

Understanding reaction mechanisms in organic chemistry from catastrophe theory applied to the electron localization function topology.

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Streszczenie

Thom's catastrophe theory applied to the evolution of the topology of the electron localization function (ELF) gradient field constitutes a way to rationalize the reorganization of electron pairing and a powerful tool for the unambiguous determination of the molecular mechanisms of a given chemical reaction. The identification of the turning points connecting the ELF structural stability domains along the reaction pathway allows a rigorous characterization of the sequence of electron pair rearrangements taking place during a chemical transformation, such as multiple bond forming/breaking processes, ring closure processes, creation/annihilation of lone pairs, transformations of C–C multiple bonds into single ones. The reaction mechanism of some relevant organic reactions: Diels–Alder, 1,3-dipolar cycloaddition and Cope rearrangement are reviewed to illustrate the potential of the present approach.

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