

Ionic Liquid-Based Deep Eutectic Solvents as Novel Solvent-cum-Catalyst Media for Thermal Dehydrogenation of Chemical Hydrides [†]

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Abstract: This work presents a comparative study between Ionic Liquids (ILs) along with the neoteric IL-based Deep Eutectic Solvents (DESs) for the thermal dehydrogenation of chemical hydrides, namely Ammonia Borane (AB) and Ethylene diamine bisborane (EDAB). In the first instance, the quantum chemistry-based COSMO-SAC (COnductor like Screening Model Segment Activity Coefficient) model was used to select the pertinent solvent. On the basis of their obtained Infinite Dilution Activity Coefficient (IDAC) value, the following solvents from the IL and the DES family were selected: 1-butyl-3-methylimidazolium methanesulfonate ([BMIM][MeSO₃]), 1-butyl-3-methylimidazolium methanesulfonate:urea ([BMIM][MeSO₃]:[urea]) at a molar ratio of 1:1 and, 1-Butyl-3-methylimidazolium methanesulfonate: Imidazole ([BMIM][MeSO₃]:[Im]) at a molar ratio of 1:2. The DES was synthesized by combining the Hydrogen Bond Acceptor (HBA), namely 1-Butyl-3-methylimidazolium methanesulfonate, combined with Urea and Imidazole as Hydrogen Bond Donor (HBD) at a suitable molar ratio and heated at $T = 70^{\circ}\text{C}$. The formation of DES was confirmed by recording the NMR spectra. Further, the thermal dehydrogenation study was performed at a vacuum of 4×10^{-2} mbar (gauge pressure) of chemical hydrides mixed with IL/DES systems at different temperatures (95°C and 105°C), where a significant equivalent of hydrogen was produced in different reported systems, respectively. Gas Chromatography (GC) analysis was further performed in order to determine the purity of the released hydrogen gas. The residual samples were further analyzed through ¹H NMR analysis for the reaction mechanism and to confirm IL and DES's role as catalyst cum solvent media. ¹¹B NMR analysis was further performed in order to confirm the existence of sp² boron moieties.

Keywords: ionic liquids; NMR spectroscopy; gas chromatography; Deep Eutectic Solvents.

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Conflicts of Interest

The authors declare no conflict of interest.