

[3+2] cycloaddition reaction of N-methyl-C-(2-furyl) nitron with maleimide derivatives: mechanistic study and selectivity, solvent and temperature effects

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Abstract

The [3+2] cycloaddition (32CA) reactions of N-methyl-C-(2-furyl) nitron with maleimide derivatives have been studied in gas phase, ethanol and acetonitrile solvents within the Molecular Electron Density Theory (MEDT) framework at the B3LYP-D3/6-31G(d) level. Topological analysis classifies the nitron as a zwitter-ionic (zw-) three atom component (TAC) associated with high energy barrier, while the high global electron density transfer (GEDT) decreases the requested energy cost for the rupture of the olefinic double bond of the maleimide derivatives and consequently decreases the activation barrier. Computations show that these 32CA reactions follow a one-step mechanism with highly asynchronous bond formation, while no new covalent bonds are formed at the transition states (TSs). Moreover, strongly repulsive non-covalent interactions at the endo TSs are found, presumably leading to their energetic destabilization relative to the exo ones. The predicted exo-selectivity agrees well with the experimental findings. Inclusion of solvent effects increases the activation energy, in particular for the endo TSs. Also, the influence of temperature was investigated at 289.15 K, 298.15 K and 393.15 K.

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