

α -tocopherol impact on oxy-radical induced free radical decomposition of DMSO : spin trapping EPR and theoretical studies.

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Streszczenie

EPR spin trapping and theoretical methods such as density functional theory (DFT) as well as combined DFT and quadratic configuration interaction approach (DFT/QCISD) were used to identify the radicals produced in the reaction of oxy-radicals and dimethyl sulfoxide (DMSO) in the presence and absence of α -tocopherol. Additionally, the mixtures of α -tocopherol with linolenic acid and glyceryl trilinoleate as well as bioglycerols (glycerol fractions from biodiesel production) were tested. α -Tocopherol inhibited oxidation of the main decomposition product of DMSO, $\bullet\text{CH}_3$ to $\bullet\text{OCH}_3$ but did not prevent the transformation process of *N-t*-butyl- α -phenylnitron (PBN) into 2-methyl-2-nitrosopropane (MNP). Theoretical investigations confirmed the structures of proposed spin adducts and allowed to correlate the EPR parameters observed in the experiment with the spin adducts electronic structure.

Słowa kluczowe

EPR, DFT, QCISD, Spin trapping, PBN, α -Tocopherol, DMSO

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