The mechanism of the formation of the hemiaminal and Schiff base from the benzaldehyde and triazole studied by means of the topological analysis of electron localisation function and catastrophe theory.

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Streszczenie

The mechanisms of reaction of benzaldehyde (ald) with 4-amine-4H-1,2,4-triazole (4at), leading to Schiff base (Sch) and water, were investigated using topological analysis of the electron localisation function and catastrophe theory. Two reactions (synthesis of hemiaminal and synthesis of Schiff base) are represented by one catastrophe sequence: ald+4at: 1-14-[FF†F†FFTS1FF†F†FF†F†CF†]-2-9-[C†FFTS3F†F†FFF]-0:Sch+H2O with only fold (F) and cusp (C) catastrophes. The first reaction, in which a molecule of the hemiaminal is formed, consists of 14 steps separated by 13 catastrophes. The mechanism is non-concerted. The covalent bond C–N is formed after the formation of the O–H bond is terminated. The Schiff base formation through the water molecule elimination in the second reaction requires nine steps with eight catastrophes. The mechanism is non-concerted because first the C–O bond is broken and then the proton transfer occurs that results in the O–H bond creation.

Słowa kluczowe

Electron localization function (ELF), bonding, attractor, chemical bond, topology

Adres publiczny

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