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Molecular Electron Density Theory Study on the Mechanism and Selectivity of the 1,3 Dipolar Cycloaddition Reaction of N-Methyl-C-(2-Furyl) Nitrone with Activated Alkenes

Authors : Moulay Driss Mellaoui, Abdallah Imjjad, Rachid Boutiddar, Haydar Mohammad-Salim, Nivedita Acharjee, Hassan Bourzi, Souad El Issami, Khalid Abbiche, Hanane Zejli

Abstract : We have investigated the underlying molecular processes involved in the [3+2] cycloaddition (32CA) reactions between N-methyl-C-(2-furyl) nitrone and three acetylene derivatives: 4b, 5b, and 6b. For this investigation, we utilized molecular electron density theory (MEDT) and density functional theory (DFT) methods at the B3LYP-D3/6 31G (d) computational level. These 32CA reactions, which exhibit a zwitterionic (zw-type) nature, proceed through a one-step mechanism with activation enthalpies ranging from 8.80 to 14.37 kcal mol−1 in acetonitrile and ethanol solvents. When the nitrone reacts with phenyl methyl propiolate (4b), two regioisomeric pathways lead to the formation of two products: P1,5-4b and P1,4-4b. On the other hand, when the nitrone reacts with dimethyl acetylene dicarboxylate (5b) and acetylene dicarboxylic acid (but-2-ynedioic acid) (6b), it results in the formation of a single product. Through topological analysis, we can categorize the nitrone as a zwitterionic three-atom component (TAC). Furthermore, the analysis of conceptual density functional theory (CDFT) indices classifies the 32CA reactions of the nitrone with 4b, 5b, and 6b as forward electron density flux (FEDF) reactions. The study of bond evolution theory (BET) reveals that the formation of new C-C and C-O covalent bonds does not initiate in the transition states, as the intermediate stages of these reactions display pseudoradical centers of the atoms already involved in bonding.

Keywords : 4-isoxazoline, DFT/B3LYP-D3, regioselectivity, cycloaddition reaction, MEDT, ELF
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