International Journal of Scientific Trends- (IJST)
ISSN: 2980-4299
Volume 3, Issue 12, December - 2024
Website: https://scientifictrends.org/index.php/ijst
Open Access, Peer Reviewed, Scientific Journal

Ethylene Telomerization Reaction with Alcohols Chromatographic Mass Spectrometry Analysis of The Product

Khudayberganova Sevara Zokirjonovna
Tashkent State Technical University, Senior Lecturer

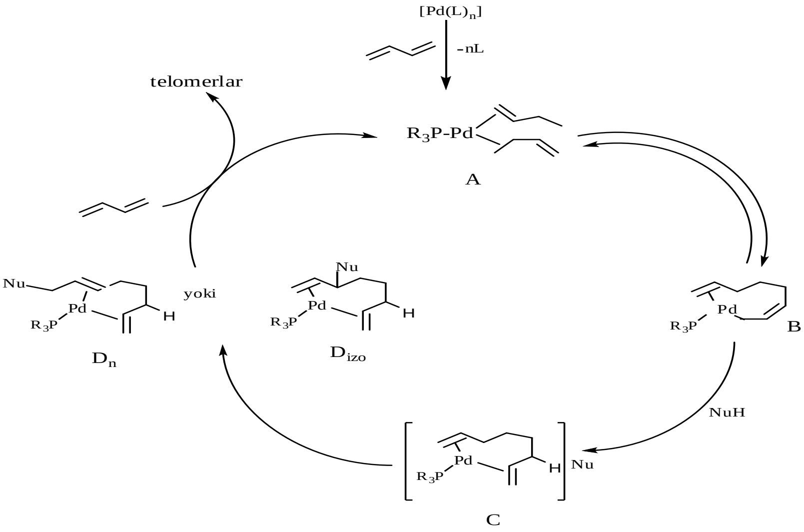
Abstract

Scientific research is being conducted worldwide to improve the quality of substances synthesized through the processing of oil and natural gas, create new technologies that meet environmental requirements, and modernize existing technologies. Nowadays, it is of significant importance to develop new and efficient methods for the production of various chemicals using oil and gas products, as well as secondary raw materials obtained from their processing, and to create modern equipment for these processes.

Keywords: Ethylene, methanol, acetone, radical, telomer, telogen.

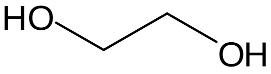
Introduction

In our country, through the use of modern technologies, new types of organic compounds are being produced, based on which polymers, plastic materials, hormones, fungicides, solvents, stimulants, emulsifiers, plasticizers, antibiotics, adhesives, paints, and other products are being manufactured through the chemical processing of oil and gas. In the new development strategy of Uzbekistan for 2022-2026, important tasks have been set, such as widely introducing innovations into the economy, and developing cooperation between industrial enterprises and scientific institutions. In this regard, it is of great importance to conduct scientific and practical research to develop the chemistry of unsaturated compounds and implement a localization program in production through the use of industrial products and substances obtained from their processing.

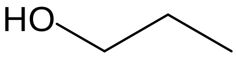


The telomerization reaction of 1,3-butadiene with palladium and nickel catalysts.

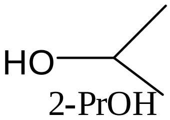
In this reaction, 1,3-butadiene undergoes telomerization in the presence of palladium and nickel catalysts. The process involves the addition of short-chain molecules (telogens) to the butadiene, resulting in the formation of shorter polymer chains, known as telomers. Palladium and nickel catalysts play a key role in initiating and controlling the reaction. This reaction typically follows a free radical mechanism, where free radicals are generated and react with the butadiene to form the final products. The telomers produced in this reaction can be used in various industrial applications, including the synthesis of polymers and other chemical products.



