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RESEARCH ON THE CHEMICAL PROPERTIES OF THE THREE-BAND AND HYDROXYL GROUP IN THE MOLECULES OF ACETYLENE SPIRITS, THEIR SPECIFICITY, AND THEIR APPLICATIONS

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Abstract
In this article, copper-bismuth-nickel-kaolin (MVNK), copper-bismuth-cobalt-kaolin (MVKK), copper-bismuth-nickel-bentonite (MVNB), copper-bismuth- cobalt-bentonite (MVKB), copper-bismuth-nickel-zeolite (MVNS), copper-bismuth-cobalt-zeolite (MVKS), copper-bismuth-nickel-silica gel (MVNS) and copper-bismuth-cobalt-silica gel (MVKS) synthesis of 2-phenyl-3-butyn-2-ol was studied in the presence of catalysts. Also, the influence of the nature of catalysts, temperature, and the mole ratio of starting materials on product yield was determined. An alternative process condition has been found.

Keywords: acetylene, acetophenone, 2-phenyl-3-butyn-2-ol, heterogeneous-catalytic, catalyst

Introduction

ASETILEN SPIRTLARI MOLEKULASIDA UCH BOG’ VA GIDROKSIL GURUHINING KIMYOVIY XOSSALARINI O’ZIGA XOSLIGI VA QO’LLANILISH SOHALARINI TADQIQ QILISH.

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Annotatsiya

Ushbu maqolada atsetilenning atsetofenon bilan ta'sirlashuvi natijasida geterogen-katalitik usulda mis-vismut-nekil-kaolin (MVNK), mis-vismut-kobalt-kaolin (MVKK), mis-vismut-nekil-bentonit (MVNB), mis-vismut-kobalt-bentonit (MVKB), mis-vismut-nekil-seolit (MVNS), mis-vismut-kobalt-seolit (MVKS), mis-vismut-nekil-silikagel (MVNS) va mis-vismut-kobalt-silikagel (MVKS) katalizatorlari ishtirokida 2-fenil-3-butin-2-ol sintezi o'rganilgan. Shuningdek mahsulot unumiga katalizatorlar tabiati, harorat, boshlang'ich moddalarni mol nisbatining , ta'siri aniqlangan. Jarayonning muqobil sharoiti topilgan.

Kalit so'zlar: atsetilen, atsetofenon, 2-fenil-3-butin-2-ol, geterogen-katalitik, katalizator

ИССЛЕДОВАНИЕ ХИМИЧЕСКИХ СВОЙСТВ ТРЕХСВЯЗИ И ГИДРОКСИЛЬНОЙ ГРУППЫ В МОЛЕКУЛЕ АЦЕТИЛЕНОВЫХ СПИРТОВ И ОСОБЕННОСТИ И ОБЛАСТИ ИХ ПРИМЕНЕНИЯ.

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Аннотация

В данной статье рассмотрены медно-висмут-никель-каолин (МВНК), медно-висмут-кобальт-каолин (МВКК), медно-висмут-никель-бентонит (МВНБ), медно-висмут-кобальт-бентонит (МВКБ), медно-висмут-кобальт-бентонит. висмут-никель-цеолит (МВНС), медь-висмут-кобальт-цеолит (МВКС), медь-висмут-никель-силикагель (МВНС) и медно-висмут-кобальт-силикагель (МВКС) синтез 2-фенил-3 -бутин-2-ол исследовали в присутствии катализаторов. Также определяли влияние природы катализаторов, температуры и мольного соотношения исходных материалов на выход продукта. Найдено альтернативное условие процесса.

Ключевые слова: ацетилен, ацетофенон, 2-фенилбутин-3-ола-2, гетерогенно-каталитический, катализатор.

