Supporting Information

Metal Chloride-anion based Ionic Liquids: Synthesis, Characterization and Evaluation of Performances in Hydrogen Sulfide Oxidative Absorption

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Selection of MCABILs process by COSMO-RS screening method

In our previous work[1], COSMO-RS was used to predict the Henry's law constants, activity coefficient and selectivity of a total 300 different types of MCAB ILs. In general, ILs can be designed by combining various kind of cations and anions. A total combination of 20 cations and 15 anions of chloride ion and metal chloride anions were chosen to form 300 different kinds of metal chloride anion based ILs, which covers almost all reported ILs and their derivatives. The wide range of cations and anions combinations were screened and predicted by COSMO-RS to determine the most efficient catalyst to perform oxidative absorption of H_2S. The cations used were imidazolium, phosphonium, pyridinium and pyrrolidinium. The anions used were chloride and metal chloride anions such as silver, zinc, cobalt, copper, gold, titanium, iron, chromium, tin, platinum, aluminium, gallium, nickel and indium. Based on the performance index, PI predicted by COSMO-RS on 300 MCABILs' performance in H_2S conversion, trihexyl(tetradecyl)phosphonium ion, $[P_{66614}]^+$ and tetrabutyl(tetradecyl)phosphonium ion, $[P_{44414}]^+$ were the two best cations of ILs after being compared with every anion in the screening process. However, recent findings revealed that ILs containing $[P_{44414}]^+$ are extremely toxic and carcinogenic to human beings. Hence, its production is no longer continued worldwide. Therefore, only trihexyl(tetradecyl)phosphonium cation, $[P_{66614}]^+$ were chosen for synthesis. Meanwhile, tetrachlorogallate ion, $[GaCl_4]^-$ is predicted as the best anion with the highest performance for H_2S conversion when paired with every cation during the screening process followed by tetrachloroindium ion, $[InCl_4]^-$, tetrachloroaluminate ion, $[AlCl_4]^-$ and tetrachloroferrate ion, $[FeCl_4]^-$. In the economic value aspects, iron(III) chloride, $FeCl_3$ and tin(II) chloride, $SnCl_2$ are lower in cost compared to the rest of metal chlorides. Therefore, by considering various aspects of ILs selection such as H_2S conversion performance, safety reasons and economic value, 3 ILs has been selected for synthesis such as trihexyl(tetradecyl)phosphonium tetrachlorogallate, $P_{66614}GaCl_4$, trihexyl(tetradecyl)phosphonium tetrachloroferrate, $P_{66614}FeCl_4$ and trihexyl(tetradecyl)phosphonium trichlorostannate, $P_{66614}SnCl_3$.

Table S1: Density values for MCABILs at 20°C

ILs structure code	Density(ρ), (g/cm^3)
$[P_{66614}][GaCl_4]$	1.00274
$[P_{66614}][FeCl_4]$	0.98470
$[P_{66614}][SnCl_3]$	0.98139

Table S2: Viscosity data for MCABILs at 20 °C

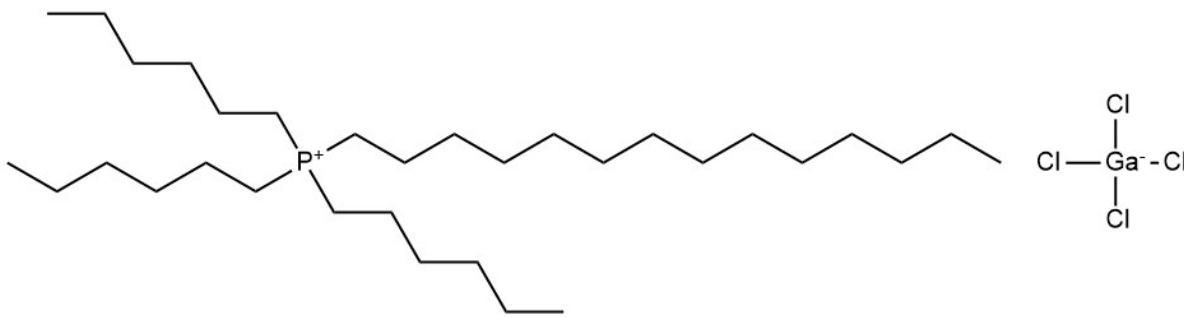
ILs structure code	Viscosity, (cP)
$[P_{66614}][GaCl_4]$	880.42
$[P_{66614}][FeCl_4]$	712.66
$[P_{66614}][SnCl_3]$	543.11

