The effect of the carbonyl moiety on the spin density delocalization in the iminoxy radicals. Hybrid density functional studies.

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Streszczenie

UB1LYP method was used to study the influence of carbonyl group in 1,2-diphenyl-1-oxoethan-2-iminoxyl and 1-oxoethan-2-iminoxyl, on radical structure and unpaired electron spin density distribution. A significant change of radical properties was found due to the second carbonyl group in 2,4-dioxopenthan-3-iminoxyl and 1,3-dioxopropan-2-iminoxyl. A specific impact of the carbonyl groups on the EPR hyperfine couplings with and nuclei (calculated at UB1LYP/EPR-III level in comparison with the experimental data) was determined for the stable isomeric forms of the radicals.

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