL phase [39] as shown in the following equation (1);

$$S_{12}^\infty = \left(\frac{\gamma_2^\infty}{\gamma_1^\infty} \right)^{IL\ phase} \quad (1)$$

where, γ_2^∞ is the activity coefficient of O₂ at infinite dilution and γ_1^∞ is the activity coefficient of H₂S at infinite dilution. The selectivity for H₂S in 300 different ILs from a combination of 20 cations and 15 anions were predicted via COSMO-RS method.

2.2.4 Capacity

Capacity of H₂S in any specific ILs is the maximum amount of H₂S that the specific ILs can contain [40]. Capacity also determines the amount of ILs needed for the removal of H₂S by extraction as given in the equation (2) below;

$$C_{12}^\infty = \left(\frac{1}{\gamma_1^\infty} \right)^{IL\ phase} \quad (2)$$

The capacity for H₂S in 300 different ILs from a combination of 20 cations and 15 anions were predicted via COSMO-RS method at 298.15 K.

2.2.5 Performance Index

Performance index (*PI*) measures the performance and effectiveness of any solvent in performing the extraction [41]. Performance index is the product of selectivity and capacity of any solvent at infinite dilution as given in the following equation (3).

$$PI = S_{12}^\infty \times C_{12}^\infty \quad (3)$$

2.3 Screening of Metal Chlorides Anion-based ILs for H₂S Conversion

In this research, COSMO-RS is used to predict the activity coefficient and selectivity of 300 different types of ILs. In general, ILs can be designed by combining different cations and anions. In this particular research, a total combination of 20 cations and 15 anions of chloride and metal chloride anions are chosen to form a total of 300 metal chloride anion based ILs, which covers almost all reported ILs and their derivatives.

The wide range combination of cations and anions are screened and predicted by COSMO-RS to determine the most efficient reaction media to perform oxidative

absorption of H₂S. Their structures and abbreviations are listed in Table 1. The cations used are imidazolium, phosphonium, pyridinium and pyrrolidinium. The anions used are chloride and metal chloride anions such as silver, zinc, cobalt, copper, gold, titanium, iron, chromium, tin, platinum, aluminium, gallium, nickel and indium.

Table 1. List of cations and anions

<i>Formal name</i>	<i>Abbreviation</i>	<i>MW (g/mol)</i>	<i>Structure</i>
1,3-methyl-imidazolium	[C ₁ Im] ⁺	83.11	
1-ethyl-3-methyl-imidazolium	[Emim] ⁺	111.16	
1-butyl-imidazolium	[C ₄ Im] ⁺	125.19	
1-butyl-3-methyl-imidazolium	[Bmim] ⁺	139.22	
1-hexyl-3-methyl-imidazolium	[Hmim] ⁺	167.27	
1-octyl-3-methyl-imidazolium	[Omim] ⁺	195.32	
1-decyl-3-methyl-imidazolium	[C ₁₀ mim] ⁺	219.27	
1-methyl-pyridinium	[Mpy] ⁺	94.13	
1-butyl-2-methyl-pyridinium	[B ₂ mpy] ⁺	150.25	
1-butyl-3-methyl-pyridinium	[B ₃ mpy] ⁺	150.25	
4-methyl-N-butylpyridinium	[4-MBpy] ⁺	150.25	
1-hexyl-pyridinium	[Hpy] ⁺	168.32	
Tetrabutyl-phosphonium	[P(C ₄) ₄] ⁺	259.43	
Tributyl-tetradecylphosphonium	[P ₄₄₄₁₄] ⁺	399.97	
Trihexyl-tetradecylphosphonium	[P ₆₆₆₁₄] ⁺	483.86	