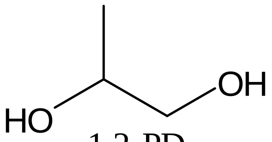
EG



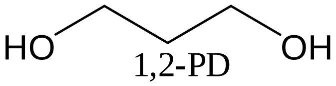
1-PrOH



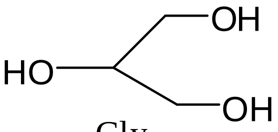
2-PrOH



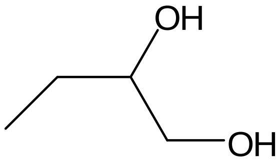
1,2-PD



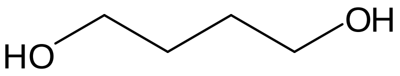
1,2-PD



Gly

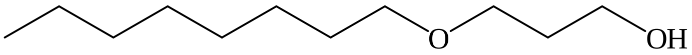


1,2-BD

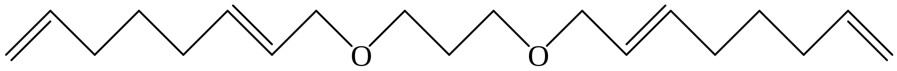


1,4-BD

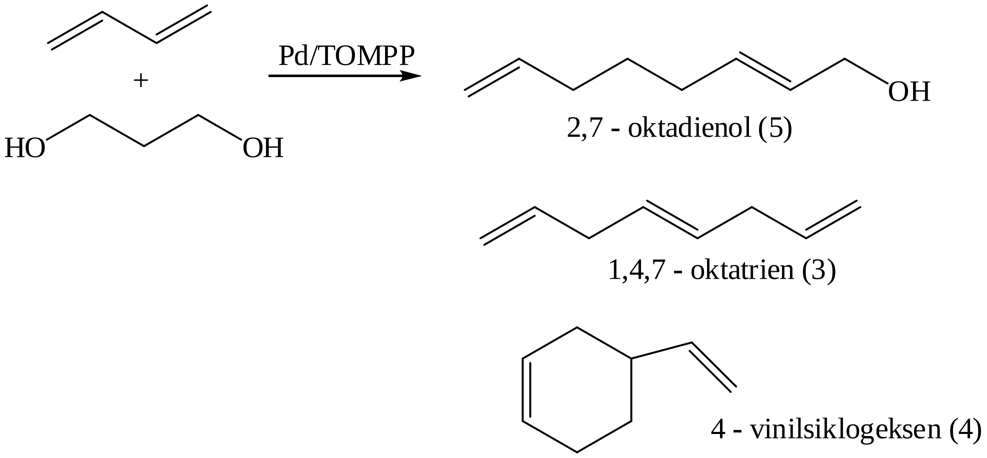
In this study, the products formed by the telomerization of 1,3-butadiene with 1,3-propanediol (1,3-PD) are as follows:



Oktadienilefir (1)



Bis-oktadienilefir (2)



2,7 - oktadienol (5)

1,4,7 - oktatrien (3)

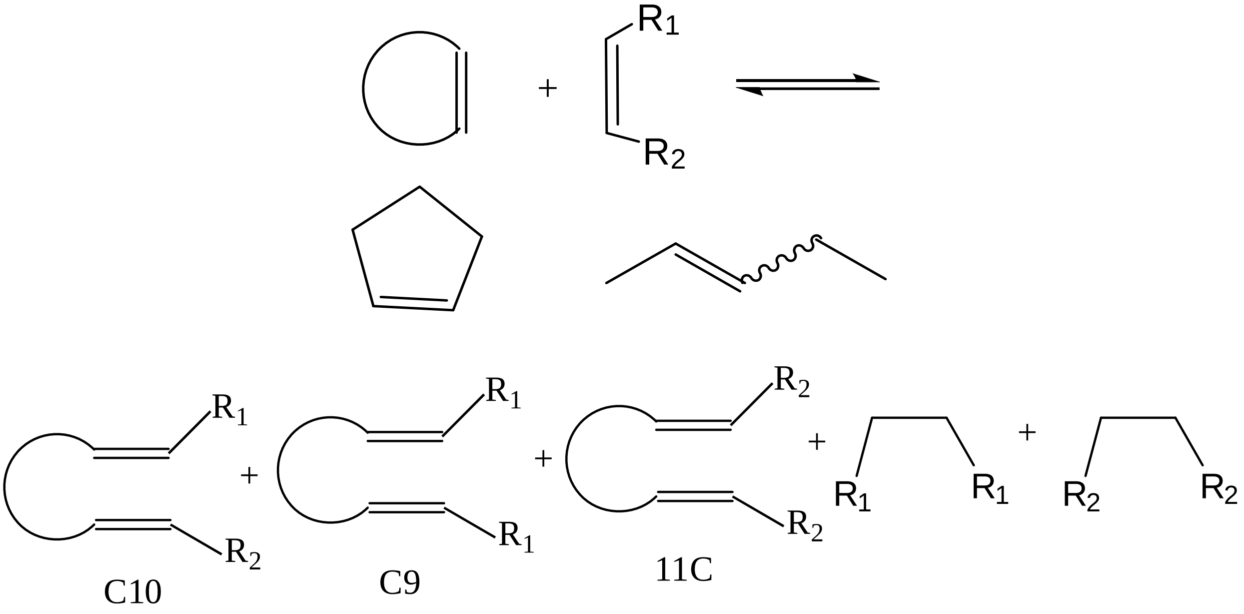
4 - vinilsiklogeksen (4)

