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Investigation of the Mechanism, Régio and Sterioselectivity Using the 1,3-Dipolar Cycloaddition Reaction of Fused 1h-Pyrrole-2,3-Diones with Nitrones: Molecular Electron Density Theory Study

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Abstract : Molecular Electron Density Theory (MEDT) elucidates the regioselectivity of the [4+2] cycloaddition reaction between 3-aroylpyrrolo[1,2-α]quinoxaline-1,2,4(5H)-trione and butyl vinyl ether Regioselectivity and stereoselectivity. The regioselectivity mechanisms of these reactions were investigated by evaluating potential energy surfaces calculated for cycloaddition processes and DFT density-based reactivity indices. These methods have been successfully applied to predict preferred regioisomers for different method alternatives. Reactions were monitored by performing transition state optimizations, calculations of intrinsic reaction coordinates, and activation energies. The observed regioselectivity was rationalized using DFT-based reactivity descriptors such as the Parr function. Solvent effects were also investigated in 1,4-dioxane solvent using a field model for self-consistent reactions. The results were compared with experimental data to find good agreement.

Keywords : cycloaddition, DFT, ELF, MEDT, parr, stereoselectivité
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