Currently, fundamental changes have occurred in the use of primary raw materials for the synthesis of organic substances and the industrial production of some of them. While plants, animals, and coke industry products were initially used as such raw materials, oil and natural gas, which are currently inexpensive and possess very large reserves, are now primarily used. A large number of organic compounds have been synthesized based on the hydrocarbons contained in these raw materials and their derivatives, and a number of such substances are also produced on an industrial scale [1]. Acetylene and its derivatives possess high reactivity, allowing for the implementation of various chemical transformations based on them. The presence of a triple bond and a hydroxyl group in the acetylene alcohol molecule ensures the uniqueness of their chemical properties and further expands the field of application [2, 3, 4, 8]. There are organic compounds that can only be synthesized from acetylene or its homologs. In recent years, the industrial production of various chemical products based on acetylene hydrocarbons has been carried out, namely various monomers, plastics, rubbers, synthetic fibers, organic solvents, pesticides, medicinal substances, reagents used for military purposes, corrosion inhibitors, and others. In the future, a further increase in the variety and quantity of such products is expected [5,6,7,9,10]. In the chemistry of acetylene compounds, new methods are being developed for reactions involving the formation of various hetero- and carbo compounds and the formation of a -C≡C bond as a result of the addition of various nucleophiles to its molecule. In particular, the reaction of acetylene and various carbonyl compounds, the formation of acetylene alcohols with the preservation of a new -C≡S- bond is of particular practical importance. The synthesis of acetylene alcohols and vinyl derivatives based on them by the heterogeneous-catalytic method, the creation and application of various selectively acting catalysts in these processes, is one of the urgent tasks of the chemistry of acetylene compounds.

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Methods and Materials

100 g of MVNK-5 for the process and the peptizer NNO3-NH4OH-methylcellulose catalyst are placed in the reactor. Refined acetylene gas is supplied to the reactor from the tap, and the catalyst pores are saturated. During the synthesis of 2-phenyl-3-butyne-2-ol, acetylene is supplied to the reactor at a temperature of 30-35 °C for 4 hours to activate the catalyst. After increasing the catalyst activity, 250 ml of acetophenone is administered dropwise. The reaction was carried out at 90 °C. The reactor is heated by an electric heater and controlled using a temperature regulator. The mixture of substances and gases formed as a result of the reaction is passed through the cooler through the outlet of the reactor and removed from the reaction medium. The synthesized substance (diethyl ether) is extracted in an absorber. The reaction mixture is dried with Na2SO4 and extracted 3-4 times with diethyl ether. The obtained catalyst is separated into fractions in a rectification unit.
The reliability of the research results was proven using modern analytical methods for the composition and structure of the synthesized substances: thin-layer chromatography (TLC), gas-liquid (GLC "CHROM 5"), elemental analysis (WDX400), PMR ("100 MHz"), and IR ("SF-4A") spectroscopic methods.

Results and Discussion

2-phenyl-3-butyne-2-ol, synthesized based on acetophenone and acetylene, contains three highly reactive functional groups. The presence of an unsaturated acetylene bond (triple bond), a mobile hydrogen of acetylene, and a hydroxyl group further expands the applications of 2-phenyl-3-butyne-2-ol in many sectors of the economy. 2-phenyl-3-butyne-2-ol and its derivatives are used in the production of metal corrosion inhibitors, herbicides, fungicides, and antiseptics.
The nature and quantity of catalysts used in the synthesis of 2-phenyl-3-butyne-2-ol depend on the nature of the core, the properties of the peptizers, and the rate of acetylene release into the reaction medium. The mechanism of 2-phenyl-3-butyne-2-ol formation in the presence of heterogeneous catalysts using acetylene and acetophenone generally proceeds as follows:

$$HC\equiv CH + CuO \longrightarrow HC\equiv \underset{\vdots \atop CuO}{\overset{\sigma^-}{C}} - \overset{\sigma^+}{H}$$

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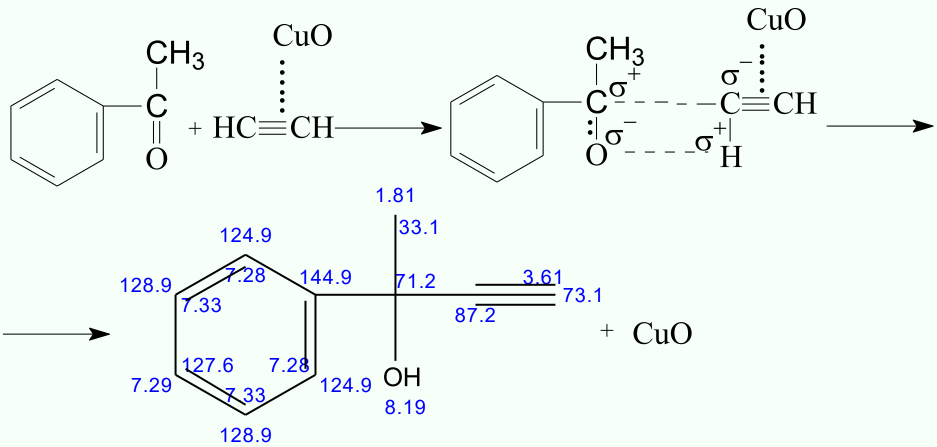

