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The Reactivity of Addends in the 1,3-Dipolar Cycloaddition Reaction

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Abstract

The influence of donor-acceptor interactions and localisation energies on the reactivity of addends in the 1,3-dipolar cycloaddition reaction is examined. It is shown that the interactions between the symmetric frontier orbitals and between the antisymmetric frontier orbitals are qualitatively different in $(4\pi+2\pi)$ -cycloaddition reactions. The effects arising as a result of the interaction of the symmetric frontier orbitals lead to an alteration of the position of the transition state on the potential energy surface for the reaction and increase the sensitivity of the 1,3-dipolar cycloaddition reactions to localisation effects. The bibliography includes 113 references.
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