

# A theoretical study on the reaction mechanism for the Bergman cyclization from the perspective of the electron localization function and catastrophe theory

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The reaction mechanism associated with the Bergman cyclization of the (Z)-hexa-1,5-diyne-3-ene to render p-benzyne has been analyzed by means of a combined use of the electron localization function (ELF) and the catastrophe theory on the basis of density functional theory (DFT) calculations (B3LYP/6-31G(d)). The complex electronic rearrangements of this reaction can be highlighted using this novel quantum mechanical perspective. Five domains of structural stability of the ELF occurring along the intrinsic reaction path as well as four catastrophes (fold-cusp-fold-cusp) responsible for the changes in the topology of the system have been identified. The multiple factors that occur along the intrinsic reaction coordinate path are presented and discussed in a consistent way. The topological analysis of ELF and catastrophe theory reveals that mechanical deformation of the C1-C2-C3 unit and closed-shell repulsion between terminal acetylene groups lead to an early formation of diradicaloid ch