

ELF Analysis along the C–C Bond Formation in Organic Reactions

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The electron localization function (ELF) established by A. D. Becke and K. E. Edgecombe [1] and further developed by A. Savin and B. Silvi [2] has become a powerful tool for the study of the bonding changes along an organic reaction. Recent ELF studies along Diels-Alder (DA) reactions have allowed establishing that the C–C bond formation in both non-polar and polar processes takes place by coupling of two carbons with some electron-density, which have been named *pseudoradical* centres [3,4].

A DFT study of the DA reactions between cyclopentadiene (Cp) and ethylene and tetracyanoethylene (TCE) showed that the large reactivity of the latter is a consequence of the high electrophilic character of TCE that makes the reaction to be very polar [5]. However, a recent ELF analysis of both DA reactions has shown that they present a similar C–C bond formation pattern characterized by the C-to-C coupling of two *pseudoradical* centres formed at the end of the two π reactant systems (see Figure) [3].

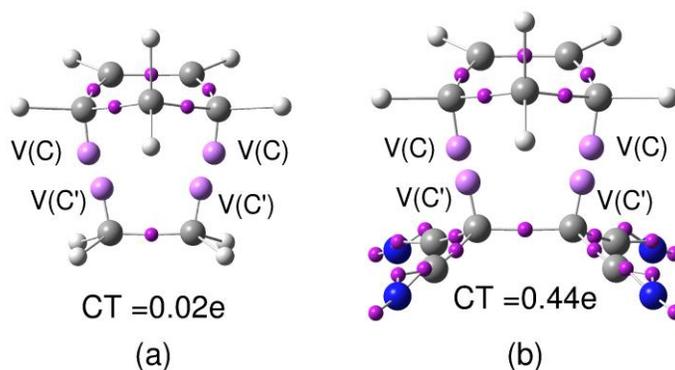


Figure 1: ELF attractors of the structures at $d(\text{C}-\text{C}) = 2.14$ and 2.08 \AA associated to the non-polar and polar DA reactions between Cp and ethylene (a) and TCE (b), respectively. The monosynaptic basins $V(\text{C})$ and $V(\text{C}')$ characterize the C and C' *pseudoradical* centres.

References

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