INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

Hydrogen Fuel is considered globally as the new face of energy sector and Ethylene diamine Bisborane (EDAB) from the amine borane family is known to releases 10 wt. % of Hydrogen. However on a standalone basis, the release of hydrogen from EDAB is limited. To improve this, the use of Ionic Liquid (IL) as solvent cum catalyst medium is recommended. IL's are known to play a dominant role for dehydrogenation. IL are molten salts, but most are liquids at room temperature due to the structure of two asymmetric ion i.e. large organic structure of the cation and a small inorganic structure of the anion .Some of the interesting features of incorporating IL are (a) it helps in reducing the induction period of EDAB and the working temperature of thermal dehydrogenation. This invariably leads to higher production of hydrogen. In this study, COSMO-SAC (COnductor like Screening MOdel Segment Activity Coefficient) model was used to select the Ionic liquids (IL) for dehydrogenation experiment. The ILs with the lowest Infinite dilution activity coefficient (IDAC) were selected, as the lower the IDAC- higher the solubility of EDAB in IL. The following ILs are 1-ethyl-3-methyl imidazolium acetate ([EMIM][OAc]) ,1-butyl-3-methyl imidazolium acetate ([BMIM][OAc]),), 1-Allyl-3-methylimidazolium bromide ([AMIM][Br]), 1-Allyl-3-methylimidazolium dicyanamide ([AMIM][$N(CN)_2$]), 1-Allyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([AMIM][Tf_2N]),

Trihexyl(tetradecyl)phosphphonium bis (2,4,4- trimethylpentyl) phosphinate ([TDTHP][Phosph]) and Trihexyl(tetradecyl)phosphphonium dicyanamide ([TDTHP][DCA]).

The experiments were carried out at a vacuum of 4 x 10^{-2} mbar (gauge pressure) and at temperature of 95°C, 105°C 115°C .The highest Equivalent of Hydrogen (3.96) was released from [BMIM][OAc]. Further analysis such as ^{1}H NMR, ^{11}B NMR, TGA and HR-MS of the residue was done for better understanding about the role of IL as catalyst and EDAB as consummate for hydrogen production.

We have further used ReaxFF MD simulation to have a better idea about the nature of EDAB at extreme high temperature. We have further incorporated AB/EDAB in IL dehydrogenation kinetics study. Rate constants for decomposition of EDAB in [AMIM][Br] using Avrami-Erofeyev model was also considered. In order to explain the effects of dehydrogenation, we regressed the experimental kinetic data using the Avrami Erofeyev model in order to obtain the activation energy, rate constant and reaction order. The reaction kinetics has been predicted for six reported ILs at 85 °C with AB and EDAB with Allyl based IL using the GA toolbox.

Finally, concluding with the future scope and new techniques that can be used to get the maximum result at optimum cost**.**