

# 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.

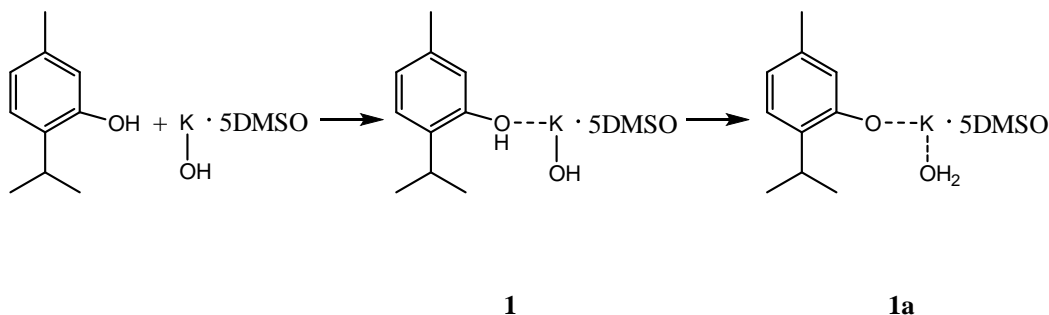
**KEYWORDS:** thymol, acetylene, vinyl acids, super-based media, quantum chemistry.

## 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

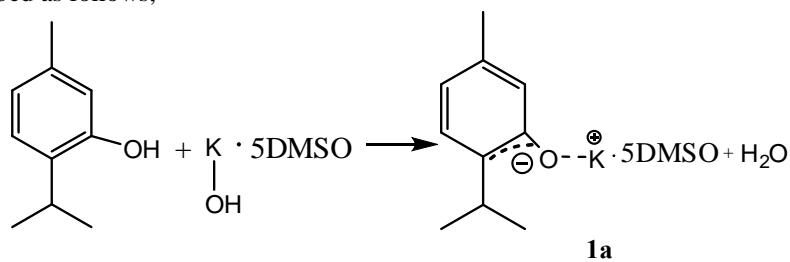
atoms, or rather the hydroxyl group in the thymus. In this case, the distance between  $K^+$  and the nearest atom is  $R(K^+ - H) = 4.974 \text{ \AA}$  (Figure 1).

Table 1. Intermediate complexes surface potential energy relative enthalpy ( $\Delta H$ , kcal / mol)

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

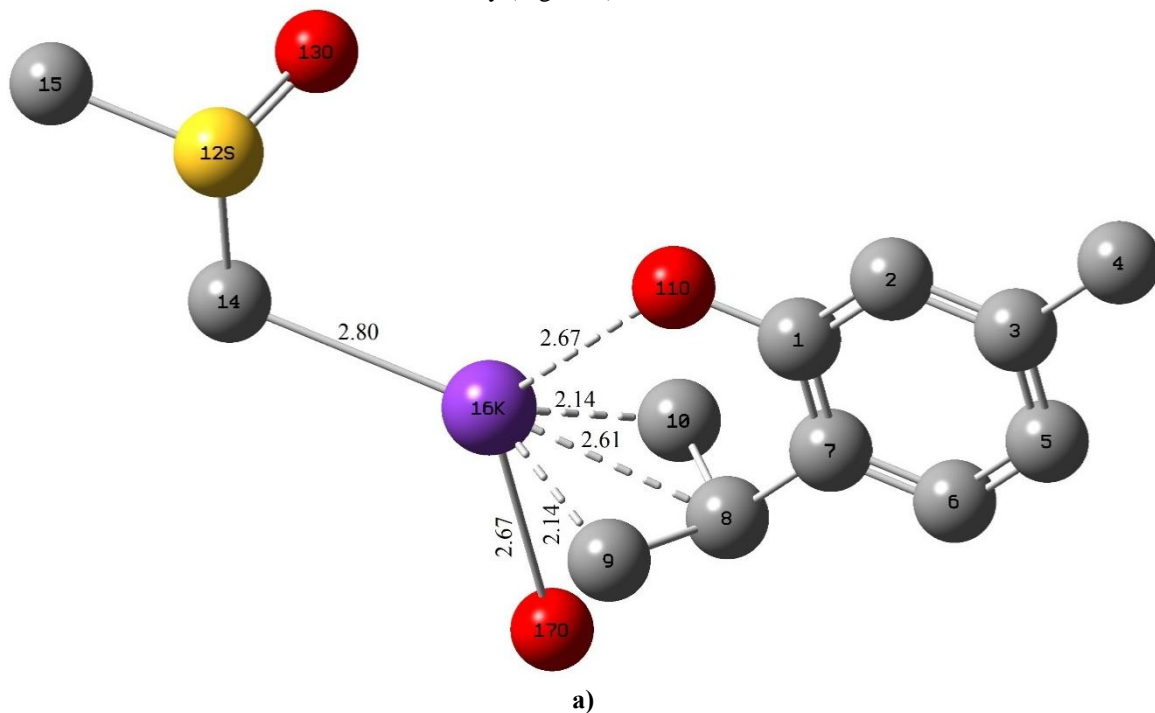
It is known that the hydroxyl group proton in the thymus is higher in comparison to all protons in the complex **1**. Therefore, this proton reacts with the hydroxyl group in potassium hydroxide and leaves the complex. For this purpose, the complex passes through a barrier relative to **1**. As a result,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

