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Analysis of the mechanism of radical chain oxidation of ethylbenzene in the presence of additive of*N*-2-ethylhexyl-*N'*-phenyl-*p*-phenylenediamine

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Abstract

A primary consideration of modern production in chemistry, medicine and the food industry is preventing unwanted oxidation processes. Currently, the quantitative characteristic of the antioxidant activity of potential antioxidant is the value of the inhibition rate constants, whose definition is available by known methods of chemical kinetics. To select an effective inhibitor of oxidative processes, it is necessary to define the optimum conditions of its validity and maximum braking, that it can provide in the process that becomes possible only after establishing the mechanism of its action. It is not sufficient for the application of methods of physical-chemical experiment for an explanation of the mechanism of action of antioxidants, because the process that inhibited by oxidation includes a large number of stages involving intermediate particles-atoms and radicals concentration and lifetime of them is extremely small. A necessary component that allows us to solve this complex problem is mathematical modeling of mechanism of action of compounds based on the available experimental results.

Therefore, the aim of this work was the study of the mechanism of antioxidant action of *N*-2-ethylhexyl-*N'*-phenyl-*p*-phenylenediamine (Novantoks, 8-PFDA) reactions initiated by the oxidation of ethylbenzene by using mathematical modeling. To achieve this goal, was used the program complex "HimKinOptima" and the obtained previously experimental data. By solving the inverse problem of chemical kinetics was restored everything, including previously unknown, key rate constants of the elementary stages. By solving the direct problem of chemical kinetics was received full kinetic painting of all the reaction participants, including unstable intermediates. It is shown that the presence of impurities of alcohol in the starter compound leads to an increase in its antiradical action at the expense of regeneration reaction inhibitor in the act of truncating the chain with the participation of peroxy radicals.

The reliability of research results obtained in theory ensured the correctness of computer modeling methods used in accordance with the established objectives and ensures a satisfactory settlement and coincidence experimental significance of quantitative parameters.

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