

Understanding the molecular mechanism of the 1,3-dipolar cycloaddition between fulminic acid and acetylene in terms of the electron localization function and catastrophe theory.

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Streszczenie

The potential-energy profile of the 1,3-dipolar cycloaddition of fulminic acid and ethyne has been investigated theoretically within the framework provided by the electron localization function (ELF) analysis. This has been achieved by carrying out density functional theory (B3 LYP approach) calculations using the bonding evolution theory. Eight different domains of structural stability have been identified along the reaction path, as well as the bifurcation catastrophes responsible for the changes in the topology of the system. The analysis provides a chemical description of the reaction mechanism in terms of heterolytic concerted nonsynchronous bond formation: the first four catastrophes enable the simultaneous formation of the C-C bond and a lone pair on the nitrogen atom, whereas the remaining ones lead to the ring closure. The valence basin populations calculated along the reaction path do not support any mechanism involving pentavalent nitrogen. The simulation of the solvent effect, by means of a continuum model, does not indicate any significant difference of the mechanism of reaction between the gas phase and solution.

Adres publiczny

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