2-фенилбутин-3-ол-2

The synthesis of 2-phenyl-3-butyne-2-ol by the heterogeneous-catalytic method was carried out at a pressure of 0.3 MPa in the presence of copper-bismuth-necyl-kaolin (MBNK), copper-bismuth-cobalt-kaolin (MBKK), copper-bismuth-necyl-bentonite (MBNB), copper-bismuth-cobalt-bentonite (MBKB), copper-bismuth-necyl-zeolite (MBNS), copper-bismuth-cobalt-zeolite (MBKS), copper-bismuth-necyl-silica gel (MBNS), and copper-bismuth-cobalt-silica gel (MBKS) catalysts prepared using various peptizers. The experimental results are presented in Table 1.

Table 1.Influence of the nature of the catalyst and peptizers on the yield of 2-phenyl-3-butyne-2-ol formation (temperature 90 °C, pressure 0.3 MPa)

Catalyst	Peptizer	2-phenyl-3-butin-2-ol yield, %
MNK-5	NNO_3-NH_4OH-$[C_6H_7O_2(OH)_{3-x}(OCH_3)_x]_n$	58,0
MNK-5	NNO_3-NH_4OH-SN_3SOON	56,4
MNK-5	NNO_3-NH_4OH-$(\text{-}CH_2\text{—}CR'(COOR)\text{-})_n$	55,8
MVK-5	NNO_3-NH_4OH-$[C_6H_7O_2(OH)_{3-x}(OCH_3)_x]_n$	59,9
MVK-5	NNO_3-NH_4OH-SN_3SOON	58,5
MVK-5	NNO_3-NH_4OH-$(\text{-}CH_2\text{—}CR'(COOR)\text{-})_n$	57,4
MVNK-5	NNO_3-NH_4OH-$[C_6H_7O_2(OH)_{3-x}(OCH_3)_x]_n$	71,3
MVNK-5	NNO_3-NH_4OH-SN_3SOON	69,8
MVNK-5	NNO_3-NH_4OH-$(\text{-}CH_2\text{—}CR'(COOR)\text{-})_n$	69,2

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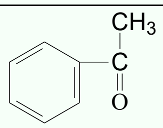
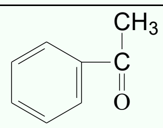
According to the results of the conducted research, it was established that the product yield is higher when MVNK-5 is used as a catalyst and the peptizer is NNO_3-NH_4OH-methylcellulose. When kaolin is used as a core, the active surface area of the catalyst is large, and the total porosity and strength are high. The product yield increases proportionally to the amount of copper oxide (40%) in the catalyst.

The yield of the synthesized 2-phenyl-3-butyne-2-ol is also significantly influenced by the molar ratios of the starting materials acetylene and acetophenone. The experimental results obtained on its basis are presented in Table 2.

Table 2.Influence of the molar ratio of acetylene and acetofenone on the yield of 2-phenyl-3-butyne-2-ol formation (temperature 90 °C, pressure 0.3 MPa).

C_2H_2 (mol)	 **(mol)**	**2-fenil-3-butin--2-ol, %**	**C_2H_2 (mol)**	 **(mol)**	**2-fenil-3-butin-2-ol, %**
1	1	58,2	1	2	50,8
2	1	60,6	1	3	51,2
3	1	64,0	1	4	51,7
4	1	66,9	1	5	52,3
5	1	69,5	1	6	52,9
6	1	71,3	1	7	53,8
7	1	68,4	1	8	53,3

From the analysis of the results obtained, it is known that the formation of 2-phenyl-3-butyne-2-ol occurs mainly at an acetylene:acetophenone ratio of 1:1 (58.2%) and a 6:1 ratio, with the maximum product yield (71.3%).

