

EFFECT OF REACTION DURATION ON ISOPROPANOL PRODUCT

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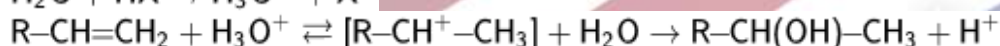
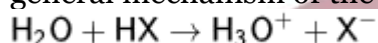
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Today, the synthesis of import-substituting organic compounds from the available resources in the country, on the basis of which the creation of solvents, disinfectants (antiseptics), antibiotics, stabilizers, fragrances in cosmetic products is an urgent task.

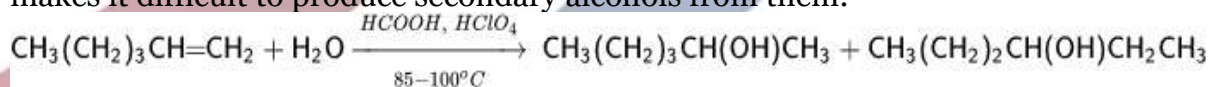
Saturated alcohols containing C₃-C₅ are used in various industries as solvents, disinfectants, antibiotics, stabilizers, fragrances in cosmetic products and as additives in perfumery.

Acid hydration of alkenes is one of the first classical methods for the production of alcohols. The general mechanism of the process is given below [1]:

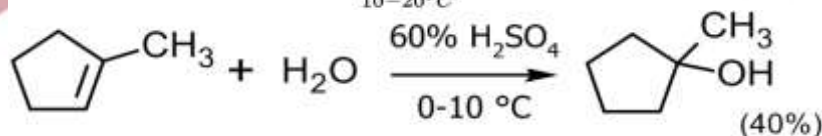
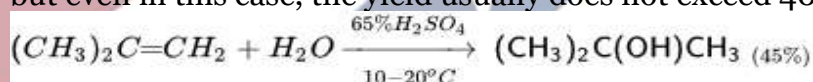


The merger will take place according to Markovnikov's rule. If sulfuric acid is used as a catalyst, sulfuric acid ester (R-CH (OSO₂OH) -CH₃) is formed as an intermediate product, which is completely hydrolyzed to alcohol under reaction conditions [2].

Other reagents for the reaction other than sulfuric acid are used: a mixture of formic acid and a catalytic amount of sulfuric acid (in some cases allows to achieve stereospecificity), a mixture of formic acid and hydrochloric acid, triforic acid and others. The reactions of secondary alkenes often lead to the formation of a mixture of products due to the rearrangement of carbocations, which makes it difficult to produce secondary alcohols from them:

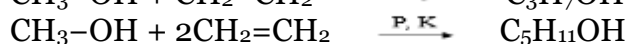
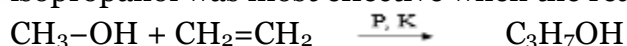


In laboratory practice, the ability to separate the product mixture is also limited by the acid hydration method due to the low yield. Most often, this method is used to produce tertiary alcohols, but even in this case, the yield usually does not exceed 40-45% [3]:



Issues such as the synthesis of saturated alcohols with C₃-C₅ content on the basis of ethylene and methyl alcohol, calculated from the available resources in the country, the definition of technological parameters of the process, the development of effective methods to increase product productivity are relevant.

The synthesis process was carried out in a high-pressure resistant hermetic reactor. Methyl alcohol and ethylene gas were used as starting materials. In the process, methyl alcohol acts as a telogen and ethylene as a monomer. The synthesis of isopropanol was carried out under different conditions, with a temperature of 40 ° C, a pressure of 10 atm and a reaction time of 2-6 hours. The release of isopropanol was most effective when the reaction time and product yield were 4 hours.



Table

The effect of reaction duration on product yield

No	Pressure	Temperature, °C	Reaction duration, hours	Isopropanol, %
1	10	40	2	5,2
2			3	8,0
3			4	13,7
4			5	11,1
5			6	9,9

In the IR spectrum of isopropanol, hydrogen bonding of the hydroxyl group was observed in the area of intensive bond signal 3333 cm^{-1} and deformation vibration signal of carbon-bonded hydroxyl group (C-OH) was observed in the area of 950 cm^{-1} . Asymmetric deformation oscillations of carbon and hydrogen with high intensity in the area of 1460 cm^{-1} , symmetrical deformation vibration signal in the area of 1376 cm^{-1} ; asymmetric valence oscillations of the methyl (CH₃) group were observed in the 2960 cm^{-1} area and asymmetric deformation oscillations were observed in the 1460 cm^{-1} area. Asymmetric valence oscillations of carbon and hydrogen with high intensity were observed in the area $2932\text{-}2960\text{ cm}^{-1}$, symmetric valence oscillation signal was observed in the area 2883 cm^{-1} .

References

1. Baylis-Hillman Reaction (англ.). Name Reactions. Organic Chemistry Portal. Дата обращения 23 сентября 2009. Архивировано 21 августа 2011 года.
2. Ho C.R.; Shylesh S.; Bell A.T. Mechanism and Kinetics of Ethanol Coupling to Butanol over Hydroxyapatite. ACS Catal. 2016, 6, 939-948.
3. Smith A.C. Morita Baylis Hillman Reaction (англ.). New Methodology and Synthesis of Natural Product. The University of North Carolina at Chapel Hill. Дата обращения 23 сентября 2009. Архивировано 23 апреля 2012 года.