



**FORM-02**

**The Patent Act 1970**

**Provisional Specification**

**Section 10**

**TITLE**

**“A Method for Preparing 4-Hexene-3-one”**

**APPLICANT**

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**The following specification describes the invention**

**FIELD OF INVENTION:**

[001] The present invention relates to the field of preparing a method of preparing 4-Hexene-3-one by condensation of Acetaldehyde and Methyl Ethyl Ketone (MEK) in presence of base

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**DESCRIPTION OF THE RELATED ART:**

[002] 4-Hexen-3-one (CAS: 2497-21-4) is a unique spice (China GB 2760-2007), mainly used for blending food flavors such as old, white, horseradish and so on.

The hydroxy compound dehydration reaction is a reaction in which a hydroxyl group and a hydrogen atom on two adjacent atoms in a reactant molecule are removed as water in the presence of a catalyst. Since the oxygen atom of the hydroxyl group contains a lone pair of electrons, it can combine with the proton (H < + > ) to form an oxonium ion. Since the oxygen atom has a positive charge, it becomes a strong electron-withdrawing group, and the CO bond is easily dissociated. . The entire dehydration reaction involves the formation of a protonated oxonium salt (R-OH<sub>2</sub><sup>+</sup>), the oxonium salt slowly dissociates into a positive carbon ion, and a hydrogen ion is quickly eliminated from the normal carbon ion to form an olefin, which occurs. The β-elimination reaction. In the reaction of dehydration of α-hydroxyketone to α,β-unsaturated ketone, the formation of oxonium ions by the α-hydroxy group is difficult due to the influence of the carbonyl group, and the reaction is difficult to occur.

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[003] Reference may be made to the following:

[004] Patent No. US5300654 relates to (beta)-hydroxyketones are prepared by reacting an aldehyde with acetone in the presence of perhydroisoindole or pyrrolidine and water. The resulting (beta)-hydroxyketone is further reacted in the presence of a solvent mixture to produce (alpha)-(beta)-unsaturated ketones.

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[005] Publication No. CN103030541 relates to a production method of 4-hexene-3-one by catalyzed dehydration of 4-hydroxy-3-hexanone, and mainly solves the problem of low catalyst activity, high reaction temperature and low space velocity in the prior art. According to the invention, 4-hydroxy-3-hexanone is used as a raw material, and the reaction raw material is in contact with a catalyst to produce 4-hexen-3-one at the conditions of a reaction temperature of 200-450 DEG C and

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the airspeed of 0.5-15 hr-1 with respect to the mass of 4-hydroxy-3-hexanone liquid, wherein the catalyst is WO<sub>3</sub>/ZrO<sub>2</sub>-SiO<sub>2</sub> or MoO<sub>3</sub>/ZrO<sub>2</sub>-SiO<sub>2</sub>, and the molar ratio of W or Mo:Zr:Si is (0.05-0.3):1:(5-50). The technical solution solves the problem preferably. The method can be used in the industrial production of 4-hexen-3-one from 4-hydroxy-3-hexanone.

**[006]** Patent No. **US4245122** relates to the preparation of allyl acetone (5-hexen-2-one) according to the reaction: wherein R is methyl or ethyl; X is chloro or bromo; M is sodium or potassium; and Q is sodium or potassium, the reaction being carried out (i) using a phase transfer agent and (ii) in a two phase system.

10 **[007]** Patent No. **US9707201** relates to allium extracts. In particular, improvements in or relating to extending the therapeutic half-life or duration of Allium extracts. The invention further relates to the synthesis of methyl methyl thiosulfinate in a mixture with varying molar or mass ratios depending on the reaction conditions, in particular from either methiin or alliin alone or a mixture  
15 of both. Methods of treatment methicillin-resistant Staphylococcus aureus are also provided. Also provided is a kit comprising methiin in a first container and alliin in a second container.

