

VINILLA Reactivity of THYMOLIN a Particular Purpose of Super-AIR Condition

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ABSTRACT: This article describes the mechanism of vinyl acid reacting in the super-based enzyme. The main results are based on quantum-chemical calculations and are consistent with experimental results. Modeling of quantum-chemical calculations and intermediate complexes was carried out in combination with methods RHF/6-31-G* baMP2/6-311++G**//B3LYP/6-31+G* in the MM + base and Gaussian09 program in HyperChem 8 softw.

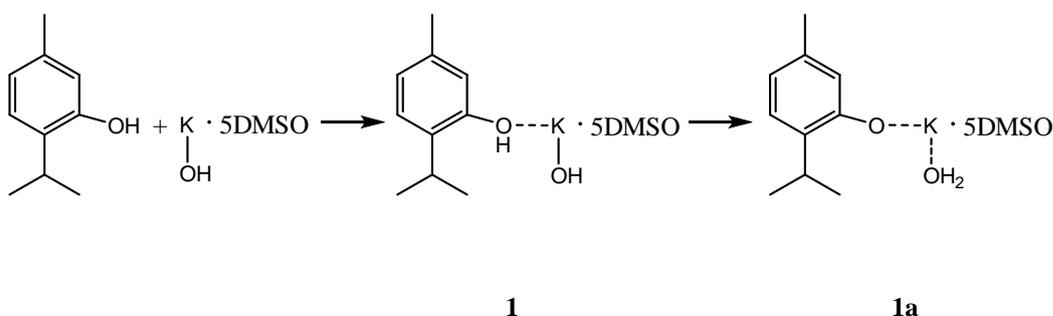
KEYWORDS: thymol, acetylene, vinyl acids, super-based media, quantum chemistry.

I. INTRODUCTION

Use of super-based systems in organic synthesis, particularly the potassium hydroxide-dimethylsulfoxide, has led to the discovery of new capacities in acetylene chemistry. It is known that the acetylene electrophile enters the reaction of vinylidation by triangular nucleophilic adhesion and the decomposition reactions through nucleophilic bonding to the carbonyl group of acetylene. The acetylene's double reactive ability is particularly evident in the effect of super-based media.

By utilizing a super-based environment, you can improve the synthesis process of vinyl esters that are important to the industry. Despite the many years that fetethylene has been investigating in a super-based environment, it has not yet lost its relevance to the explanation of these reactions mechanisms, the super-based catalytic nature. In the experimental study of reaction mechanisms in super-based systems, many components of the reaction mixture, high speed and multi-stage chemical reaction speed are a great problem. Therefore it is important to introduce high-level quantum-chemical calculations for the formation of pronounced pronouncements of the main reactions in the organic synthesis (rhinestone or rhythm), the proper orientation and description of the synthesis of complex organic compounds, and justification of these assumptions.

Formation of thymolate ion. At the initial stage of the reaction, the thymol molecule is coordinated with potassium hydroxide and potassium thymolyate 2 is the result of the proton emission by complex 1 production.



The intermediate complex 1, which initially was weakly bounded by the co-ordination of the thymol molecule with the super-based system, is formed. This complex consists of the interaction of the proton with the KOH·5DMCO super-based complex in the hydroxyl group of the complex, and the H-O interstellar distance is 2,255 Å (Figure 1). The weakness of this intermediate complex is located outside the coordination point of the potassium cation of the thymol

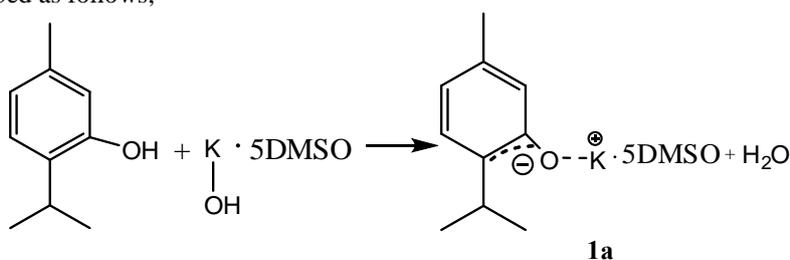
atoms, or rather the hydroxyl group in the thymus. In this case, the distance between K^+ and the nearest atom is $R(K^+ - H) = 4.974 \text{ \AA}$ (Figure 1).