In this reaction, the products formed are mono-telomers (octadienyl ethers) (1), di-telomers (bis-octadienyl ethers) (2). As a result of the reaction of the formed products with water, 2,7-octadienol (5) is obtained, and the dimerization products are 1,4,7-octatriene (3) and 4-vinylcyclohexene (4). The telomerization of 1,3-butadiene with various alcohols and its effect on diols have been studied using Pd/TOMPP catalysts [1].

The raw materials that can undergo telomerization (ethylene and other olefins, as well as their halogenated derivatives) allow for the production of high mono- and bifunctional compounds, including acids. The halogen-exchanged acids obtained during telomerization are used for the synthesis of both saturated and unsaturated acids [2].

A number of scientists, including S. Bigot, J. Lai, I. Shveysariya, and M. Sauthier, studied the telomerization of 1,3-butadiene with glycerin under aqueous two-phase conditions and the influence of reaction conditions on product yield. During the reaction, butadiene continuously added, and the reaction was maintained under constant pressure. Various parameters were tested to improve the activity and selectivity of the resulting mono-, di-, or tritelomers.

Y. Chuamin and his students carried out the telomerization reactions of cyclopentane and pentene-2 [3].



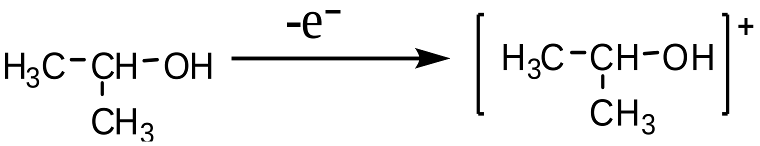
A. Rjevskiy, A. Topchiy, and others studied the telomerization of isoprene with methanol in the presence of heterogeneous palladium complexes without a solvent. The telomerization processes of butadiene with arylamines in the presence of palladium complexes were studied by R. Aripov, Ye. Ganieva, R. Izhberdina, R. Khusnutdinov, K. Khusnutdinova, and I. Abdurakhmanov. O. B. Penrhyn-Lou and his students investigated the radical telomerization reactions of ethylene glycol dimethacrylate, 1,6-hexandiol dimethacrylate, and 1,12-dodecandiol dimethacrylate. The telomerization reaction of styrene with mercaptans to prepare macromonomers with variable molar mass functional telomers was studied by A. Bechkok, M. Belbachir, B. Guyot, and B. Butevin [4,5].

Telomerization reactions have significant practical importance in the production of macrocyclic lactones, ω-amino acids, high-carbon acids, and other organic compounds. The rearrangement of radicals in the telomerization reaction of ethylene has been extensively studied using carbon acids and their derivatives as examples. However, fewer studies have been conducted on the rearrangement in the telomerization of alcohols [6,7].

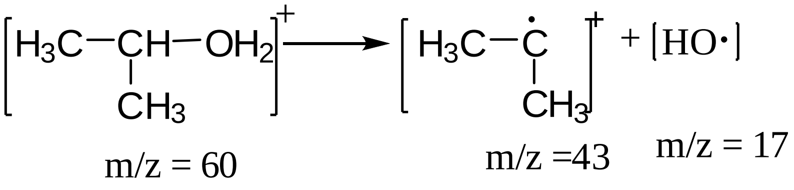
Chromatographic-Mass Spectral Analysis of Isopropyl Alcohol

In this process, the molecular ion peak of isopropyl alcohol was observed at m/z 59.0. Below is the schematic representation of the fragmentation ions generated from the molecular ion of isopropyl alcohol.