**[008]** Publication No. **CN105418392** relates to veratryl acetone. The method comprises the steps that an etherification reaction is performed under the  
20 conditions of solvent water, a phase transfer catalyst and high pressure by taking a by-product 4-(2-methyl allyl)-1,2-benzenediol and methane chloride as raw materials and taking strong base as an acid-binding agent to obtain an intermediate 1,2-dimethoxy-4-(2-methyl allyl)benzene; the 1,2-dimethoxy-4-(2-methyl allyl)benzene is subjected to an oxidation reaction with ozone in solvent  
25 acetic acid, reduction is performed through zinc powder, and then the product veratryl acetone is prepared, wherein the reaction formula is as followed (please see the reaction formula in the specification). According to the preparation method, waste utilization is achieved, and the requirements for environmental protection and circular economy development are met; the obtained intermediate  
30 4-(2-methyl allyl)-1,2-benzenediol is high in quality, and a good base is laid for preparation of the high-quality product veratryl acetone; the technology is simple, operation is convenient, the raw materials are easy to obtain, the production cost is low, and industrialized production is facilitated; the product yield is higher, the

total yield is larger than 70%, the product quality is high, and the mass content is 98% or above.

5 **[009]** In order to overcome above listed prior art, the present invention provides a method of preparing 4-Hexene-3-one by condensation of Acetaldehyde and Methyl Ethyl Ketone (MEK) in presence of base

#### **OBJECTS OF THE INVENTION:**

10 **[010]** The principal object of the present invention is to provide a method of preparing 4-Hexene-3-one by condensation of Acetaldehyde and Methyl Ethyl Ketone (MEK) in presence of base

15 **[011]** Another object of the present invention is to provide a simple and eco friendly process with very minimum by-products for preparing 4-Hexene-3one

**[012]** Yet another object of the present invention is to provide a method of preparing 4-Hexene-3-one which enhances the yield of the production

20 **[013]** At the outset of the description that follows, it is to be understood that the ensuing description only illustrates a particular form of this invention. However, such a particular form is only an exemplary embodiment and is not intended to be taken restrictively to imply any limitation on the scope of the present invention.

#### 25 **BREIF DESCRIPTION OF THE INVENTION:**


**[014]** The present invention relates to a method of preparing 4-Hexene-3-one by condensation of Acetaldehyde and Methyl Ethyl Ketone (MEK) in presence of base. The process is a simple two-step synthesis process providing 4-Hexene-3-one in high yields.

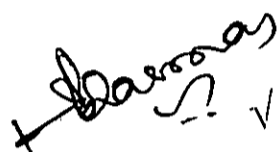
30 **[015]** MEK is employed in large excess such that, it acts as a solvent as well as reactant for the condensation with Acetaldehyde in presence of catalytic base. The reaction can be carried out at temperature varying from -10 to 40°C to afford mixture of crossed Aldol product. The base is selected from the series of alkali group, metal alkoxides & organic bases but not limited to NaOH, KOH, Sodium

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Carbonate, Sodium methoxide, Sodium ethoxide, Potassium methoxide, Potassium ethoxide, Triethanol amine, Triethyl amine, Ammonia etc. In particular, the Aldol mixture is then subjected to dehydration utilizing the Organic acids and or Carboxylic acids such as Formic acid, Acetic acid, Oxalic acid, Salicylic acid etc and Zeolites and Ion Exchange resins, but not limited to these, such that a double bond is generated, selectively at 4th carbon atom in the chain. This upon purification afforded the selective Hexenone in satisfactory yields. The process accordingly is simple, eco friendly with very minimum by-products and provides high yield.

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Dated .....day of ....., 2019

## ABSTRACT

### A Method for Preparing 4-Hexene-3-one

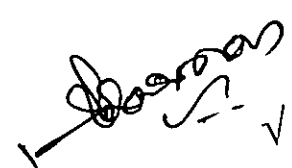
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The present invention relates to a method of preparing 4-Hexene-3-one by condensation of Acetaldehyde and Methyl Ethyl Ketone (MEK) in presence of base. The process is a simple two-step synthesis process for obtaining 4-Hexene-3-one with high yields.

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