MECHANISTIC ELUCIDATION OF DIELS-ALDER CYCLOADDITION REACTIONS BETWEEN QUINO-FLAVONOIDE DERIVATIVES AND SUBSTITUTED BUTADIENE USING LOL, ELF, QTAIM AND DFT STUDIES.

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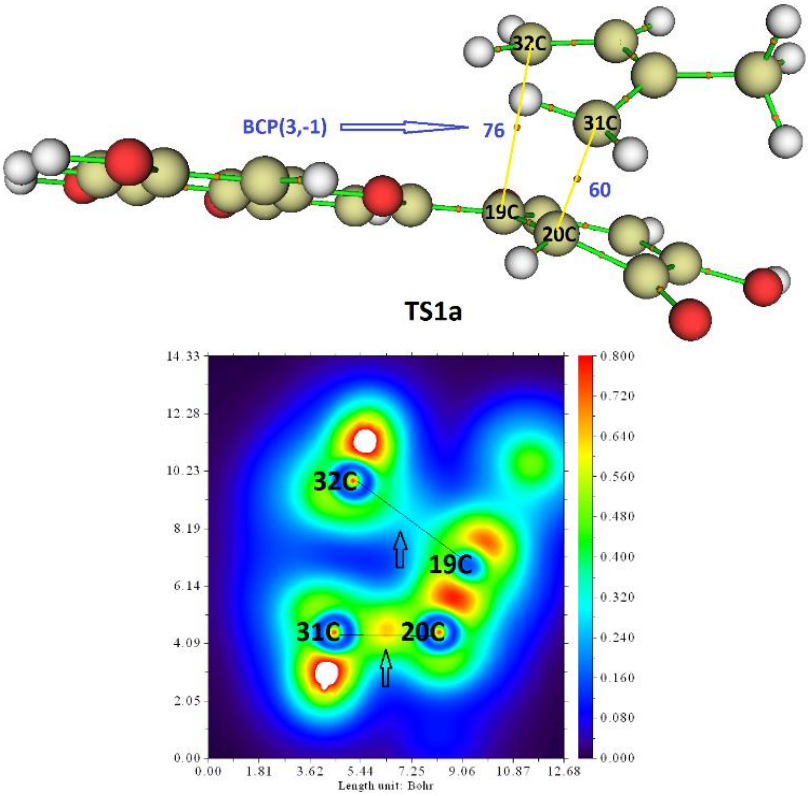
Abstract:

This study is devoted to the elucidation of the mechanism of the Diels–Alder reactions between quinoflavonoids and butadiene using DFT/B3LYP/6-311(d,p) level. The results obtained reveal that the reactions take place in a concerted mechanism via asynchronous transition states. Moreover, the low activation energies obtained for the studied reactions mean that these reactions are not energetic. The results show also that the solvent decreases significantly the activation energy barrier. The reaction 6 is not experimentally done; on the other hand, theoretically we have shown that it is possible to realize it. High values of Electron Localization Function (ELF), Localized Orbital Locator (LOL) and electron density as well as negative values of laplacian confirm the stability of the transition state structures over all for the reaction 6.



Keywords: DFT, Diels-Alder reaction, quinoflavonoids.

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