Condensation Reactions of Bicycle Sulfur Organic Compounds

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ABSTRACT

In this article, the reaction of 5-acetyl-2-methyl-1-thiaindan molecule with benzaldehyde, propion aldehyde, oil aldehyde and isovalerian aldehyde as a substrate in aldol condensation reactions of bicyclic sulfur organic compounds is studied. According to the result of the reaction, the reaction of 5-acetyl-2-methyl-1-thiaindan molecule with various aldehydes proceeds in the same way as aliphatic aldehyde and ketones, and the yield of the reaction product is high.

Keywords: 5-acetyl-2-methyl-1-thiaindan, benzaldehyde, propion aldehyde, fatty aldehyde, isovaleric aldehyde, ketone, carbonyl component, methylene component, condensation, aldol, acetylthiandan, acetyl group.

Introduction

In recent years, the volume of production of new types of medicinal preparations is based on medical sources [1-3]. Several aldehyde groups can be seen in the molecular structure of medicinal compounds. With its high reactivity, these a1ldehyde groups are considered one of the main functional groups in the synthesis of compounds with carbocyclic and heterocyclic structures[4-10]. One of the characteristic reactions of aldehydes and ketones is aldol condensation reactions. In general, reactions with the formation of a new carbon-carbon bond are called condensation reactions. The participation of methylene component and carbonyl component is necessary for condensation reactions to proceed. All organic compounds containing a carbonyl group can be used as a carbonyl component. However, for a methylene component vs. a carbonyl component, however, for a methylene component, the carbonyl k atom must have at least one exchangeable hydrogen atom on the α-state carbon atom. Condensation reactions take place at the expense of the hydrogen atom located in the α-position relative to the carbonyl group. This hydrogen atom becomes activated as a result of the polarization of the carbonyl group. Alkalis and acids are used as catalysts for condensation reactions.It is known from the mechanism of aldol condensation reaction that in order to increase the reactivity of ketones, it is necessary to convert them into enol or enolate anion under the catalysis of alkali or acid. In a base-catalyzed aldol condensation reaction, the ion ion of a ketone attacks the carbonyl group of another molecule, a ketone or aldehyde, resulting in the formation of β-hydroxyketones. It is also possible to isolate the last β-hydroxyketones, but under the influence of a base, especially in the presence of an acid, this substance undergoes dehydration and separates a water molecule, resulting in the formation of α-, β-unsaturated ketones.

Materials And Methods

Synthesis from 2-Methyl-5-benzylideneacetyl-1-thiain

Equipping a round-bottomed two-necked flask with a mechanical stirrer and a dropping funnel, dissolve 0.5 g of sodium alkali in 5 ml of water and add 10 ml of ethanol. We cool the flask from the outside in cold water, while stirring the mixture in the flask, we drop 2 g (0.01 mol) of 2-methyl-5-acetyl-1-thiain and 1 g of freshly distilled benzaldehyde through a dropper funnel, and the temperature is 0 C° + 5 C° we keep it between. Stir the mixture in the flask for another 2-3 hours. The reaction product is formed in crystalline form. We filter the crystals, wash them in cold water until they become neutral and dry them. The yield of the reaction was 93% (2.7 g). The melting temperature is 136-137 0C.

2-Methyl-5-propyleneacetyl-1-thiaindane

Equipping a round-bottomed two-necked flask with a mechanical stirrer and a dropping funnel, dissolve 0.5 g of sodium alkali in 5 ml of water and add 10 ml of ethanol. We cool the flask from the outside in cold water, while stirring the mixture inside the flask, drop 2 g (0.01 mol) of 2-methyl-5-acetyl-1-thiain and 1 g of freshly distilled propionaldehyde through a dropping funnel and bring the temperature to 0 C. We keep it in the range of +5 0C. Stir the mixture in the flask for another 2-3 hours. The reaction product is formed in crystalline form. We filter the crystals, wash them in cold water until they become neutral and dry them. The yield of the reaction was 75% (1.8 g). Liquefaction temperature 38-39 0C.

2-Methyl-5-butyleneacetyl-1-thiaindane

Equipping a round-bottomed two-necked flask with a mechanical stirrer and a dropping funnel, dissolve 0.5 g of sodium alkali in 5 ml of water and add 10 ml of ethanol. We cool the flask from the outside in cold water, while stirring the mixture inside the flask, drop 2 g (0.01 mol) of 2-methyl-5-acetyl-1-thiain and 1 g of freshly distilled oleic aldehyde through a dropping funnel and keep the temperature at 0 C°+5C°. Stir the mixture in the flask for another 2-3 hours. The reaction product is formed in crystalline form. We filter the crystals, wash them in cold water until they become neutral and dry them. The yield of the reaction is 80% (2 g). Liquefaction temperature is 36-37 0C.

2-Methyl-5-izovalerianidenatsetil-1-thiaindane

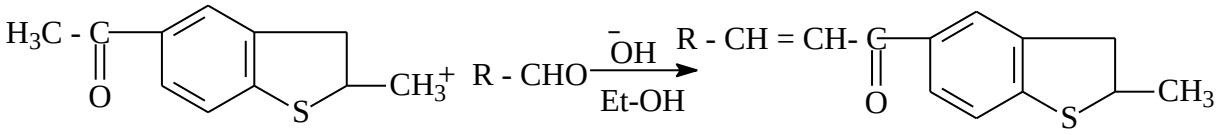
Equipping a round-bottomed two-necked flask with a mechanical stirrer and a dropping funnel, dissolve 0.5 g of sodium alkali in 5 ml of water and add 10 ml of ethanol. We cool the flask from the outside in cold water, while stirring the mixture in the flask, drop 2 g (0.01 mol) of 2-methyl-5-acetyl-1-thiain and 1 g of freshly distilled isovaleric aldehyde through a dropping funnel and bring the temperature to 0 C°. We keep it in the range of +5 0C. Stir the mixture in the flask for another 2-3 hours. The reaction product is formed in crystalline form. We filter the crystals, wash them in cold water until they become neutral and dry them. The yield of the reaction is 82% (2.2 g). Liquefaction temperature 39-40 0C.

