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Repozytorium

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The DFT study on the reaction between benzaldehyde and 4-amine-4H-1,2,4-triazole and their derivatives as a source of stable hemiaminals and schiff bases. Effect of substitution and solvation on the reaction mechanism.

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Streszczenie

Reaction mechanism for the benzaldehyde (ald) and 4-amine-4H-1,2,4-triazole (4at) has been investigated at the DFT (B3LYP)/6–31+G(d) computational level. Three transition states (TS) have been identified. The TS1 corresponds to hydrogen transfer from the NH_2 group to the C = O bond and nucleophillic attack of the carbon atom from the aldehyde group on the nitrogen atom from the NH_2 group in 4at. The result of this reaction is the hemiaminal molecule. The TS2 characterises an internal rearrangement of the benzene and triazole rings in the hemiaminal molecule. The TS3 leads to breaking of the O-H bond, the elimination reaction of the H_2O molecule, and formation of the C=N bond. The final product of this reaction is a Schiff base. In order to determine the most favorable conditions for hemiaminal formation, the influence of electronic structure modification on the energetic p

Słowa kluczowe

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