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Prediction of the Regioselectivity of 1,3-Dipolar Cycloaddition Reactions of Nitrile Oxides with 2(5H)-Furanones Using Recent Theoretical Reactivity Indices

Authors : Imad Eddine Charif, Wafaa Benchouk, Sidi Mohamed Mekelleche

Abstract : The regioselectivity of a series of 16 1,3-dipolar cycloaddition reactions of nitrile oxides with 2(5H)-furanones has been analysed by means of global and local electrophilic and nucleophilic reactivity indices using density functional theory at the B3LYP level together with the 6-31G(d) basis set. The local electrophilicity and nucleophilicity indices, based on Fukui and Parr functions, have been calculated for the terminal sites, namely the C1 and O3 atoms of the 1,3-dipole and the C4 and C5 atoms of the dipolarophile. These local indices were calculated using both Mulliken and natural charges and spin densities. The results obtained show that the C5 atom of the 2(5H)-furanones is the most electrophilic site whereas the O3 atom of the nitrile oxides is the most nucleophilic centre. It turns out that the experimental regioselectivity is correctly reproduced, indicating that both Fukui- and Parr-based indices are efficient tools for the prediction of the regiochemistry of the studied reactions and could be used for the prediction of newly designed reactions of the same kind.

Keywords : 1,3-dipolar cycloaddition, density functional theory, nitrile oxides, regioselectivity, reactivity indices
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