

5- Methyl -2-(1-Methylethyl) Phenol with Chloroacetyl Chloride under Alkaline Conditions

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Article Information

Received: February 05, 2023

Accepted: March 06, 2023

Published: April 08, 2023

Keywords: Bacteria and fungus, infection, incubation, chloroacetylchloride, DMSO, cresol, catalyst, benzene, solvent, extraction, vacuum, flask, O-acylation, C-acylation, mixture.

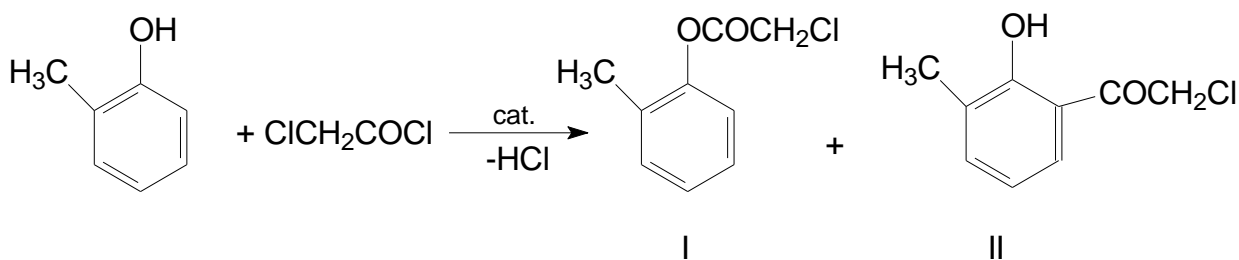
ABSTRACT

In this article, the reaction of 5-methyl-2-(1-methylethyl)phenol with chloroacetyl chloride was carried out for the first time in DMSO solution. It was found that the yield of the substance in this reaction depends on the solvent and the reaction conditions. The mechanism of the reaction of chloroacetyl chloride with 5-methyl-2-(1-methylethyl) phenol in DMSO solution was developed and proposed. Some geometrical and energetic parameters of 5-Methyl-2-(1-methylethyl)phenylchloroacetate Chemical, Obtained in MMFF94, MMFF94s, UFF methods. The structure of the new substance formed was confirmed by IR-, H1 NMR and C13 NMR spectra.

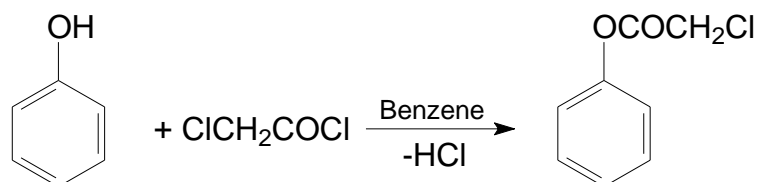
5-Methyl-2-(1-methylethyl)phenol compounds are used for the pathogenesis of bacterial and fungal infections. Because microorganisms settle in the mucous membrane cells to multiply and form colonies before certain symptoms of the disease are detected. This is especially true for urinary tract infections, bacterial vaginosis and female genetic infections such as vaginitis.

5-Methyl-2-(1-methylethyl)phenol compounds incubated with human neutrophils significantly reduced the oxidant release-up to 2.73. Among other results related to bacterial and fungal adhesion, the antioxidant activity of 5-Methyl-2-(1-methylethyl)phenol compounds is used against vaginosis and vaginitis. In addition, it exhibits antibacterial, antifungal and antioxidant properties and can have a synergistic effect.

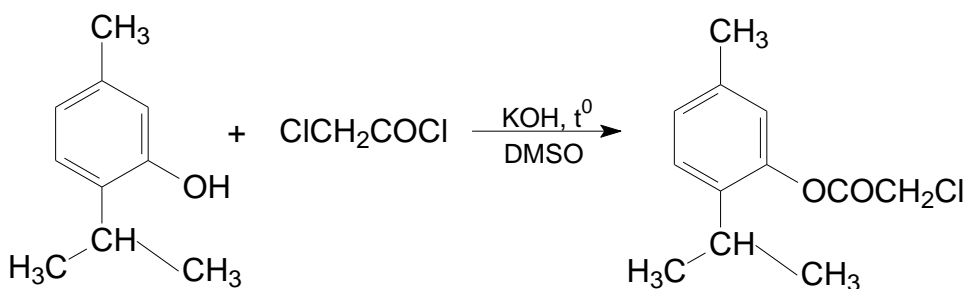
Uzbek chemists have determined that o-tolylchloroacetate (I) and 2-hydroxy-3-methylphenacyl chloride are formed as a result of the reaction of o-cresol with chloroacetyl chloride using a catalytic amount of iron salts [1-2].



As a result of the reaction of phenol and cresols in benzene solution with chloroacetyl chloride, only one substance, phenylchloroacetate, was formed. Biologically active substances were synthesized with this substance through nucleophilic exchange reactions [3-4].

