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

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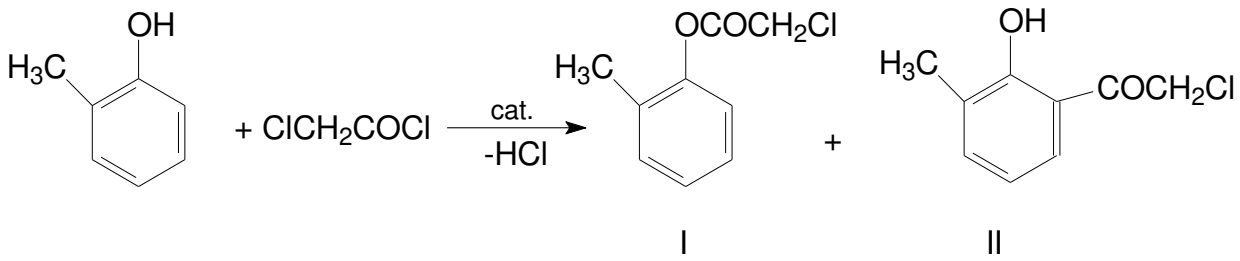
**ABSTRACT**

*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.

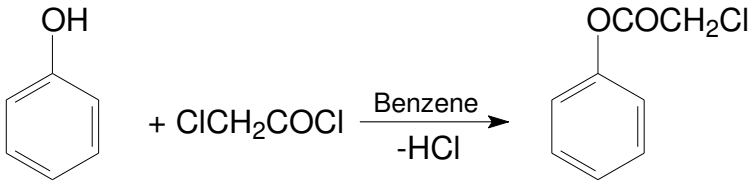
5-Methyl-2-(1-methylethyl)phenol compounds incubated with human neutrophils significantly reduced the oxidant release-up to 2.73.Among other results related to bacterial and fungal adhesion, the antioxidant activity of 5-Methyl-2-(1-methylethyl)phenol compounds is used against vaginosis and vaginitis. 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].

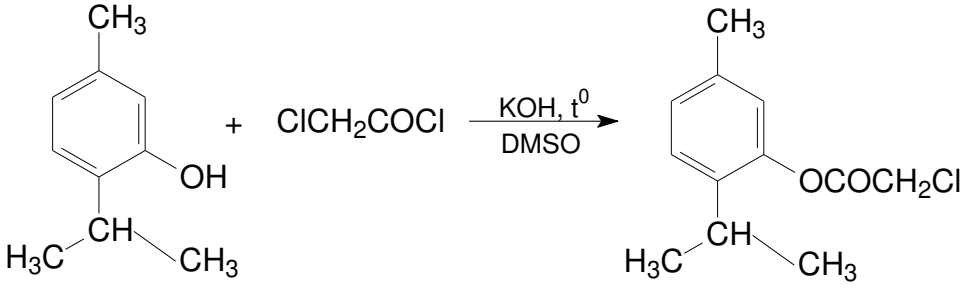



I II

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] .

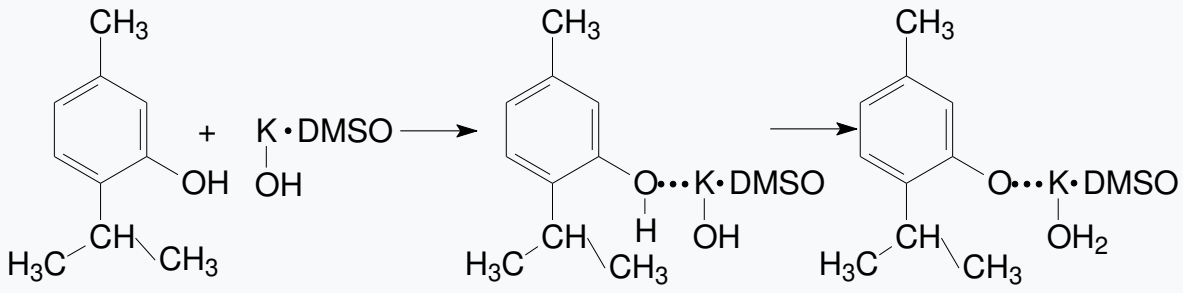



Chloroacetylation reactions were carried out with 5-methyl-2-(1-methylethyl)phenol under different conditions in order to synthesize an individual substance similar to the above and to synthesize substances with biological activity based on it. The method of obtaining 5-methyl-2-(1-methylethyl)phenylchloroacetate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




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

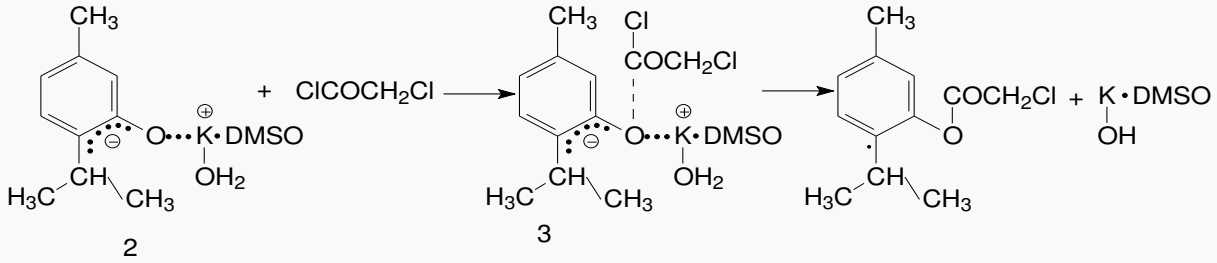
At the initial stage of the reaction 5- methyl -2-(1- methylethyl ) phenol The molecule is coordinated with potassium hydroxide and potassium turns into 5- methyl -2-(1- methylethyl ) phenol . As a result of the displacement of protons due to 2 complex formation 1 . In this case, it is initially more 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.



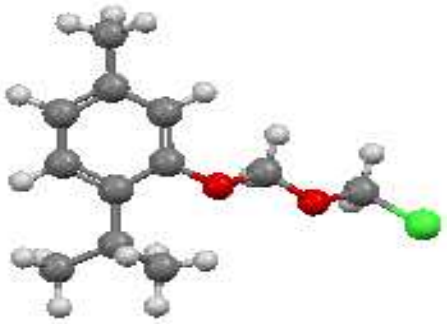

1 2

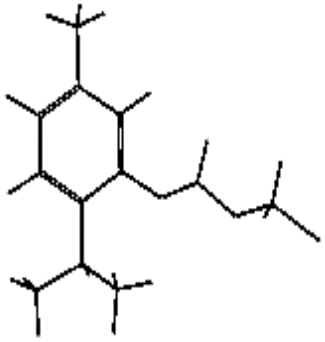
It is known that due to the high mobility of the hydroxyl proton in 5- methyl -2-(1- methylethyl ) phenol , the proton in complex 1 interacts with the hydroxyl group in potassium hydroxide. Complex 1 then passes through a relatively small energy barrier. As a result complex 2 is formed.

***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 (A $^0$) 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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