

Development of the mechanism of action and reaction of O-chloracetylation.

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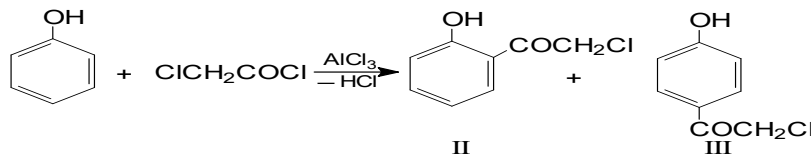
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Abstract: In this article, the reaction of phenol with the catalytic quantities of FeCl_3 , $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$, $\text{Fe}_2(\text{SO}_4)_3$, TAA and benzene solution. The resulting product was isolated and analyzed. The mechanism of the O-targeting reaction has been proposed.

Keywords: Phenol, Chloracetylchloride, Catalyst, Phenylchloracetate, Temperature, Absolute Benzene, Acid, Hydrogen Chloride, Alkaline Water, Benzene, Extraction Vacuum, Substance, Gas-Liquid Chromatogram, Column, Stationary Phase.

I. INTRODUCTION

English scientists carried phenol [1] at higher temperatures (10-20° C) and overdose of phenol C-acetylene reaction resulted in 2- (I) and 4-hydroxyphenylchloride (II):



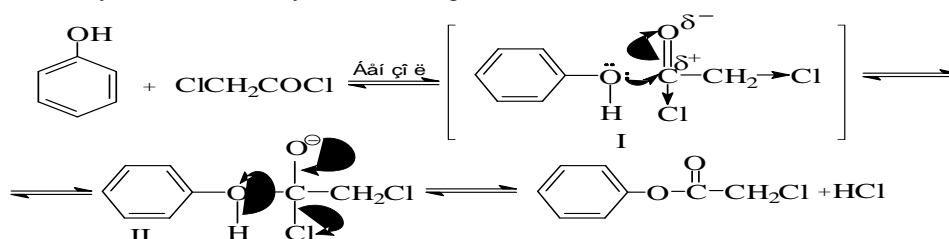
Russian scientists G. Dorofenko and Sadykov [2] also studied the reaction of chloracetylation of phenol. However, they were able to heat an equimolar phenol and chloroacetylchloride mixture for 14 hours and obtain an O-acetylphenylchloroacetate with 79% yield.

The literature shows that the chloracetylation of phenol was carried out without catalyst or in equimolar quantities of AlCl_3 . There is no information on the reaction of chloracetylation with the catalyst of phenol catalyst.

II. SIGNIFICANCE OF THE SYSTEM

We conducted phenol in a solvent solvent without catalyst and catalyst in the presence of catalysed FeCl_3 , $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$, $\text{Fe}_2(\text{SO}_4)_3$, TAA in order to study the chloracetylation reaction greater depth.

Phenol chloracetylation reaction abs. When administered in benzene solution, only the O-acetylation reaction occurs and Phenylchloracetate yields 94%. Phenylchloracetate generation scheme can be described as follows: [3]:



Phenol During the reaction of phenol and chloroacetylchloride, the electron density in the chloroacetylchloride molecule is shifted to electromagnetic oxygen and the oxygen is partially negative. As a result of the electromagnetic chlorine and oxygen atoms, the carbon atom is partially positively charged and interacts with the double electrons of the hydroxyl group in the phenol molecule to form complex I. In the reaction, the valence bond between oxygen and carbon forms a complex II, which produces a reaction product with hydrogen chloride.

The proposed O-Cyclic scheme for this reaction is also related to the reaction of isomeric cresols with absolute benzene with Chloracetylchloride, which also undergoes the same mechanism.

It is known that alkylation and acetylation reactions of aromatic compounds with haloid alkyls or acylhalogens in the ionic mechanisms, these reactions are better in polar solvents. Because the above reaction occurs in a polar solvent (benzene) and without catalyst, no ethyl cation is formed. Therefore, this reaction is in the form of nucleophilic substitution in the carbonyl group of the chloracetylchloride molecule, and (for example, in the reaction of o-cresol in the benzene solution of chloracetylchloride) forms an ether product. The nucleophilic reagent acts as an oxygen atom in the phenolic cellulose molecule.

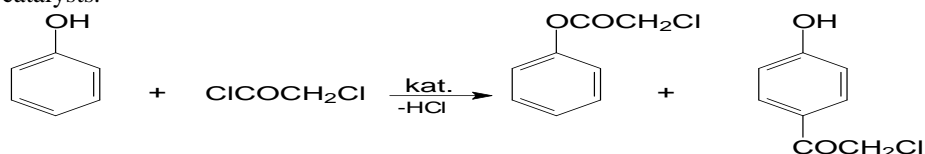
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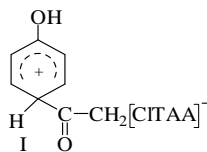
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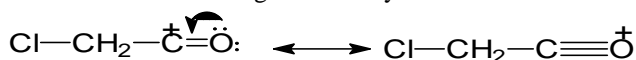
When using TAA as a catalyst, a single substance forms 4-hydroxyphenyl chloride. Therefore, this method can be proposed as a method for the synthesis of 4-hydroxyphenyl acetyl chloride. This substance is explained by the complex (1) complex formation of large and stable:



The chloracetylation of phenol can be explained by the fact that the acyl group does not reach 2 states [4]

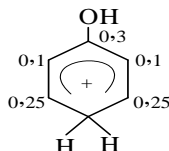
1) Due to the high volume of the complex formed by the catalyst with chloracetylchloride, the reaction does not go to the ortho state due to space difficulties.