<i>Formal name</i>	<i>Abbreviation</i>	<i>MW (g/mol)</i>	<i>Structure</i>
1-ethyl-1-methyl-pyrrolidinium	[Empyrr] ⁺	122.31	
1-butyl-1-methyl-pyrrolidinium	[C ₄ mPyrr] ⁺	144.29	
1-butyl-1-ethyl-pyrrolidinium	[C ₄ ePyrr] ⁺	156.29	
1-hexyl-1-methyl-pyrrolidinium	[Hmpyrr] ⁺	170.31	
1-octyl-1-methyl-pyrrolidinium	[Ompyrr] ⁺	198.37	
Chloride	[Cl] ⁻	35.45	
Tetrachloroaluminate	[AlCl ₄] ⁻	168.79	
Dichloroargentate	[AgCl ₂] ⁻	178.78	
Tetrachlorochromate	[CrCl ₄] ⁻	193.81	
Tetrachloroferrate	[FeCl ₄] ⁻	197.66	
Tetrachloronickelate	[NiCl ₄] ²⁻	200.51	
Tetrachlorocobaltate	[CoCl ₄] ²⁻	200.75	
Tetrachlorocuprate	[CuCl ₄] ²⁻	205.36	
Tetrachlorozincate	[ZnCl ₄] ²⁻	207.22	
Tetrachlorogallate	[GaCl ₄] ⁻	211.54	
Trichlorostannate	[SnCl ₃] ⁻	225.07	
Tetrachloroindium	[InCl ₄] ⁻	256.56	
Hexachlorotitanate	[TiCl ₆] ²⁻	260.59	
Dichloroaurate	[AuCl ₂] ⁻	267.87	

Formal name	Abbreviation	MW (g/mol)	Structure
Trichloroplatinate	[PtCl ₃] ⁻	301.44	

3 Results and discussion

3.1 Electronegativity of the metals in the metal chloride anions based ILs

Electronegativity refers to the atomic ability to attract the electrons from the atoms bonded to it. The electronegativity of the anions play a major role in affecting the selectivity and capacity [42] of the metal chloride anion based ILs for direct conversion of H₂S into elemental sulfur. The electronegativity values for all metals used in the screening of metal chloride anion based ILs by COSMO-RS is shown in Table 4.3 below [43]. Based on Table 4.3, Ga is the most electronegative metals followed by Fe, Au, Al and In. Meanwhile, the least electronegative metal is Ti.

Table 1. Table of metals electronegativity in the metal chloride anion based ILs [43]

Metal chloride anions	Electronegativity
[TiCl ₆] ²⁻	1.225
[CoCl ₄] ²⁻	1.321
[CrCl ₄] ⁻	1.322
[AgCl ₂] ⁻	1.333
[ZnCl ₄] ²⁻	1.336
[NiCl ₄] ²⁻	1.367
[CuCl ₄] ²⁻	1.372
[SnCl ₃] ⁻	1.427
[PtCl ₃] ⁻	1.432
[InCl ₄] ⁻	1.480
[AlCl ₄] ⁻	1.513
[AuCl ₂] ⁻	1.550
[FeCl ₄] ⁻	1.556
[GaCl ₄] ⁻	1.579

3.2 Henry's law constants

The Henry's law constants of H₂S in 300 ILs are predicted by COSMO-RS method at 298.15 K, given in a graph of shown in Figure 1. As is well-known, a higher Henry's law constant indicates a lower solubility. A lower prediction value of Henry's law constant indicates a lower solubility of H₂S in ILs.

Solubility of H₂S is found to be inversely proportional with the electronegativity of the anions. As the electronegativity of the anion decreases, the solubility of H₂S in ILs increases. By referring to Table 1, hexachlorotitanate anion, [TiCl₆]²⁻ based which is the least electronegative compared to the rest of metals used in metal chloride anion based ILs displayed a very low Henry's law constant values, indicating the highest solubility compared to the rest of metal chloride anion based ILs. Meanwhile, metals with higher electronegativity such as Ga, Fe, Au, Al and In recorded

large Henry's law constant values, indicating a relatively low solubility of H₂S in the ILs.

