

The joint use of catastrophe theory and electron localization function to characterize molecular mechanisms. A density functional study of the Diels-Alder reaction between ethylene and 1,3-butadiene.

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The catastrophe theory has been used to investigate the reorganization of the localization basins, within the electron localization function formalism, along the intrinsic reaction coordinate associated with the reaction pathway of the Diels–Alder reaction between ethylene and 1,3-butadiene. There are distinguished seven phases (I–VII) characterized by a decay and formation of the double bonds, an accumulation of the nonbonding electron density on the C atoms involved in the formation of two sigma bonds and a ring closure processes. During the reaction 10 catastrophes occur belonging to two elementary types: fold and cusp. The transition structure is located in phase III, being determined by a “reduction” of the double CC bond of ethylene to the single bond, and it is not associated with any special event on the intrinsic reaction coordinate path. For the first time, it is shown that formation of two new sigma C–C bonds between ethylene and 1,3-butadiene begins in phase VI at 2.044Å.

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