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ALKYLATION OF P-NITROPHENOL WITH BENZYL CHLORIDE

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Abstract: This article focuses on the study of alkylation reactions of p-nitrophenol in the presence of nanocatalysts. The formation of C-alkyl and O-alkyl products was observed in the alkylation reactions and the composition of isomers was determined. Benzyl chloride was selected as the best alkylating agent for the reactions, and alkylation under mild conditions gives mainly O-benzyl products. As a catalyst, $TiO_2 \cdot SiO_2/FeCl_3$ catalyst, $FeCl_3$ nanocatalyst soaked in polyvinyl chloride (PVC) was used and it was found that the selectivity increased.

Key words:p-nitrophenol, benzyl chloride, PVC-based $FeCl_3$ nanocatalyst, nanostructured $TiO_2 \cdot SiO_2/FeCl_3$ catalyst

Enter. Currently, compounds containing phenol are widely used in various fields of industry (polymer, rubber, pharmaceuticals, cosmetics), as well as in medical practice. One of the most important areas of use is the production of antioxidants from phenols [1]. The most traditional and studied area of application of phenolic antioxidants is the polymer industry. Due to their low toxicity, they are primarily used in materials widely used by humans, medical equipment, food packaging, children's toys, and also in the production of food products [2].

Analysis of literature on the topic Recently, 2,4-dinitrophenol drug has been widely used as a weight loss agent. Side effects of 2,4-dinitrophenol drug cause poisoning of the body. A single poisoning dose of 2,4-dinitrophenol for people weighing 60 kg is 1 g. 2,4-dinitrophenol has a strong toxic effect, in particular, it causes dizziness, headache, back pain, nausea and vomiting, hyperhidrosis, fear. During the experiments, on the second day of taking the drug, paresthesia, shallowing of consciousness, shocking depression, dysarthria, increased heart rate, increased blood pressure, increased respiratory rate, and increased fever were found in the experiments [3].

Most of the phenols are used in the production of phenol-formaldehyde resins, which are raw materials for press powders, laminates, varnishes, adhesive resins. Phenols are one of the main raw materials in the synthesis of higher alkylphenols, which are used to obtain surfactants and stabilizers. Electrophilic exchange reactions are used to obtain such compounds of phenols. Currently, electrophilic reagents can be conditionally divided into three types: strong electrophiles, moderately strong electrophiles, weak electrophiles. One of the most important and basic reactions of phenols is the electrophilic substitution reaction, which has been thoroughly and thoroughly studied from the point of view of the mechanism and is widely used in organic synthesis.

Strong electrophiles include complexes of nitronium cation N^+O_2, Cl_2 and Br with Lewis acids – $FeCl_3$, $FeBr_3$, $AlCl_3$, $SbCl_5$ etc.

Moderately strong electrophiles include Lewis acids of alkyl halides and acyl halides $RCl{*}AlCl_3$, $RBr{*}GaBr_3$, $RCOCl{*}AlCl_3$ and complexes of alcohols with strong Lewis and Brønsted acids $ROH{*}BF_3$, $ROH{*}H_3PO_4$, $ROH{*}HF$.

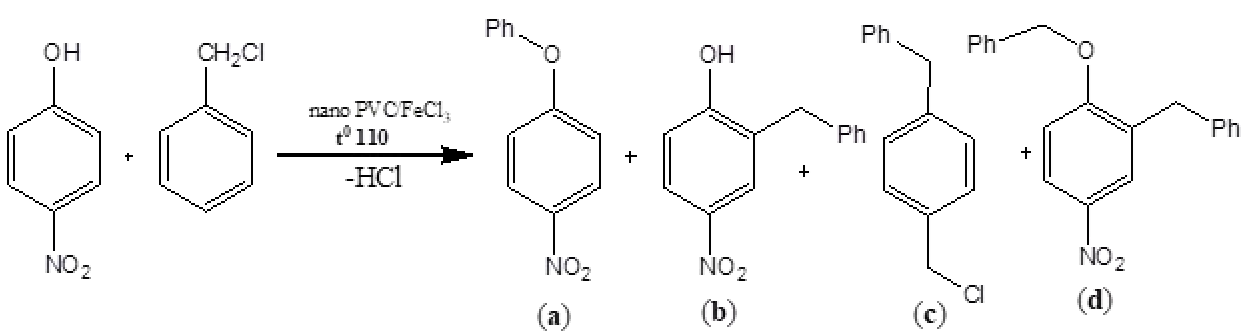
Strong electrophiles easily react with benzene series compounds with electron-donating and electron-withdrawing substituents. Moderately strong electrophiles react with benzene and its activating electron-donating substituents, halogen atoms.

Allyl and benzyl halides are considered to be strong electrophiles compared to alkyl halides containing saturated radicals. Allyl and benzyl halides can easily form carbocations under the influence of solvents or catalysts and undergo an active reaction.

Research methodology The reaction of 4-chloro-3-methyl phenol and 1-iodo-4-nitrobenzene at 130 °C was studied in the presence of Fe_3O_4-Co_3O_4 catalyst. The influence of time, solvent base, and amount of catalyst on the reaction was studied. Fe_3O_4-Co_3O_4 nanocatalyst was used in the O-arylation of 4-chloro-3-methylphenol and the o-aryl product was obtained [4]. When using a catalyst in the alkylation of phenols, alkylphenol products are obtained, and the total yield of products (C-alkyl and O-alkyl) is found to be up to 60% [5,6]. Alkylation reactions of substituted phenols, effect of nano catalysts on reaction processes, H_3PO_3-catalyzed alkylation of phenols with alkenes are carried out easily, efficiently and selectively. The reaction shows the process of alkylation of the benzene ring, and the synthesis of ortho-, meta- or para-alkylated phenol derivatives has been carried out [7].

As a result of allylation reactions of phenol, 1-naphthol, 2-naphthol, 2-naphthylmethyl ether, anisole, veratrol and dimethyl ether of resorcinol with various allylating agents, O- and C-allyl products were obtained with high yield; iron(III) chloride crystal hydrate catalyst was used to obtain para-substituted products in allylation reactions of phenols and naphthols, nanostructured $TiO_2 \cdot SiO_2/FeCl_3$was used to obtain ortho-substituted allyl derivatives; It was found that the nanostructured $TiO_2 \cdot SiO_2/FeCl_3$ catalyst used in the synthesis of o-substituted derivatives with high biological activity is more effective for allylation reactions [8].

The composition of the reaction product was determined by chromo-mass spectroscopy as follows: benzyl ether of 4-nitrophenol, 2-benzyl 4-nitrophenol, benzyl ether of 2-benzyl 4-nitrophenol, bis-benzyl substituted 4-nitrophenol, molecular structure corresponding to 4-benzyl benzyl chloride and fragment ions were found to be present.



Chromato-mass spectrum "Agilent Technologies 7890 N GC system" with mass selective detector "5977 A MSD" DRUGS_SKAN.A1 M method, inner surface covered with 5% phenylmethylsiloxane, length 30 m. Capillary column was used and Agilent Technologies 7890 inert mass spectra were obtained at injector temperature of 280°C and thermostat temperature from 150°C to 289°C.

Summary. O- and C-alkyl products were formed in this process. The highly reactive benzyl chloride reacts to form parabenzylated benzyl chloride as the major product, leading to an electrophilic exchange reaction of the aromatic ring of p-nitrophenol. shows that the ability is lower than that of benzyl chloride.

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