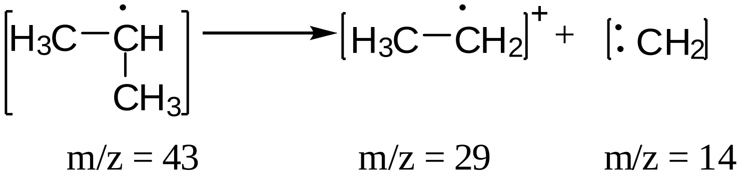
To verify isopropyl alcohol, it was introduced into the chromatograph-mass spectrometer. Under the specified conditions, a molecular ion of isopropyl alcohol with m/z 60.0 appeared in the range of 1.816 to 1.818 minutes.



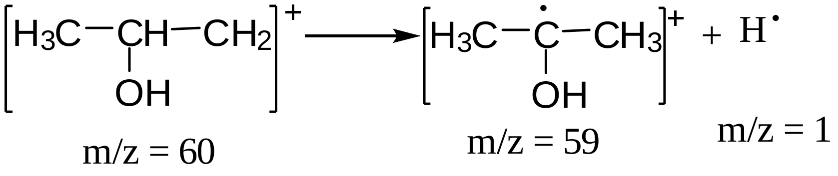
In the chromatographic-mass spectrum, the appearance of fragment ions with masses m/z 46, m/z 45, m/z 43, m/z 31, m/z 29, and m/z 27 was observed. At 1.818 minutes, the fragmentation of the isopropyl alcohol ion occurred due to the detachment of the hydroxyl (-OH) ion, leading to the formation of the fragment ion with m/z 43. This corresponds to the isopropyl ion with a peak at m/z 43.



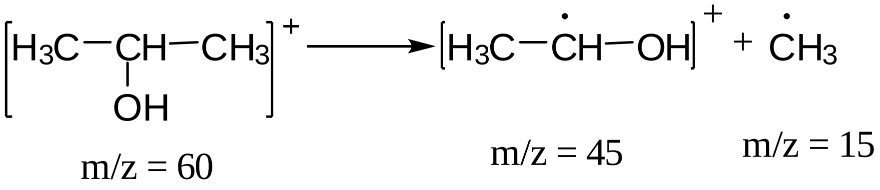
The detachment of a methylene (=CH2) ion from the isopropyl ion results in the formation of a fragment ion with m/z 29. This corresponds to the ethyl ion with a peak at m/z 29.



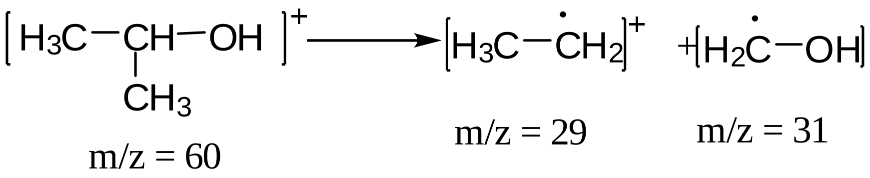
In addition, the fragmentation of the isopropyl alcohol ion along a different pathway resulted in the formation of a fragment ion with m/z 59. This corresponds to the isopropanol ion with a peak at m/z 59.



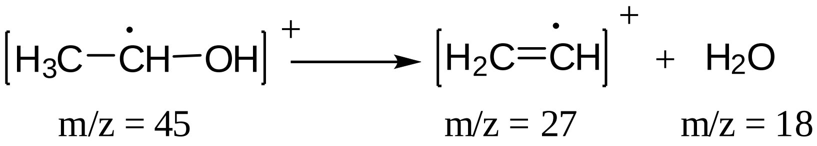
It should also be noted that from the propanol-2 ion, the fragmentation at 1.818 minutes resulted in the release of a –CH3 ion, forming a fragment ion with m/z 45. This corresponds to the ethanol ion with a peak at m/z 45.



