Quantum chemical topology description of the hydrogen transfer between the ethynyl radical and ammonia ($C_2H^{\cdot}$ + NH_3) - the electron localization function study.

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Streszczenie

The topological analysis of the Electron Localization Function (ELF) has been carried out for the hydrogen abstraction pathway
between ethynyl radical (HCC) and ammonia (NH3). The IRC path, minima (HCC HNH2, HCCH NH2) and transition structure
have been calculated at the UB3LYP/6-311++G(2d,2p) computational level. The ‘closed-shell’ and ‘spin-polarized’ formula of ELF are
used for an analysis. A detailed study of the topology of ELF (the basin population and spin density redistribution) shows that the reaction consists of three main steps distinguished on the IRC path. First, the N–H bond in ammonia is broken, then the hydrogen atom with a population of ca. 0.7 e is transferred and finally the C–H bond in acetylene is formed. It is interesting to note that all chemically important changes occur after the transition state.

Adres publiczny

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