Table 1. Intermediate complexes surface potential energy relative enthalpy (ΔH , kcal / mol)

Surface potential energy points	The potassium dimyl KOH · 5DMCO	Complex1	Complex1a	Complex2	Complex2a	Complex3
ΔH	44,34	366.98	322.09	52.85	359.41	152.73

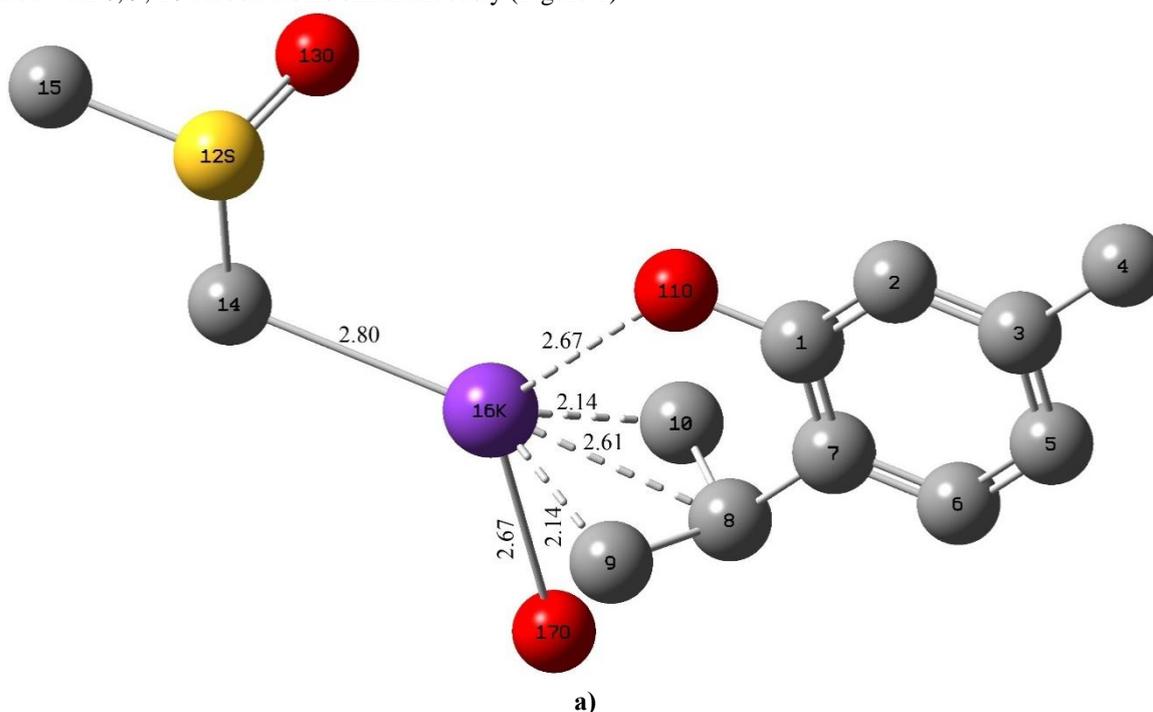
It is known that the hydroxyl group proton in the thymus is higher in comparison to all protons in the complex **1**. Therefore, this proton reacts with the hydroxyl group in potassium hydroxide and leaves the complex. For this purpose, the complex passes through a barrier relative to **1**. As a result, complex **1** from complex **1** is $\Delta H = -44.89 \text{ kcal / molar complex 1a}$ (Table 1).

