

## The quantitative analysis of the antioxidants antiradical activity on the example the initiated radical-chain 1,4-dioxane oxidation model reaction

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### Abstract

In the present work on the example the radical-chain inhibited organic compound oxidation are shown methods for finding quantitative parameters characterizing the antioxidant. These parameters are the reaction rate constant of the peroxy radical with the inhibitor ( $k_7$ ) and the stoichiometric inhibition factor ( $f$ ). Examples are given the mathematical analysis of the experimental kinetic oxygen absorption curve obtained during the initiated radical chain oxidation of 1,4-dioxane. To determine the rate constant ( $k_7$ ) of the peroxy radical with the inhibitor molecule were used following methods: experimental (semi-logarithmic method the kinetic curve processing, method kinetic curve transformation, determining the effective reaction rate constant of the peroxy radical with the inhibitor on the initial oxidation rate) and theoretically using the intersecting-parabolas method.

The important inhibitor characteristic is the stoichiometric inhibition factor ( $f$ ). The parameter is numerically equal to the number of peroxy radicals interacting with one inhibitor molecule. To determine  $f$ , it is necessary to measure the induction period and use the equation  $f = \tau \cdot W_i / [InH]$ . Here  $\tau$  is the induction period. To determine  $\tau$  can be applied the method of tangents to the kinetic curve. It is often difficult to determine the initial rate of inhibited oxidation. In this case, for measuring  $\tau$  it is suitable to use the integral method, as well as graphical method, when  $\tau$  is the point of intersection of two tangents, 0.5 and 0.75 to the slope angle of the oxygen absorption kinetic after inhibited oxidation. Also, the assessment of  $f$  can be carried out using the method kinetic curve transformation.

The article shows that the methods for determining  $k_7$ ) and  $\tau$  are in good agreement with each other.

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