Table S3: Thermal onset, T_{Onset} and decomposition, $T_{Decomposition}$ temperatures for each MCABILs

ILs	T_{onset} (°C)	$T_{decomposition}$ (°C)
$[P_{66614}][GaCl_4]$	459.19	480.34
$[P_{66614}][FeCl_4]$	431.18	478.57
$[P_{66614}][SnCl_3]$	425.50	468.77

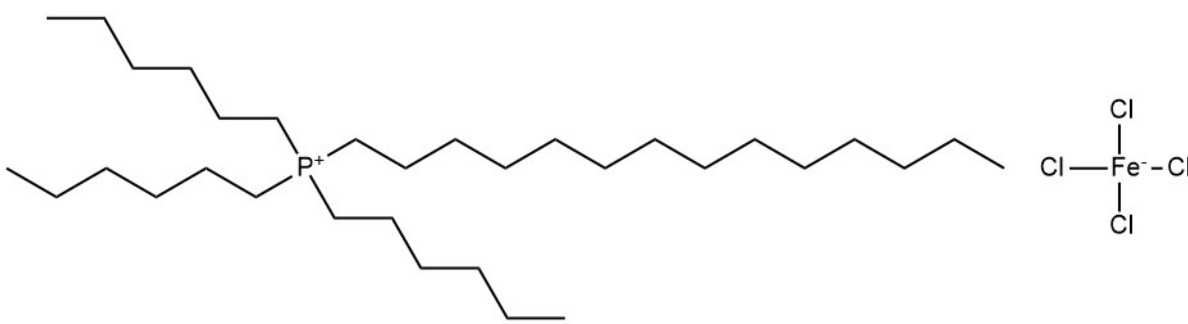
Table S4: Melting points of MCABILs

ILs structure code	Melting point (°C)
[P_{66614}][$GaCl_4$]	90.58
[P_{66614}][$FeCl_4$]	90.51
[P_{66614}][$SnCl_3$]	90.62



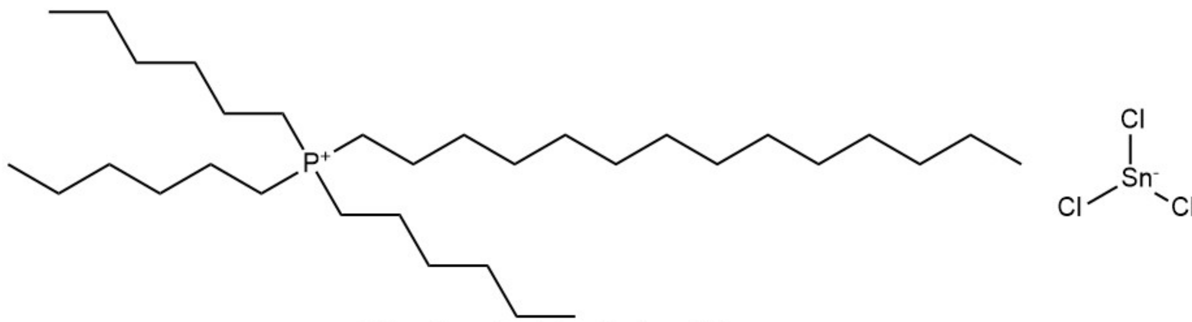
Trihexyl(tetradecyl)phosphonium tetrachlorogallate

Fig. S1: $P_{66614}GaCl_4$ structure



Trihexyl(tetradecyl)phosphonium tetrachloroferrate

Fig. S2: $P_{66614}FeCl_4$ structure



Trihexyl(tetradecyl)phosphonium trichlorostannate

Fig. S3: $P_{66614}SnCl_3$ structure

References

1. M. S. Aminuddin, Z. Man, M. A. Bustam Khalil and B. Abdullah, *E3S Web Conf.*, 2021, **287**, 02003.