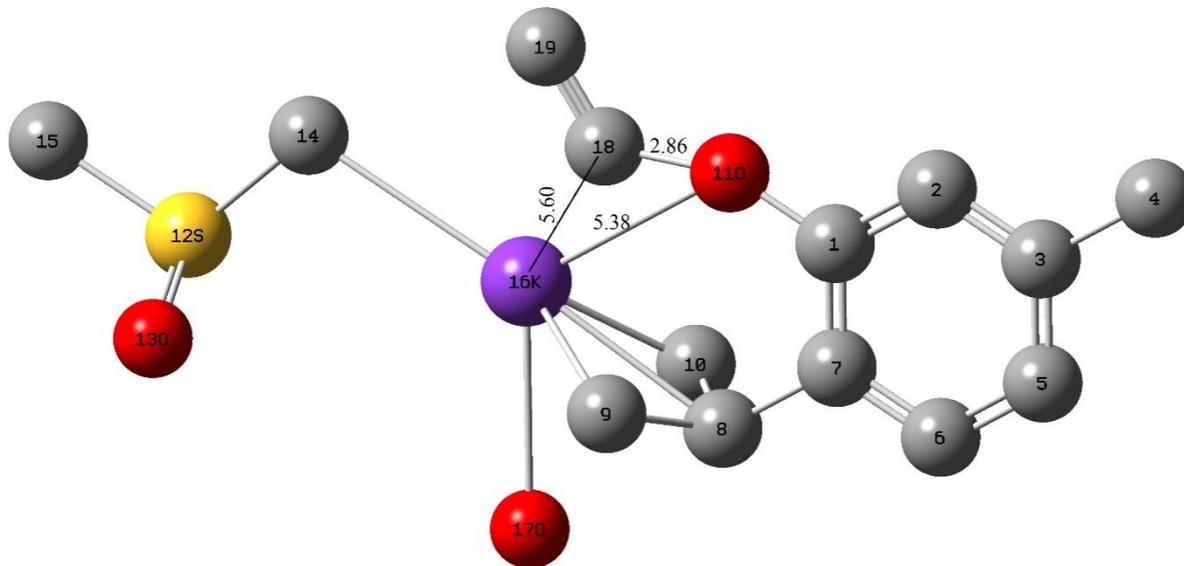
This process is described as follows,



Gibbs free energy for the process is reduced to $\Delta G = -5.0 \text{ kcal / mol}$.

In addition to the oxygen atom (11) with the thymolate-ion potassium cation of complex complex 2, coordinated with 8, 9, 10 carbon atoms simultaneously (Figure 1):

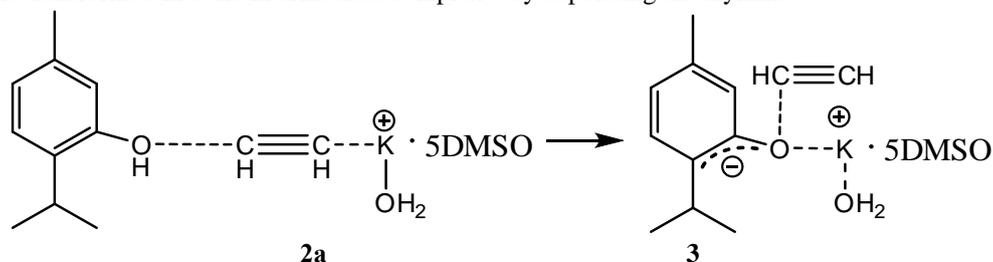




Picture 2. The structure of the intermediate complex of vinyl sulphate 3.

The stability of this intermediate complex is also significant, with the acetylene DMSO molecule being affected by the protons in the methyl group. The result is partly polarized.

The deprotonation of thymole and the formation of the intermediate complex 3 from the co-ordination of the acetylene into the thymolytic complex that is formed is not the only mechanism of the vinyl reaction. The direct effect of the acetylene on the KOH · 5DMSO super-based complex results in the molecule's partial polarization, complex 2a, and its effect is transformed into the intermediate complex 3 by deprotonating the thymine.



However, given the computation results in Table 1, the relative concentration of complex 2a (352.41 kcal / mol) is much higher than complex 2 (52.85 kcal / mol). It is clear that the stability of the system is much lower in such a high energy, and therefore the complex 2a transition to a more stable complex 2.

II. CONCLUSIONS

In deduction, in the super-based atmosphere, the acetylene-based vinyl acetate is initially a solubilising and potassium-cylindrical intermediate complex formed as a catalyst, and complex 2 intermediate complexes forming a thymol molecule are formed. As a result of the introduction of the acetylene into the reaction mixture, complex 2 is formed from acetylene complex 3, resulting in vinyl ether of thymol.

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ISSN: 2350-0328

**International Journal of Advanced Research in Science,
Engineering and Technology**

Vol. 6, Issue 6 , June 2019

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