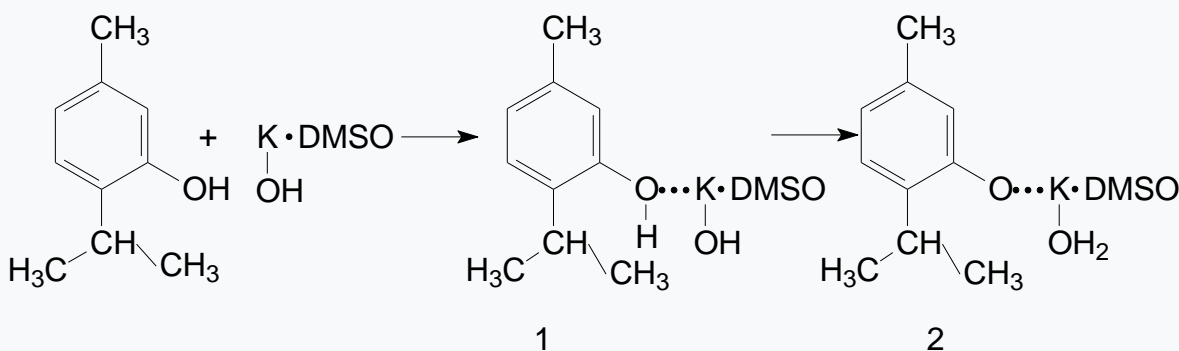


Chloroacetylation reactions were carried out with 5-methyl-2-(1-methylethyl)phenol under different conditions in order to synthesize an individual substance similar to the above and to synthesize substances with biological activity based on it. The method of obtaining 5-methyl-2-(1-methylethyl)phenylchloroacetate with the highest yield was found. The reaction goes according to the following scheme.



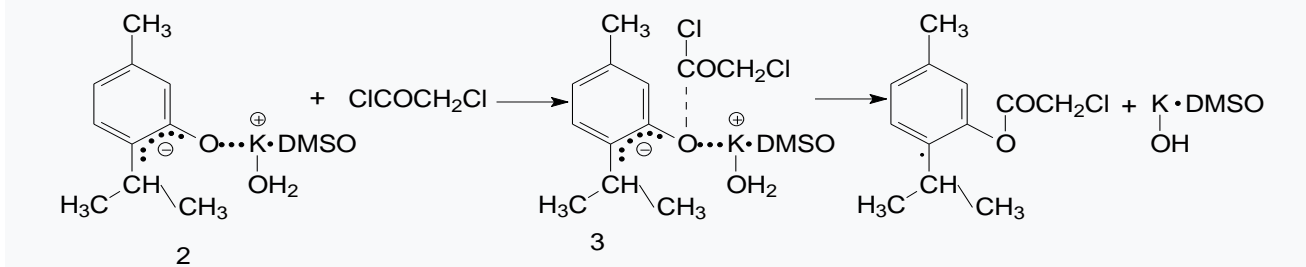
5- Methyl -2-(1- methylethyl) formation of phenolate ion.

At the initial stage of the reaction 5- methyl -2-(1- methylethyl) phenol The molecule is coordinated with potassium hydroxide and potassium turns into 5- methyl -2-(1- methylethyl) phenol . As a result of the displacement of protons due to 2 complex formation 1 . In this case, it is initially more loosely tied intermediate complex 1 is formed . The reason for the weakness of this intermediate complex 5- methyl -2-(1- methylethyl) phenol atoms, hydroxyl group outside the coordination range of the potassium cation.

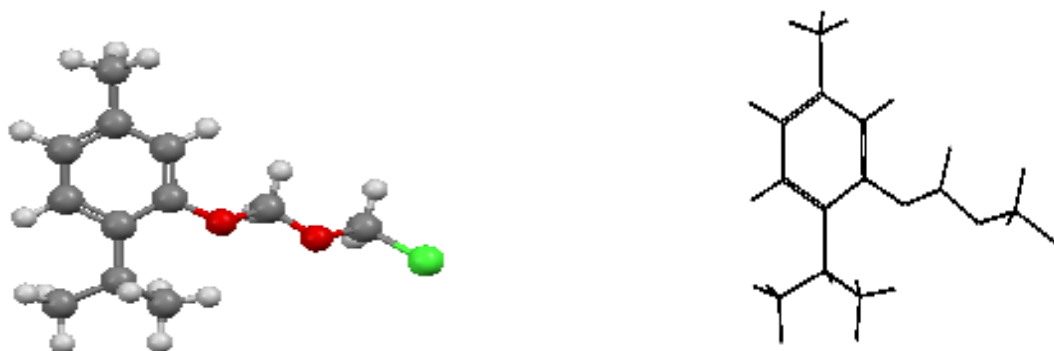


It is known that due to the high mobility of the hydroxyl proton in 5- methyl -2-(1- methylethyl) phenol , the proton in complex 1 interacts with the hydroxyl group in potassium hydroxide. Complex 1 then passes through a relatively small energy barrier. As a result complex 2 is formed.