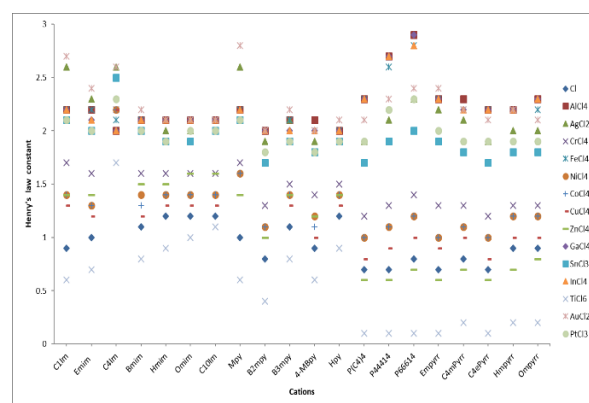


Fig. 1. Henry's law constants of H₂S in 300 ILs at T=298.15 K and P=101.325 kPa.

3.3 Activity coefficient

The activity coefficient (γ) of H₂S at infinite dilution in 300 ILs at 298.15 K is calculated from the COSMO-RS prediction results and is displayed in Figure 2 below. The activity coefficient values exhibit the same trends as Henry's law constant values which means the effect of anions and cations are important in designing new ionic liquids.

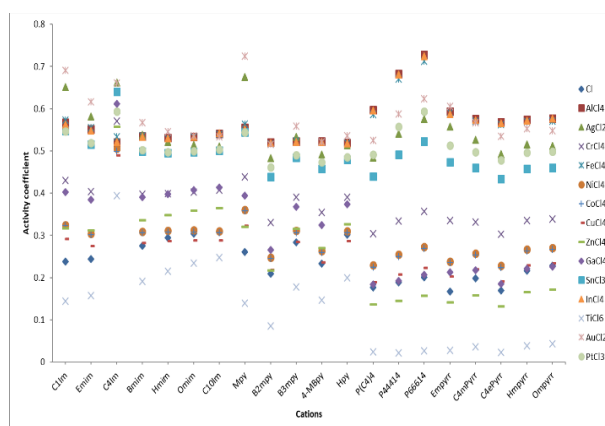


Fig. 2. The activity coefficient (γ) of H₂S at infinite dilution in 300 ILs at T=298.15 K and P=101.325 kPa.

Based on the comparison of γ^∞ values, there is no specific trend observable regarding the change of cations and anions in the metal chloride anion based ILs. Further calculations of selectivity, capacity and performance index were performed at 298.15 K and 1 atm pressure to screen the most promising metal chloride anion based ILs for direct conversion of H₂S [44].

3.4 Selectivity

The selectivity for H₂S in 300 different ILs from a combination of 20 cations and 15 anions were predicted via COSMO-RS method. The selectivity for H₂S over O₂ in 300 ILs at 298.15 K predicted by COSMO-RS is shown in a graph presented in Figure 3.

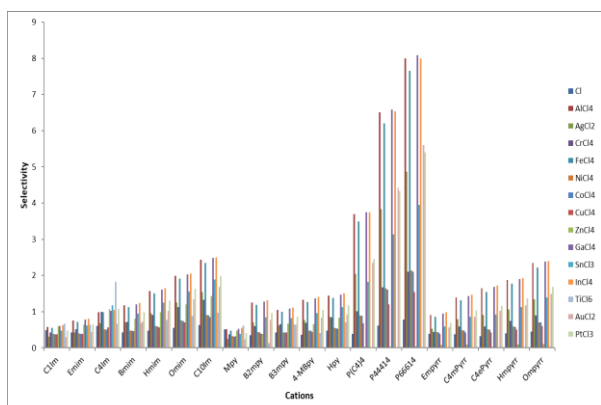


Fig. 3. Selectivity at infinite dilution for H₂S over O₂ in 300 ILs at T=298.15 K and P=101.325 kPa.

Based on the comparison of cations, the selectivity for H₂S at infinite dilution increases in the following order. Pyridinium < imidazolium < pyrrolidinium < phosphonium. Phosphonium-based ILs cations such as [P(C₄)₄], [P₄₄₄₁₄] and [P₆₆₆₁₄] displayed a high selectivity compared to the rest of cations. The interactions between cations are mainly due to hydrogen bonding between the cation and the polyaromatic molecule heteroatom and with the polyaromatic compounds π -electron cloud [45].