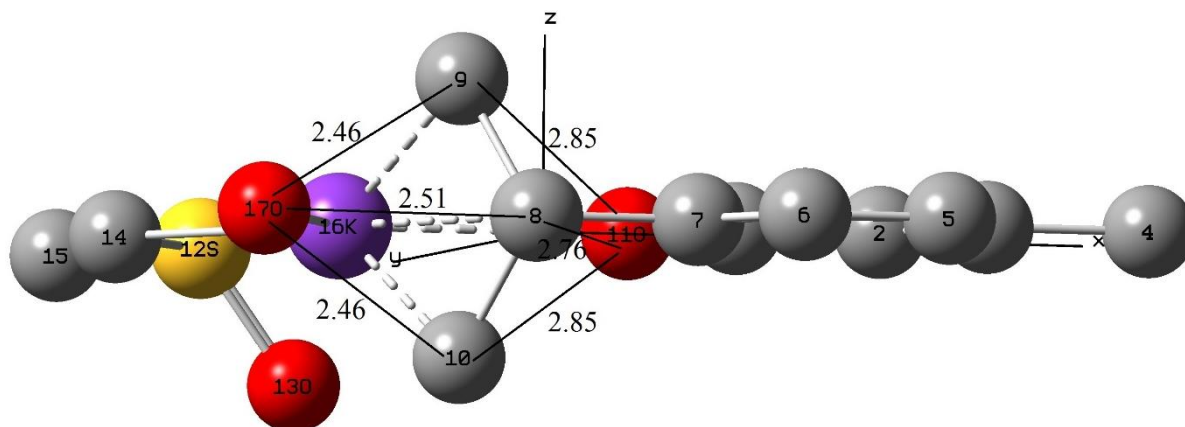
This process is described as follows,



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):





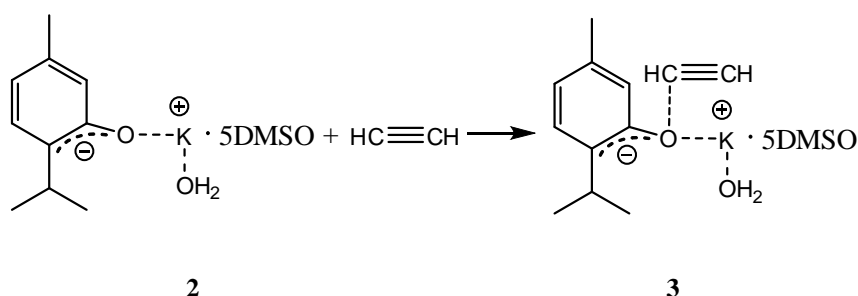
6)

Picture 1. Structure of potassium thiolytic complex 2

This feature of the thymolytic ion is explained by the distribution of negative charges in atoms. According to the results of the RHF/6-31-G\* method, the charge of the oxygen atom (11) is -0.75 atomic units, (8) carbon atoms -0.37 and (9, 10) carbon atoms respectively -0, 540250 and -0,540248 equal to the atomic unit. In this case, attention is drawn to the distances between potassium cation and the atoms close to it by other molecules. Figure 2 depicts the catalytic medium - the intermediate complex formed with the thymol of the potassium complex. This picture shows that the potassium cation in the center is co-ordinated with the thiol, ion, 8, 9, 10 carbon atoms and the single oxygen atom (Figure 2). It is also bound to carbon dioxide (14) in the dimer ion and oxygen (17) formed by the production of potassium. Although the distance between thrombolium ions 9 and 10 and the potassium cation is the closest (2.14 Å), the negative charge power in them is less than that of the 21 atomic oxygen atom (11).

It should be noted that in the complex 2, all atoms, except those of the 9<sup>th</sup> and 10<sup>th</sup> carbon atoms of the thromolyte ion, are in almost the same plane (Fig. 2b). The water molecule formed in the environment is close to the ionic ion, which forms hydrogen bonds with hydrogen atoms in the 8, 9, 10 carbon atoms. Figure 2b shows that these carbon atoms are close to oxygen (17) relative to oxygen (10) of thymolate ion. Such an arrangement of atoms in complex 2 further enhances the nucleophilicity of oxygen atoms 10 and facilitates the attack of the acetylene.