The yield of 2-phenyl-3-butyne-2-ol also depends on temperature. It is necessary to fully regulate the temperature within a specific temperature range. Otherwise, the formation of diols is accelerated. 2-phenyl-3-butyne-2-ol and, in general, some acetylene alcohols have an asymmetrical structure, which increases their reactivity with increasing temperature. As a result, the yield of acetylene diols increases.

Figure 3 shows the temperature dependence of the yield of 2-phenyl-3-butyne-2-ol formation. As can be seen from the figure, the yield of 2-phenyl-3-butyne-2-ol increases with increasing temperature to 80-90 °C, and then begins to decrease. This is primarily explained by the formation of acetylene diols or the formation of oligomers and polymers.

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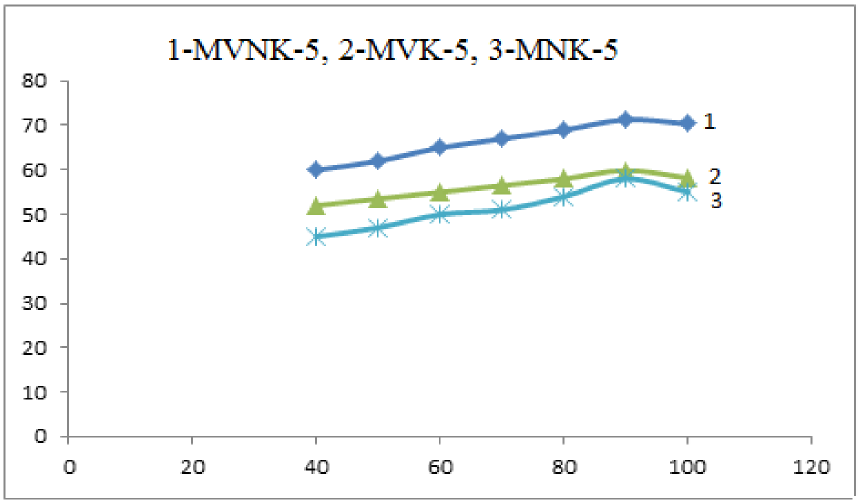
Product yield, %



Temperature ^{0}C

Figure 3. Dependence of product yield on the nature of the catalyst and temperature

The product yield also depends on the nature of the catalyst. When the MVNK-5 catalyst is used in the process, the product is formed with a high yield. It was established that the optimal temperature for the synthesis of 2-phenyl-3-butyne-2-ol is 90 °C, and the product yield is 71.3%.

The IR spectrum of the synthesized compound 2-phenyl-3-butyne-2-ol was obtained. In the IR spectrum, there is absorption when the valence oscillations (CH) of the methyl group are 968 cm^{-1}. The deformation vibrations of the hydroxyl group (OH) were observed at 3600 cm^{-1}, the absorption of aromatic ring (CH) bonds at 700–860 cm^{-1}, and for the -C≡CH group (C≡S) at 2120 cm^{-1}.

Results of ^{1}H nuclear magnetic resonance spectroscopy (YMR) of 2-phenyl-3-butyne-2-ol showed that protons in the aromatic ring are 7.33, 7.29, 7.28 ppm,

CH_3 (3N) -1.81 ppm,

-C≡CH (1H) was observed at 3.61 ppm, and OH (1H) at 8.19 ppm.

Based on the research results, the molecular weight of the obtained 2-phenyl-3-butyne-2-ol was 146.1 g/mol, and elemental analysis yielded the following results: C-82.90%; H - 6.88%; O-10.0%. The theoretically calculated elemental composition is as follows: C-82.89%; H - 6.89%; 0.1%.

Conclusion

Optimal conditions for the process of synthesizing 2-phenyl-3-butyne-2-ol based on acetophenone and acetylene by the heterogeneous-catalytic method have been found.

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When using the MVNK-5 catalyst in the process, at a temperature of 90 °C and a molar ratio of acetylene and acetophenone of 6:1, the product is formed with a higher yield of 71.3%.

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