How a quantum chemical topology analysis enables prediction of electron density transfers in chemical reactions. The degenerated cope rearrangement of semibullvalene.

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Streszczenie

Recent works on the reaction mechanism for the degenerated Cope rearrangement (DCR) of semibullvalene (SBV) in the ground state prompted us to investigate this complex rearrangement in order to assign experimentally observed contrast features in the simulated electron distribution. We present a joint use of the electron localization function (ELF) and Thom's catastrophe theory (CT) as a powerful tool to analyze the electron density transfers along the DCR. The progress of the reaction is monitored by the structural stability domains of the topology of ELF, while the change between them is controlled by turning points derived from CT. The ELF topological analysis shows that the DCR of SBV corresponds to asynchronous electron density rearrangement taking place in three consecutive stages. We show how the pictures anticipated by drawing Lewis structures of the rearrangement correlate with the experimental data and time-dependent quantum description of the process.

Słowa kluczowe

electron localization function, catastrophe theory, electronic flux, semibullvalene, cope rearrangement, Lewis structures

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