

MICELLAR SYSTEM THE DECONTAMINATION OF ACTIVE PHARMACEUTICAL INGREDIENTS AND PESTICIDES OF ORGANOPHOSPHORUS NATURE

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Introduction. Protecting the environment and population from the negative effects of toxic substances such as organophosphorus compounds is, at present, an important task for the government as a whole and for managers of chemical and pharmaceutical companies. Therefore, the development of this direction is important for any chemical production [1–3].

Aim. Development micellar system degradation of active pharmaceutical ingredients (APIs) and pesticides of organophosphorus nature.

Methods. QSAR analysis, kinetic studies of nanostructured model decontamination systems of organophosphorus compounds [4–6].

Results. Kinetic spectrophotometric study of the model of nanostructure systems the decontamination of organophosphorus compounds implemented.

Initial aqueous solutions prepared by on the basis cetylpyridinium chloride (CPC), KOH, H₂O₂, pH of the solution - 12; model substance - metylparation.

The volume of the sample of kinetic solution made 1515 μl, in which the volume of methylparathion was 15 μl. Kinetic solutions were prepared by pouring working solutions. During the study, a comparison of rates of the reaction of alkaline and peroxide hydrolysis of methylparathion in micellar medium of CPC was conducted. In addition, reactions using the activator of peroxyanion B(OH)₃, were studied. The measurement of optical density of 4-nitrophenol, formed during

the reaction, was conducted by spectrophotometry at wavelength 400 nm; during measurement, temperature of the solution was 25 ± 0.1 °C.

Constants of rates of first-order reactions were calculated by formula (1):

$$k_H^1 = \frac{1}{t} \cdot \ln \frac{D_\infty - D_0}{D_\infty - D_t}, \quad (1)$$

where t is the time of reaction; D_∞ is the value of optical density after the end of the reaction; D_t is the value of optical density at a certain moment of time; D_0 is the value of optical density at the beginning of the reaction.

$$k_H^2 = \frac{k_H^1}{[H_2O_2]_0} = \frac{k_B^2 + (k_m^2 / V) K_S K_{HOO^-} D_n}{(1 + K_S D_n)(1 + K_{HOO^-} D_n)}, \quad (2)$$

where K_{HOO^-} and K_S are the constants of micellar binding by peroxyanion and substrate; $[H_2O_2]$ is the concentration of solution of hydrogen peroxide; k_H^1 is the constant of rate of the first-order reactions; V is the molar volume of SAS; k_B^2 is the constant of rate of the second-order reactions for aqueous solution; D_n is the concentration of SAS at a moment of time, $D_n = [SAS] - CCM$ (critical concentration of micellar formation).

Peroxoanions are mostly active at values of $pH \leq 9$. For successful flow of nucleophilic reactions involving HOO^- ion, one should use more alkaline media. This is due to the fact that the constant of ionization of hydrogen peroxide has the value of $pK_a = 11.6$. Thus, at $pH \leq 9.0$ only 0.03–0.3% of hydrogen peroxide is located in the ionic reactive form HOO^- .

Conversion of methyparathion in solution $H_2O_2 - HO^-$ in all the studied media occurs mainly in two ways: perhydrolysis with generated HOO^- - anion ($H_2O_2 + HO^- \rightarrow H_2O + HOO^-$) and alkaline hydrolysis with the help of HO^- - anions (Fig. 1).

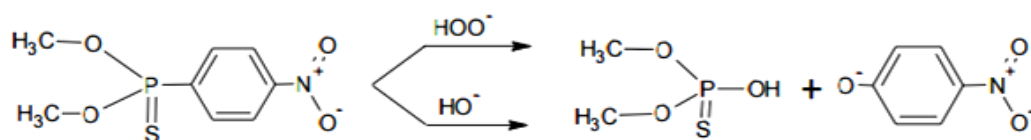
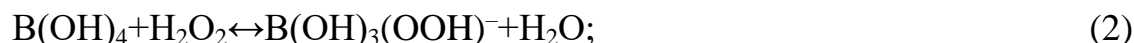


Fig. 1. Chemical scheme of converting methylparathion into $\text{H}_2\text{O}_2\text{--HO}^-$ solution.

In this case, contribution of alkaline hydrolysis is minimal and does not exceed 1–5 % of the total rate of substrate decomposition [7].

Hydrogen peroxide in micellar systems in a neutral form is known to be a weak oxidizing agent. Therefore, it is activated using hydrocarbonates, molybdates, phthalates, nitrites and other compounds that form highly active peroxyacids in the reaction with H_2O_2 [8].

Boric acid ($\text{B}(\text{OH})_3$) may serve a perspective activator, which during the interaction with hydrogen peroxide forms perborates:



To determine the optimal detergent concentration, at which the rate of reaction of hydrolysis of methylparathion under conditions of micellar catalysis is the highest, the study of dependences of values of rate constants of first-order reactions on the concentration of OPC was carried out.

Determined mean values of rate constants of second-order reaction k_H^2 for the studied systems of inactivation of methylparathion made: for decontamination

systems CPC/H₂O₂/H₂O – 0.07 M⁻¹·s⁻¹, for decontamination systems B(OH)₃/CPC/H₂O₂/H₂O – 0.17 M⁻¹·s⁻¹, respectively.

Data on the performed study show that progress of the reaction occurs much faster when adding boric acid as an activator. Therefore, it is possible to propose the presented decontamination system as a model of cleaning solution with the following composition: cetylpyridine chloride, H₂O₂, water, boric acid, pH=12 (KOH).

Toxicological parameters of developed system studied *in silico*.

The results of endotoxicity calculation suggest that the components of the basic reaction media for decontamination of organophosphorus pesticides and APIs are of low toxicity.

Conclusions. Micellar system the decontamination of organophosphorus APIs and pesticides on the basis CPC, hydrogen peroxide, KOH and boric acid are highly effective in terms of reaction rate and low toxicity.

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