

The Role of Water in Proton Transfer Reactions of Formamide and Thioformamide

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A theoretical study of the mechanism of proton transfer reactions in formamide and thioformamide is presented with focus on the characterization of the role of water in the reactions. The reaction mechanisms was analyzed with the help of energy profiles in the frame of the reaction force analysis and using the reaction electronic flux to characterize the electronic activity that takes place along the reaction. Bader's quantum theory of atoms-in-molecules is used to confirm the reaction mechanism and help elucidate the specific role of water. Results of the DFT/B3LYP 6 – 311G** level show that water-catalyze the proton transfer reaction lowering the activation energy by a factor of two.

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