It is observable that cations that do not possess aromatic rings such as phosphonium-based and pyrrolidinium-based ILs have higher selectivity than the cations having aromatic rings such as imidazolium-based and pyridinium-based ILs. This occurs because of the steric hindrance of cations towards hetero-atomic polyaromatic compounds [46] that encourage the delocalization of charge in cations possessing an aromatic ring. The steric hindrance reduces the hydrogen bonding strength between cation and heteroatoms of polyaromatic molecules hence, resulting in lower selectivity.

Meanwhile, in cations without aromatic rings, the charge delocalization in the ring does not exist due to the absence of π -electron cloud resulting in better interaction with polyaromatic molecules [47]. In addition, as the number of heteroatoms increases in the cation, the sharing of charges also increases which could lead to higher ability of the cations to interact. The interaction between hetero-atomic molecules in ILs is because of the Coulombic interaction and highly dependent on the electronegative strength and number of anions. This interaction eventually leads to the formation of hydrogen bonding with hetero-atomic polyaromatic molecule. Hence, based on the infinite dilution selectivity order of H₂S of cations, phosphonium-based ILs such as [P(C₄)₄], [P₄₄₄₁₄] and [P₆₆₆₁₄] are recommended as the favorable cations.

Based on the comparison of anions, it was clearly evident that the selectivity for H₂S is found to be related with the electronegativity of anions. Higher oxidation state elements are more electronegative as they are more capable to attract and stabilize the electrons. The order of selectivity for H₂S at infinite dilution of anions irrespective of cations increases in the following order. [TiCl₆]²⁻ < [ZnCl₄]²⁻ < [Cl]⁻ < [CuCl₄]²⁻ < [CoCl₄]²⁻ < [NiCl₄]²⁻ < [CrCl₄]⁻ < [SnCl₃]⁻ < [AgCl₂]⁻ < [PtCl₃]⁻ < [AuCl₂]⁻ < [FeCl₄]⁻ < [AlCl₄]⁻ < [InCl₄]⁻ < [GaCl₄]⁻.

Selectivity of H₂S is found to be directly related with the electronegativity of the anions. Higher oxidation state elements are more electronegative as they are more capable to attract and stabilize the electrons. Selectivity for H₂S increases as the oxidation states of the metal used in metal chloride anions increases. The greater electronegativity of the anions leads to the increase in the selectivity of H₂S [48]. Higher electronegativity of the anions such as GaCl₄, InCl₄, AlCl₄ and FeCl₄ led to higher selectivity as compared to the other metal chloride anions [49]. Hence, based on the selectivity at infinite dilution order of H₂S of anions, anion of tetrachlorogallate, [GaCl₄]⁻ is recommended as the most favorable anion.

3.5 Capacity

The capacity for H₂S in 300 different ILs from a combination of 20 cations and 15 anions were predicted via COSMO-RS method. The capacity for H₂S over O₂ in 300 ILs at 298.15 K predicted by COSMO-RS is shown in a graph presented in Figure 4.

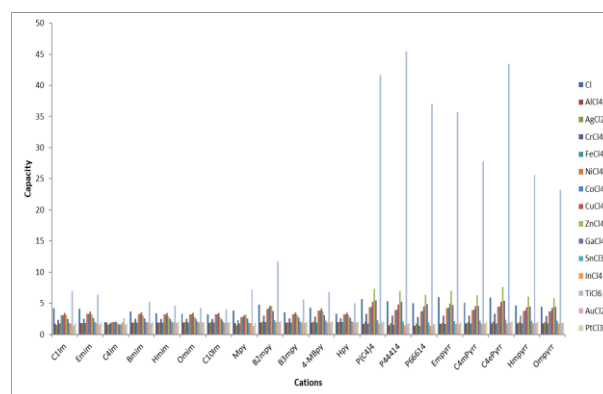


Fig. 4. Capacity at infinite dilution of H₂S in 300 ILs at T=298.15 K and P=101.325 kPa.

