

Thematic course: Quantum-chemical calculations of some of elementary reactions of the acid-catalytic decomposition of cumene hydroperoxide. Part 1.

## Protonization of hydroperoxide

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### Abstract

The acid-catalytic decomposition of cumene hydroperoxide proceeds with a high velocity through the successive formation of intermediates, which is difficult to be detected by physical methods. The quantum-chemical study of the process allowed to establish the presence of different stable conformations of cumene hydroperoxide, characterized by different mechanisms of their transformation. In the present paper we propose the possibility of protonization on both atoms (alkoxyl and hydroxyl) of oxygen hydroperoxide of different conformations. We found out that on protonization of hydroxyl oxygen of hydroperoxide dehydration is accompanied by the simultaneous rearrangement of the oxonium ion into the carbonium ion, which then interacts with the second molecule of hydroperoxide to form an intermediate complex decomposing to phenol, acetone and carbonium ion. In the case of protonization of alkoxyl oxygen atom, hydrogen peroxide splits off to form carbocation, which is converted to  $\alpha$ -methylstyrene or dimethylphenylcarbinol.