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[DBU-H]+ and H_2O as effective catalyst form for 2,3-dihydro pyrido[*2,3d*]pyrimidin-4(1H)-ones: A DFT study

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DFT investigations are carried out to explore the effective catalyst forms of DBU and H_2O; and the mechanism for the formation of 2,3-dihydropyrido[2,3-*d*]-pyrimidin-4(1H)-ones. Three main pathways are disclosed under unassisted, water-catalyzed a DBU and water co-catalyzed condition, which involves concerted nucleophilic addition and H-transfer; concerted intramolecular cyclization and H-transfer; and Dimroth rearrangement to form the product. The results indicated that the DBU and water co-catalyzed pathway is the most favored one as compared to the rest two pathways. The water donates one H to DBU and accepts H from 2-amino-nicotinonitrile(1), forming $[DBU\text{-}H]^+\text{-}H_2O$ as effective catalyst form in the proton migration transition state rather than $[DBU\text{-}H]^+\cdot OH^-$. The hydrogen bond between $[DBU\text{-}H]^+\cdots H_2O\cdots 1^-$ decreases the activation barrier of the rate-determining step. Our calculated results open a new insight for the green catalyst model of DBU-H_2O.

Biography

Haiyan Yuan has completed her PhD from Northeast Normal University and continued her Postdoctoral studies in the School of Physics. Her research interest focuses on the effect of catalyst, solvent and counter ion on the organometallic and organocatalytic reactions to optimize the experimental conditions using DFT method. She has published more than 10 papers in many reputed journals.

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