Results (Discussion)

In order to study the chemical properties of acetyl-1-thiaindanes, we conducted the condensation reactions of these compounds based on Klyazin and Schmidt reactions. In these condensation reactions, we studied the interaction reactions of 5-acetyl-2-methyl-1-thiaindan molecules with benzaldehyde, propion aldehyde, fatty aldehyde and isovaleric aldehyde as reactive substrates. The reaction was carried out in ethanol medium in equimolar proportions of the reactants. Sodium alkali was used as a catalyst in the reaction, and the reaction was carried out at a temperature of 0 C° +5 C° for 2-3 hours.

As a result of the research, it was found that the condensation of aromatic aldehyde and aliphatic aldehyde with acetyl-1-thiain molecule, sulfur bicyclic ketones condensed with benzene ring behaves like aliphatic ketones, and according to the result of this reaction, the yield of the product is much higher. It turned out. This aldol-cratone condensation reaction proceeds in an alkaline medium. Aldol condensation reaction in an alkaline medium follows the type of nucleophilic mechanism. Under the influence of a base (catalyst), a proton is removed from

the α-carbon atom of the methylene component, which leads to its activation, and it turns into a strong nucleophilic reactive anion with a delocalized negative charge. Activated methylene component attacks the carbonyl group of aldehydes on the carbon atom. As a result, an anion is formed, and an aldol is formed through the release of a proton from it. As a result of the reaction, the corresponding α-unsaturated ketones of the 1-thiaindan series were formed:



I. R = C_6H_5- II. R = $CH_3 – CH_2$ -
III. R = CH_3-CH_2 –CH_2 - IV. R = $CH_3 – CH – CH_2$-CH_3

The synthesized compounds are crystalline substances, insoluble in water, well soluble in benzene, acetone, ether and other organic solvents. The structure and composition of the obtained compounds were confirmed by physical and chemical methods. In particular, the IR spectrum of substance I with the above composition shows absorption lines characterizing methyl groups at 3005 and 1190 cm-1, while absorption lines at 2950 cm-1 are absorption lines characterizing valence vibrations of methylene groups. Also, the specific absorption lines in the region of 885 and 1100 cm-1 indicate that they belong to the deformation vibrations of the SN groups in the benzene ring, while the absorption lines in the region of 1680 cm-1 indicate that they belong to the carbonyl group. Also, the absorption lines in the region of 1660 cm-1 indicate that they belong to the S=S bond in the benzene ring. The characteristic absorption lines belonging to the double bond in the acyl group of the molecule show specific absorption lines in the region of 1430 cm-1 in the cis form and in the regions of 1300 and 1285 cm-1 in the form of the trans form. It was found that the absorption lines belonging to S-S-C bonds in the heterocyclic part of the molecule are observed in the region of 720 cm-1.

In the PMR-spectrum of 6-benzylidene-1-thiaindan from the compounds with the formulas given above or the IR-spectrum, the signals of protons of methylene groups are 1.25 in the form of quadruple and multiplet; shows its signals at 2.15 m.h. and 2.40 m.h., while the signals of the aromatic ring and phenyl group protons give their signals in the form of weak singlet and doublet at 7.93 m.h. and 8.29 m.h. And the signals of protons in the SN=SN bond in the side chain in the 6th state of the molecule are 7.75 m.h. and 7.52 m.h. appear in the form of a complex multiplet. The spin-spin interaction constant of the protons in the methylene groups (6) in the heterocyclic part of the molecule is 6 Gs, and the spin-spin interaction constant of the protons in the SN=SN groups is 4 Gs. It was found that the constant of spin-spin interactions of protons in the aromatic ring and phenyl groups is equal to 26 Gs.

As a result of the research, it was found that the products formed by the reaction of 1-thiaindan series ketones with a bicyclic structure with various aldehydes are formed with high yield, the methylene component of the methyl group located in α-position compared to the carbonyl group of the acetyl group in the 1-thiaindan molecule. is explained by easy condensation reactions. It can be seen that the increase in the molecular mass of the reactant is directly proportional to the yield of the reaction. In this reaction, the yield of the reaction with aromatic aldehyde is much higher than with aliphatic aldehydes. This is explained by the unique structure and properties of the benzaldehyde molecule. The resulting substances are crystalline substances, well soluble in benzene, acetone, ether, chloroform and other organic solvents, and insoluble in water. Purification of the obtained substances was done by recrystallization in ethanol.

Conclusion

According to the results of the research conducted above, it can be mentioned that the condensation reactions of 1-thiain acetyl derivatives with various aldehydes proceed in the same way as the condensation reactions of aliphatic ketones with aldehydes. It was found that aromatic aldehydes react better than aliphatic aldehydes in these reactions. This process can be explained by the effect of p-electron system on aromatic ring on aldehyde group.

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