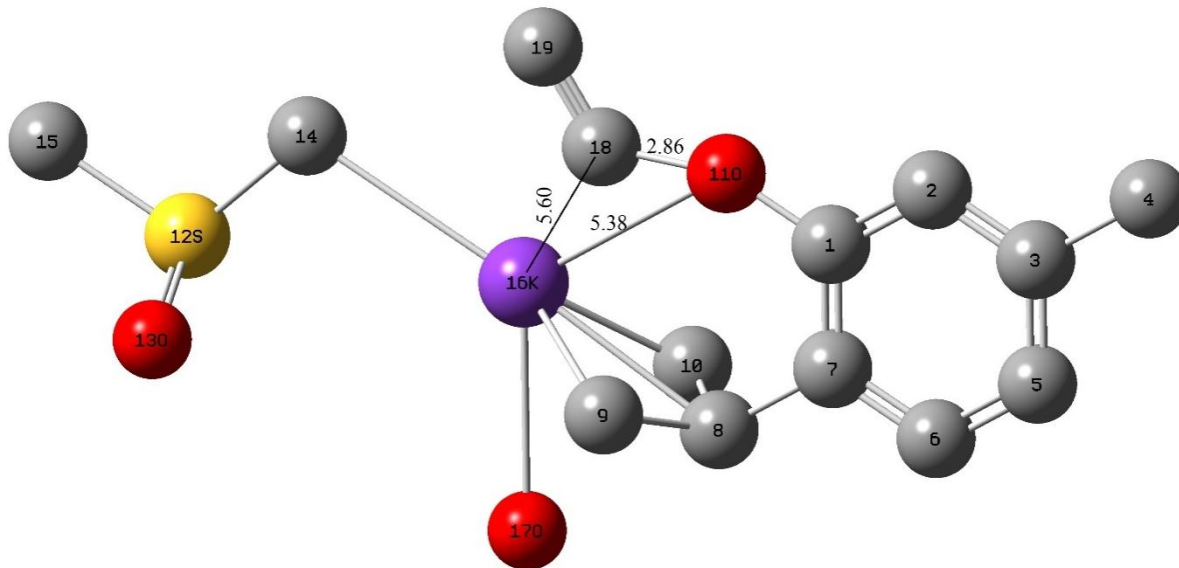
Intermediate complexes. The potassium thylolytic complex 2 contains the intermediate complex of vinyl acetate 3:



2

3

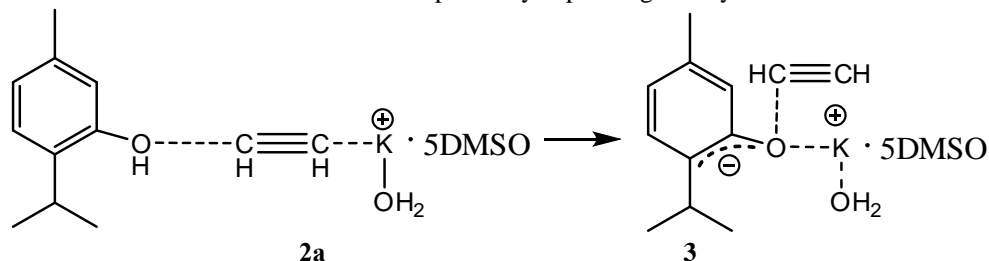
As a result of this change, systemic enthalpy change is  $\Delta H = -100,12$  kcal / mol. In the intermediate complex 3, the acetylene molecule is coordinated with the oxolyth of the thymolate-ion (11). The distance between acetylene carbon (18) and oxygen (11) is 2,86 Å, and the distance between potassium ion is 5,60 Å (Fig. 2).



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.

## REFERENCES

1. Base-Catalyzed Vinylation of Tertiary Propargylic Alcohols with Acetylene: a First Examples / B.A. Trofimov, E.Yu. Schmidt, E.V. Skital'tseva, et al. // Mendeleev Commun. – 2012. – V. 22, No. 2. – P. 62–63.
2. Quantum-chemical model of the reaction of the nucleophilic addition of methanol and methanethiol to acetylene in the superbasic system KOH — DMSO / N.M. Vitkovskaya, E.Y. Larionova, A.D. Skitnevskaya and others. // Izv. An. Ser. Chem., 2013, № 1. - P. 27–34.
3. Theoretical evaluation of some interactions in the acetylene – alkali metal hydroxide – DMSO system / N.M. Vitkovskaya, V.B. Kobychev, E.Yu. Larionov et al. // Zhurn. structures. Chemistry. – 2009. – T. 50, No. 1. – P. 24–32.



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4. Geometry optimization with QM / MM, ONIOM and other combined methods. I. Microiterations and constraints / T. Vreven, K. Morokuma, C. Farkas et al. // J. Comput. Chem.– 2003.– V. 24, No. 6.– P. 760–769.
5. Calculation of the electronic structure of the molecule of some substances based on computer programs / M.I. Soliev, Sh.N. Atakhanov, R.A. Akramboev // NEW INFORMATION TECHNOLOGIES IN SCIENCE: collection of articles of the International Scientific and Practical Conference (November 1, 2015, Ufa). / 2 hours. Part 2 - Ufa: AETERNA, 2015. - p. 12-14.