

Free-radical chain oxidation of 1,4-dioxane inhibited by 2,3-dihydro-2-thioxo-4(1H)-pyrimidinone

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Abstract

In the model chain radical oxidation of 1,4-dioxane was studied the antioxidant properties of 2,3-dihydro-2-thioxo-4(1H)-pyrimidinone (TU) and 6-amino-2,3-dihydro-2-thioxo-4(1H)-pyrimidinone (TAU). Oxidation was carried out with air oxygen, water soluble 2,2'-azobis(2-methylpropionamide) dihydrochloride was used as an initiator. The effect of water presence on the antioxidant activity of TU and TAU is considered. The reaction kinetic was monitored on the rate of oxygen uptake using a universal manometric differential setup. It was shown that both compounds inhibit the radical chain oxidation of 1,4-dioxane. In a system containing water for TAU was measured rate constant of interaction with the 1,4-dioxane peroxy radical $k_7 = (8.9 \pm 1.3) \cdot 10^4 \text{ l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$. The obtained result is lower than the rate constant measured in the absence of water. It is suggested that a decrease in the reactivity of 6-amino-2,3-dihydro-2-thioxo-4(1H)-pyrimidinone perhaps due to the formation of intermolecular hydrogen bonds. It was measured the stoichiometric inhibition coefficient for 6-amino-2,3-dihydro-2-thioxo-4(1H)-pyrimidinone: $f = (0.6 \pm 0.1)$. In the system containing 1,4-dioxane and water, the effective antioxidant activity of the TU was estimated: $f k_7 \approx 1.4 \cdot 10^4 \text{ l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$. It was found that the presence of a sulfur atom and an amino group at the 6-position of molecule increases the antioxidant activity of the compound.

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