Intermediate complexes. As a result, as a result of adding chloroacetyl chloride to 5-methyl-2-(1-methylethyl)phenolate complex, chloroacetylation reaction takes place in 2 complexes and a product is formed.



The 2D and 3D views of 5-methyl-2-(1-methylethyl)phenylchloroacetate are shown below.



Avagadro software was used to experimentally study some geometrical and energetic parameters of 5-Methyl-2-(1-methylethyl)phenylchloroacetate. Results **Chemical**, Obtained in **MMFF94**, **MMFF94s**, **UFF** methods. The optimization results of each method are presented in the following tables.

Table 1 Heat energies of formation of 5-Methyl-2-(1-methylethyl)phenylchloroacetate obtained using Avogadro's program

Chemical	MMFF94	MMFF94S	UFF
17.8846 kj / mol	102,735 kj / mol	90.0004 kj / mol	163,672 kj / mol

The formation energy of the molecule has a maximum value when it is alternated in **the UFF method**, and it has a minimum value when it is alternated in **the Chemical method**. Therefore, **the Chemical** method is effective in calculating the energy parameter for 5-methyl-2-(1-methylethyl)phenylchloroacetate.

Table 2 Real bond lengths (Å⁰) of 5-Methyl-2-(1-methylethyl)phenylchloroacetate obtained using Avagadro software.

T/r	Gardens	Chemical	MMFF94	MMFF94S	UFF
1.	C ₁ -C ₂	1.3936	1.3959	1.3969	1.3964
2.	C ₁ -C ₅	1.3965	1.3995	1.3986	1.4006
3.	C ₁ -C ₁₀	1.4995	1.5000	1.4998	1.5012
4.	C ₂ -C ₃	1.3957	1.3976	1.3976	1.3946
5.	C ₂ -H ₃₀	1.0878	1.0884	1.0878	1.0835
6.	C ₃ -C ₄	1.4090	1.4045	1.4041	1.4137
7.	C ₃ -H ₃₂	1.0872	1.9864	1.0870	1.0794
8.	C ₆ -C ₄	1.4113	1.4100	1.4097	1.4175

9.	C ₄ -H ₇	1.5352	1.5265	1.5254	1.5359
10.	C ₅ -C ₆	1.4051	1.4019	1.4015	1.4119
11.	C ₅ -H ₃₁	1.0870	1.0851	1.0860	1.0816
12.	C ₆ -O ₁₁	1.3709	1.3727	1.3728	1.3615
13.	C ₇ -C ₈	1.5409	1.5343	1.5340	1.5388
14.	C ₇ -C ₉	1.5307	1.5329	1.5318	1.5395
15.	C ₇ -H ₂₂	1.0986	1.0982	1.0980	1.1126
16.	C ₈ -H ₁₉	1.0948	1.0952	1.0954	1.1110
17.	C ₈ -H ₂₀	1.0959	1.0958	1.0958	1.1112
18.	C ₈ -H ₂₁	1.0966	1.0956	1.0954	1.1111
19.	C ₉ -H ₂₃	1.0913	1.0951	1.0954	1.1071
20.	C ₉ -H ₂₄	1.0947	1.0959	1.0958	1.1113
21.	C ₉ -H ₂₅	1.0966	1.0954	1.0954	1.1111
22.	C ₁₀ -H ₁₆	1.0938	1.0951	1.0949	1.1104
23.	C ₁₀ -H ₁₇	1.0953	1.0950	1.0952	1.1107
24.	C ₁₀ -H ₁₈	1.0956	1.0944	1.0945	1.1106
25.	O ₁₁ -H ₁₂	1.4304	1.4259	1.4268	1.3793
26.	C ₁₂ -O ₁₃	1.4264	1.4261	1.4261	1.4111
27.	C ₁₂ -H ₂₆	1.0978	1.0977	1.0979	1.1164
28.	C ₁₂ -H ₂₇	1.0955	1.0958	1.0958	1.1130
29.	O ₁₃ -H ₁₄	1.4145	1.4157	1.4160	1.4091
30.	C ₁₄ -Cl ₁₅	1.7723	1.7707	1.7705	1.7776
31.	C ₁₄ -H ₂₈	1.0940	1.0942	1.0943	1.1131
32.	C ₁₄ -H ₂₉	1.0938	1.0941	1.0942	1.1126

of 5-Methyl-2-(1-methylethyl)phenylchloroacetate were studied by the theoretical molecular mechanics method, no significant differences were observed in the 4 methods of the empirical method.

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