2) The chloracetyl cation (electrophil) in the complex composed of chloracetylchloride and catalyst is unstable due to mesomeria and has high selectivity:



Therefore, the most favorable and stable p-isomer is generated in the reaction.

3) Given the charge distribution in the sigma complex due to electrophilic exchange to the aromatic ring, the phenol nucleus -OH group is more sensitive to the complex when it is oriented to p-state and therefore p-hydroxyphenyl acetyl chloride is formed.



The selectivity of the acyl group, the orientation of the aryl group I substitutions in the acyl group to p-position is well known from the literature data, and in our experience the formation of 4-hydroxyphenacylchloride with the TAA catalyst also confirms this.

III. EXPERIMENTAL RESULTS

To confirm the results of experiment, the total energy of the phenylchloracetate, 2- and 4-hydroxyphenacylchloride systems, the bonding energy, and the heat generated, were calculated by the "Hyper Chem" program and obtained the following results:

No	Organic matter	The total energy of the system, Kcal/mol	Bond energy, kcal/mol	Heat of formation, kcal/mol
1.	Phenylchloracetate	-48633,70	-2220,996	-65,96
2.	2-hydroxyphenacyl-chloride	-48641,35	-2228,64	-73,6122
3.	4-hydroxyphenacyl	-48638,925	-2226,22	-71,18

Analysis of the results of quantum-chemical calculations shows that the total energy of the system and the heat generated by hydroxyphenacylchloride 2 and 4 are very different. Spatial effects are not considered in this calculation. However, the spatial effects of the cationic acid during the acetylation reaction are decisive and result in the formation of an inorganic product relative to the hydroxyl group. This is also confirmed by the results of the reaction.

Analyzing the literature reveals that the study of chloracetylation reactions of o-Creole is not studied. O-Creole is an easy-to-use compound that reacts with alkyl and acetylene and has two reaction centers.

Experiment. №1

Phenylchloracetate intake

a) 9.4 g (0.1 g mol) of phenol, 50 ml abs., In tubular round tubes with hydrogen chloride release for recirculation cooling. Dissolved in benzene, 11.3 g (0.1 g-mol) of chloracetylchloride was added and boiled for 10 h. After stopping hydrogen chloride, the mixture was washed with alkaline water and extracted in benzene, dried in CaCl₂. The benzene was released under normal conditions and the substance was vacuumed at 120-122° C / 20mm.sim.ust. The substance is 16 g (94.1%).

b) 9.4 g (0.1 g-mol) of phenol was dissolved in 30 ml of pyridine in a circular tube with the refrigerant installed and added 11.3 g (0.1 g-mol) of chloracetylchloride. The reaction mixture was boiled and turned dark red during boiling. To this solution was added 10 ml dilute sulfuric acid solution and cooled with ice water. The reaction product was isolated as a fatty substance. To extract the pyridine from the mixture, diethyl ether and dilute acid solution were added. The ether section was separated and dried with CaCl₂. After the solvent was pumped, the phenylchloracetate was pumped into a vacuum. The reaction yield was 10.2 g (60%). T. Kaine. 120-122° C / 20 mm.sim. over.

c) 14.1 g (0.15 g-mol) phenol, 5.65 g (0.05 g-mol) chloracetylchloride, 8.01 g (0.06 g-mol) in AlCl₃ by 00C as described above. 5.95 g (70%) of phenyl chloracetate was obtained by cysteine. T. Kaine. 120-122° C / 20 mm.sim. over.

Experience №2. Chloracetylation of phenol

9.4 g (0.1 mol) phenol, 11.3 g (0.1 g-mol) chloracetylchloride, 0.04 g (2.5 * 10⁻⁴ g-mol) FeCl₃ mixture at 118-120° C for 3 hours heated. Phenol that has not been reacted after hydrogen chloride gas stops.

Then 13.6 g (80%) of the main product is 138-140° C / 30 mm sim.ust. was seized.

Gas-liquid chromatography shows that the reaction product is phenylchloracetate and 85% 4-hydroxyphenacylchloride. Chloracellation reaction of phenol results in formation of ironacetylchloride. The yield of the reaction is 83% Activity = 148° C. 148° C according to the literature.

The gas-liquid chromatogram of the substances obtained by these methods was analyzed on <LXM-8MD> equipment under the following conditions: column length 2 m, stationary phase 20% apex L column and detector temperature 150° C, hydrogen speed 25 ml / min.



ISSN: 2350-0328

International Journal of Advanced Research in Science, Engineering and Technology

Vol. 7, Issue 1, January 2020

IV. CONCLUSION AND FUTURE WORK

The synthesized nucleophilic reactions with the synthesized phenylchloracetate with phenol, cresols, ethyl spirit and benzoic acids. This synthesis reveals the structure of new organic compounds. Their biological activity is determined. Testing of substances in laboratory and field conditions is carried out in Rostov-on-Don and RostovskogoUniversio.

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