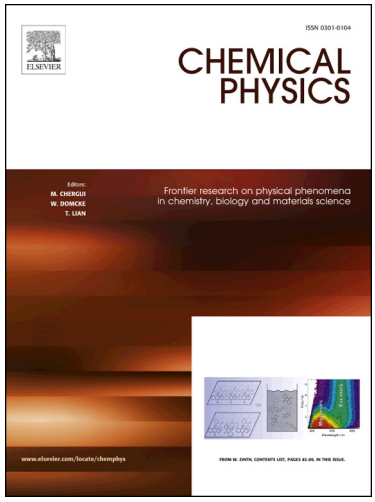

Mechanistic and kinetic insights of reduction of indophenol by sodium borohydride: A theoretical study to explore the effect of solvent and counter ion

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Mechanistic and kinetic insights of reduction of indophenol by sodium borohydride: A theoretical study to explore the effect of solvent and counter ion

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ABSTRACT

$NaBH_4$ finds plethora of applications in organic synthesis due to its unique capability of chemo-selective reduction of carbonyl functional group. Present work is focussed to explore the energetically feasible reaction pathway for reduction of indophenol by sodium borohydride. Our calculations suggest following reaction steps for reduction of indophenol. The reduction reaction is initially driven via an asynchronous nucleophilic attack of borohydride ion on carbonyl group of indophenol. Intermediate generated is subjected to concurrent, hydroxyl ion assisted, proton abstraction followed by protonation of nucleophilic rich site on the molecule. Finally, reduction process undergoes completion by hydrolysis. Potential energy surface suggest that initial step of the reduction reaction is a rate determining step (RDS). More importantly, the synergistic effect of solvent and counter ion was observed to increase the electrophilicity of carbonyl carbon and thereby assisting in lowering energy barrier of RDS. This, in turn, enhances the reaction rate significantly.

Keywords: Indophenol; Sodium Borohydride; Reduction mechanism; DFT study; Theoretical calculations.