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Computational investigation of water as catalyst and solvent in aromatic nucleophilic substitution reaction of 2-bromopyridine

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We have computationally investigated the role of water as a catalyst and solvent in the aromatic nucleophilic substitution reaction of 2-bromopyridine with thiophenol. Water as catalyst significantly lowers the transition state energy by an amount of 5.58 kcal/mol *via* forming hydrogen bonds with reactants and the transition state. The role of water as catalyst is further studied by investigating non-covalent interactions. Results show that water forms hydrogen bonding with reactant 2-bromopyridine (-5.90 kcal/mol) and two hydrogen bonds in the transition state (7.24 and 7.95 kcal/mol) that stabilize the transition state. Reduced density gradient analysis confirms these interactions. Frontier molecular orbital analysis shows water reduces the energy gap in both reactants and transition states thus lowering the reaction's energy requirement. Additionally, the reaction's energy requirement in water is 1.25 kcal/mol lower than in non protic solvent DMSO, further confirming water's dual role as a catalyst and solvent.

Keywords: DFT studies, Nucleophilic substitution, QTAIM, RDG, FMO