Describing the molecular mechanism of organic reactions by using topological analysis of electronic localization function.

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Here, we provide an essay on the analysis of the reaction mechanism at the molecular level; in particular, the evolution of the electron pair, as it is provided by the ELF, is used to decribe the reaction pathway. Then, the reaction mechanism is determined by the topological changes of the ELF gradient field along a series of structural stability domains. From this analysis, concepts such as bond breaking/forming processes, formation/annihilation of lone pairs and other electron pair rearrangements arise naturally along the reaction progress simply in terms of the different ways of pairing up the electrons. To visualize these results some organic reaction mechanisms (the thermal ring aperture of cyclobutene and cyclohexa-1,3-diene) have been selected, indicating both the generality and utility of this type of analysis.

Słowa kluczowe

quantum chemistry, bonding evolution theory, electronic localization function, molecular mechanism, thermal-ring aperture

Adres publiczny

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