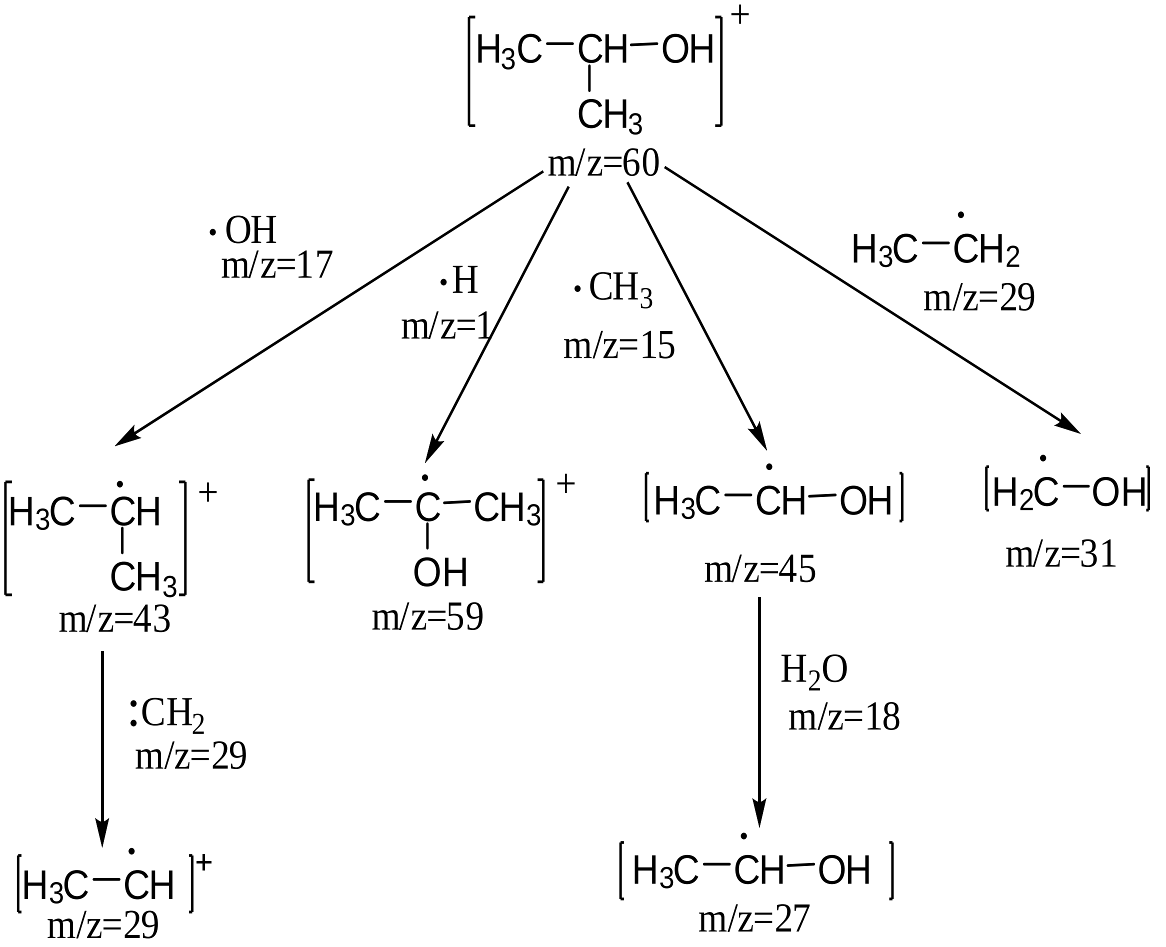
From the propanol-2 ion, at 1.818 minutes, the release of an ethyl ion resulted in the formation of a fragment ion with m/z 31. This corresponds to the methanol ion with a peak at m/z 31.



Additionally, it was shown that the fragmentation of the ethanol alcohol ion in another direction led to the formation of a fragment ion with m/z 27 due to the loss of a water (H2O) molecule. This corresponds to a methanol ion with a peak mass of m/z 27.



The general scheme of fragment ion formation can be described as follows:



Molecular Ion Formation: The parent molecule, in this case, is isopropyl alcohol (or ethanol), which undergoes ionization to form a molecular ion. Fragmentation: After ionization, the molecular ion may undergo various fragmentation pathways, breaking into smaller ions (fragment ions). Loss of Functional Groups: Fragment ions can form when functional groups like hydroxyl (-OH), methylene (=CH2), or water (H2O) are lost from the molecule. For example: Loss of a hydroxyl group (-OH) results in the formation of a fragment ion with mass m/z 43.

Loss of a methylene group (=CH2) leads to the formation of a fragment ion with mass m/z 29. Loss of water (H2O) leads to the formation of a fragment ion with mass m/z 27. Specific Fragment Ions: Depending on the structure of the parent molecule, different ions such as m/z 45 (ethanol ion), m/z 31 (methanol ion), and others may appear in the spectrum.

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