Experiment 41: Isomerization of a cyclic ketone

**Analysis**

* **Final product structure**



Carvacrol C10H14O

* **Yield**



Table of experimental data.-

|  |  |  |  |
| --- | --- | --- | --- |
|  | (R)-carvone | Sulfuric acid | Carvacrol |
| Mass (g) | 1.52 | - | 1.01 |
| Volume (mL) | - | 15 mL | - |
| Concentration (M) | - | 6.0 M | - |
| Molar mass (g/mol) | 150.22 | 98.08 | 166.26 g |

* + Theoretical yield

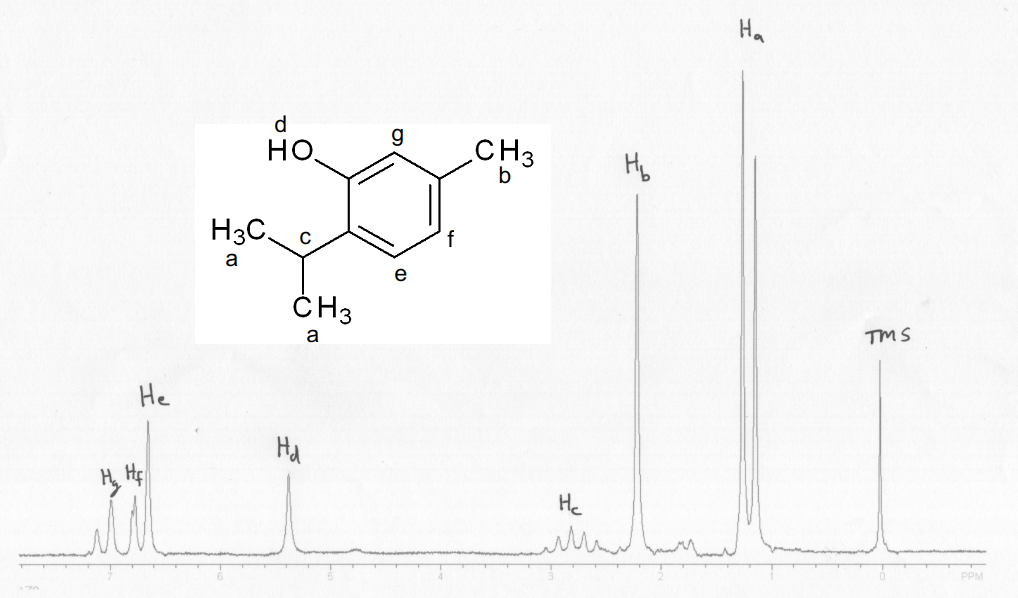
Limiting reagent:

(R)-carvone is the limiting reagent

* + Percent yield
* **IR analysis**

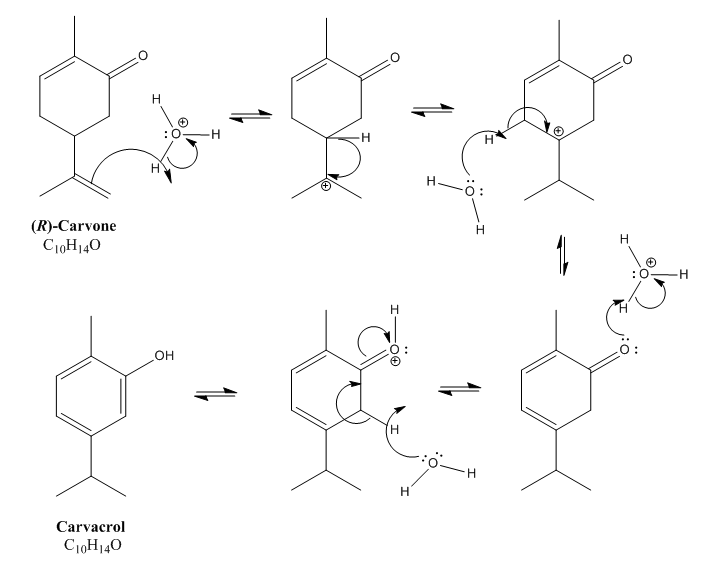
|  |  |
| --- | --- |
| **Bond type** | **Wavenumber (cm-1)** |
| O-H stretch | 3383.42 |
| C-H (sp3) stretch | 2926.77 & 2960.23 |
| C-H (sp2) stretch | 2869.30 |
| C=C aromatic stretch | 1421.57 & 1621.25 |
| O-H bending (phenol) | 1382.29 |

* **NMR analysis**



* **Answer to exercises**





1. a) **IUPAC name**: 5-isopropyl-2-methylphenol **Common name**: Carvacrol

b) Numerous plants contains Carvacrol as the major metabolite, such as oregano, thyme, pepperwort, wild bergamont, among many others.

1. a) The removal of the product would be too difficult due to the relatively high boiling point. Even when this could be solved by increasing the temperature, this would lead to decomposition of the product. Thus, it is imperative to use a very volatile solvent.

b) Sodium bisulfite is a very weak base compared to sodium bicarbonate and thus, not all of the Carvacrol product would be extracted, leading to a poor yield.

c) Too much pressure would build up inside the funnel due to the formation of carbon dioxide and it could explode.