In general, the capacity of metal chloride anion based ILs does not provide any reasonable trend. The order of capacity for H₂S in metal chloride anion based ILs based on group of cations irrespective of anions increases in the following order. Imidazolium < pyridinium < pyrrolidinium < phosphonium. By comparing the cations, the results indicated that the capacity increases as the π -electron cloud of cations decreases [44]. The cations without aromatic rings such as phosphonium-based and pyrrolidinium-based ILs possess a higher capacity compared to the cations having aromatic rings such as pyridinium-based and imidazolium-based ILs. This happens due to the presence of delocalized electrons in the cations with aromatic ring causes a strong steric hindrance towards the hetero-atomic polyaromatic compounds [46]. As a result, they possess a lower capacity for H₂S molecules.

Due to the absence of π -electron cloud in non-aromatic cations, there is no charge delocalization in the ring and results in more effective interaction with H₂S molecules. In addition, as the number of heteroatoms increases in the cation, the sharing of charges also increases which could lead to higher ability of the cations

to interact [47]. This interaction eventually leads to the formation of hydrogen bonding with hetero-atomic polyaromatic molecule. Hence, based on the comparison of H₂S capacity in the cations, phosphonium-based ILs were selected as the favorable cations since they possess a higher capacity compared to the rest of cations.

Based on the comparisons of anions irrespective of cations, it can be seen that the hexachlorotitanate anion, [TiCl₆]²⁻ based ILs demonstrated a very high capacity for H₂S absorption compared to the rest of the anions. The trend is similar with the prediction trend of H₂S solubility in metal chloride anion based ILs discussed earlier. This is probably because titanium metal in hexachlorotitanate anion [50] is the least electronegative compared to the rest of metals used in metal chloride anion based ILs. Its low electronegativity contributed to its high capacity for H₂S molecules.

However, hexachlorotitanate anion, [TiCl₆]²⁻ based ILs are not suitable anions for selection as they possess a very low selectivity towards H₂S even though they have a very high capacity for H₂S molecules. In general, the solvents which possess high capacity tends to have a very low selectivity for the solute molecules [51]. Thus, it is not economically viable to choose a solvent which requires only a small volume but has a very poor interaction to yield the main product which is elemental sulfur, S₈ in this particular study. Therefore, it is necessary to consider the solvents which possess a reasonable magnitude in both selectivity and capacity for selection.

3.6 Performance Index

The performance index (PI) values for a total of 300 ILs from a combination of 20 cations and 15 anions are presented in a graph of performance index in 300 ILs at 298.15 K as in Figure 5. The PI values are calculated using equation (3) via COSMO-RS model.

Generally, the solvents which possess a high capacity tend to have a low selectivity to yield the products instead and vice versa. Hence, it is not economically viable to choose a solvent which require a small volume but has a poor interaction instead. Thus, it is crucial to identify a solvent which possess both properties in a reasonable magnitude.

By comparing the performances of cations in 300 ILs, it is obvious that phosphonium-based ILs such as [P(C₄)₄], [P₄₄₄₁₄] and [P₆₆₆₁₄] have higher PI values due to higher selectivity and capacity values respectively. This also indicated that phosphonium-based ILs might give better results in real conversion of H₂S experiment compared to the pyrrolidinium-based, imidazolium-based and pyridinium based ILs.

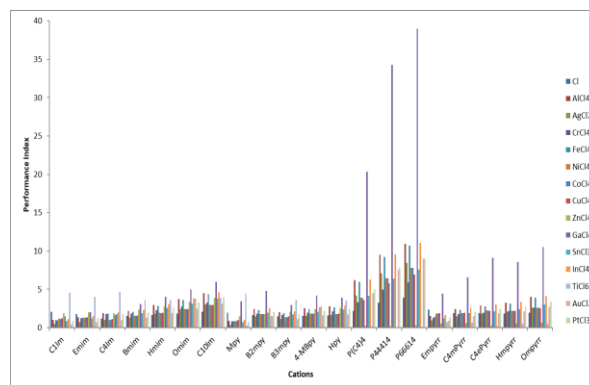


Fig. 5. Performance index for H₂S in 300 ILs at T=298.15 K and P=101.325 kPa.

By comparing the performances of anions in 300 ILs, it is obvious that certain metal chloride anion-based ILs have higher PI values such as tetrachlorogallate anion, [GaCl₄]⁻, tetrachloroindium anion, [InCl₄]⁻, tetrachloroaluminate anion, [AlCl₄]⁻ and tetrachloroferrate anion, [FeCl₄]⁻ based ILs due to their higher selectivity and capacity values respectively. However, metal chloride anion-based ILs such as hexachlorotitanate anion-based ILs, [TiCl₆]²⁻ displayed low PI value as it possesses a very high capacity, but has a very low selectivity instead.

Therefore, it can be concluded that ILs with higher values of capacity and selectivity will possess a higher performance index. These ILs are also predicted to be more efficient in performing H₂S conversion and thus, favorable to be selected for synthesis.

3.7 Selection of metal chloride anion based ILs for synthesis

Based on the performance index, PI predicted by COSMO-RS on 300 ILs' performance in H₂S conversion, trihexyl-tetradecylphosphonium ion, [P₆₆₆₁₄]⁺ and tetrabutyl-tetradecylphosphonium ion, [P₄₄₄₁₄]⁺ were the two best cations of ILs after being compared with every anion in the screening process. However, recent findings revealed that ILs containing [P₄₄₄₁₄]⁺ are extremely toxic and carcinogenic to human beings. Hence, its production is no longer continued worldwide. Therefore, only trihexyl-tetradecylphosphonium cation, [P₆₆₆₁₄]⁺ is chosen for synthesis.

Meanwhile, tetrachlorogallate ion, [GaCl₄]⁻ is predicted as the best anion with the highest performance for H₂S conversion when paired with every cation during the screening process followed by tetrachloroindium ion, [InCl₄]⁻, tetrachloroaluminate ion, [AlCl₄]⁻ and tetrachloroferrate ion, [FeCl₄]⁻. In the economic value aspects, iron(III) chloride, FeCl₃ and tin(II) chloride, SnCl₂ are lower in cost compared to the rest of metal chlorides.

Therefore, by considering various aspects of ILs selection such as H₂S conversion performance, safety reasons and economic value, 3 ILs has been selected for synthesis such as trihexyl(tetradecyl)phosphonium tetrachlorogallate, [P₆₆₆₁₄][GaCl₄], trihexyl(tetradecyl)phosphonium tetrachloroferrate, [P₆₆₆₁₄][FeCl₄] and trihexyl(tetradecyl)phosphonium trichlorostannate, [P₆₆₆₁₄][SnCl₃].

4 Conclusion

Task-Specific Ionic Liquids such as metal chloride anion based ILs have a high potential to be developed as reaction media for the conversion of H₂S. By considering high conversion efficiency can be achieved by these TSILs, they are also expected to promote a faster conversion of H₂S into S₈.

However, the process of selecting and identifying the best possible metal chloride anion based ILs is very tedious, time consuming and expensive if it is carried out experimentally. Therefore, an efficient screening method with high accuracy is required. In order to identify the best possible reaction media for performing H₂S conversion, a total number of 300 different ILs from a combination of 20 cations and 15 anions were screened via COSMO-RS model simulations.

By COSMO-RS method, thermodynamic and physicochemical properties of 300 ILs such as Henry's law constants, activity coefficient, selectivity, capacity and performance index are obtained and analyzed. Thus, by comparing the performance of ILs via COSMO-RS, a series of TSILs containing cation of [P₆₆₆₁₄] with metal chloride anions such as Ga, Fe and Sn were selected based on their performance predicted by COSMO-RS, economic and safety values.

Consequently, the physicochemical properties such as density, viscosity, thermal properties, as well as H₂S oxidation performances in those TSILs will be systematically investigated.

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